The $3n + 1$ conjecture

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Abstract

The $3n + 1$ conjecture, also known as the Collatz conjecture, is an unsolved conjecture in number theory. The $3n + 1$ function $T : \mathbb{N}_+ \to \mathbb{N}_+$ is defined as:

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

The $3n+1$ conjecture says that for any positive integer n, $1 \in \{n, T(n), T(T(n)), T(T(T(n))), \ldots\}$. After reaching 1, the sequence will then stay in the cycle $(1, 2)$ indefinitely, since $T(1) = 2$ and $T(2) = 1$.

In this report, we look at various approaches to this problem. We look at the infinite Collatz Digraph, its adjacency matrix and its eigenvectors to learn more about the $3n + 1$ conjecture, and the consequences of the existence of other cycles or divergent trajectories. We also look at Collatz Modular Digraphs to investigate properties of the $3n + 1$ conjecture when applied to congruence classes. A special case of Collatz Modular Digraphs is shown to be isomorphic to Binary De Bruijn Digraphs, which has several interesting consequences.

After looking at these graphs, we also look at generating functions, where the coefficients satisfy the $3n + 1$ recursion, and derive functional equations for these generating functions. These functional equations then also lead to reformulations of the $3n + 1$ conjecture.

Besides the $3n + 1$ problem, we also look at certain generalizations of the $3n + 1$ problem, namely $pn + q$ problems and Collatz-like functions. We apply the above methods to those problems as well, to learn more about these problems in general.

Contents

Introduction

In 1937, Lothar Collatz stated the question if the sequence defined by

$$a_{n+1} = \begin{cases} a_n/2 & \text{if } a_n \text{ is even} \\ 3a_n + 1 & \text{if } a_n \text{ is odd} \end{cases}$$

with $a_0 \geq 1$ would always eventually arrive at $a_i = 1$ for some $i = 0, 1, \ldots$, after which it will stay in the cycle $(1, 4, 2)$ forever. For example, if we look at the starting values $a_0 = 5$ to $a_0 = 10$, we get the following sequences:

$$(a_0, a_1, a_2, ...) = \begin{cases} a_0 = 5: & (5, 16, 8, 4, 2, 1, 4, 2, 1, ...) \\ a_0 = 6: & (6, 3, 10, 5, 16, 8, 4, 2, 1, 4, 2, 1, ...) \\ a_0 = 7: & (7, 22, 11, 34, 17, 52, 26, 13, 40, 20, 10, 5, 16, 8, 4, 2, 1, ...) \\ a_0 = 8: & (8, 4, 2, 1, 4, 2, 1, ...) \\ a_0 = 9: & (9, 28, 14, 7, 22, 11, 34, 17, 52, 26, 13, 40, 20, 10, 5, 16, 8, 4, 2, 1, ...) \\ a_0 = 10: & (10, 5, 16, 8, 4, 2, 1, 4, 2, 1, ...). \end{cases}$$

And as we can see, these sequences all eventually 'converge' to 1, after which the sequences repeat the cycle $(1, 4, 2)$. One might now expect that the cycles never get too wild; all of the above sequences end in the $(1, 4, 2)$ cycle after less than 20 iterations, and the highest value encountered in these sequences is 52, which compared to the values of a_0 is not so high.

However, when we look at $a_0 = 27$ we get the following sequence:

$$(a_0, a_1, a_2, ...) = (27, 82, 41, 124, 62, 31, 94, 47, 142, 71, 214, 107, 322, 161, 484, ...)$$

The sequence has gone as high as 484 after 14 iterations, and it seems like we may never encounter 1 but diverge to infinity instead. Indeed, 22 iterations later the sequence even climbs above 1000 for the first time, with $a_{36} = 1186$. If we go even further, we see that after 25 more iterations we get $a_{61} = 2158$, and after 16 more steps we even get $a_{77} = 9232$. However, this last value turns out to be the maximum of the whole sequence. After 34 more iterations the sequence finally reaches $a_{111} = 1$ and ends in the cycle $(1, 4, 2)$. The sequence is shown in Figure 1, with the values of a_n plotted against n.

As we can see from this example, the behavior of the sequences is not so predictable as it seemed at first. This illustrates why no proof or counterexample of this so-called $3n + 1$ conjecture or Collatz conjecture has been found yet. Brute force calculations have shown that the conjecture is true for all starting values a_0 up to $20 \cdot 2^{58} \approx 5.76 \cdot 10^{18}$ [eS09]. And for big numbers, we see that if a number is odd, then it is roughly multiplied by a factor 3 and then divided by 2 (odd numbers are always followed by even numbers), while if it is even, it is multiplied by $1/2$. So if the number of even and odd numbers in the sequence is about equal in the long term, then the geometric mean of the factors gives us an average multiplication factor of $\sqrt{1/2 \cdot 3/2} = \frac{1}{2}\sqrt{3} \approx 0.866 < 1$. So on average, the value decreases over time, and so it is very likely that all numbers either end in some

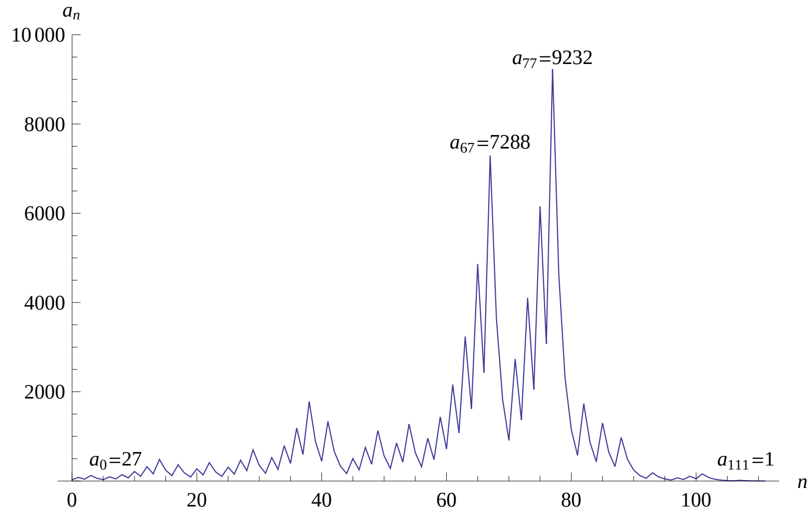

Figure 1: The values of a_n plotted against n, with $a_0 = 27$ and $a_{111} = 1$.

other cycle or end in the cycle $(1, 4, 2)$.

However, both brute force calculations for different starting values and heuristic calculations based on 'averages' can never prove the conjecture. We cannot calculate the sequences for all different starting values, and there could even exist certain complicated patterns such that a sequence does contain strictly more odd than even numbers. Then it could even be possible that certain sequences don't end in a cycle but 'diverge' to infinity. Brute force calculations can only find counterexamples and disprove the conjecture (should they exist), while heuristic 'evidence' only gives us reasons to believe the truth of the conjecture, instead of proving it. So if we should ever want to prove the conjecture for all starting values a_0, we will need different methods.

In this report, we look at several methods to analyze the $3n + 1$ conjecture. First we define some widely used terminology to describe behavior and properties of such sequences, and define variants of the $3n + 1$ problem which could be useful to investigate as well. Then we first try to analyze the $3n + 1$ conjecture using some simple calculations, to see why it is not so easy to find other possible cycles. Then we look at the so-called Collatz graphs, and at its adjacency matrix. This infinite matrix turns out to have interesting properties, when regarded as a linear mapping. We then calculate the complete spectrum of this matrix, and reformulate the $3n + 1$ conjecture in terms of this spectrum.

After that we look at modified Collatz graphs, which have only a finite number of vertices, namely Collatz Modular Graphs. These graphs turn out to have many interesting properties. One of the most important results of this chapter is that these graphs are isomorphic with a class of graphs known in literature, namely De Bruijn graphs. Finally we also look at generating functions, using the $3n + 1$ recursion on the coefficients of the power series. From these functions we derive functional equations, which have only certain known solutions, if the $3n + 1$ conjecture is true.

Note that this report does not claim to have a proof of the $3n + 1$ conjecture. The various approaches to the problem just try to provide the reader with more insight to the problem.

Chapter 1

Terminology

Before we thoroughly investigate the $3n+1$ problem, we introduce some terminology about the $3n+1$ problem and commonly used generalizations of the $3n+1$ problem, namely the class of $pn+q$ problems and the class of Collatz-like problems. The terminology introduced in this chapter is used throughout the rest of this report. Most of the terminology can be found in other literature on the $3n+1$ problem as well (see for example [Lag08b]). However, some terminology introduced in this chapter is new, such as the level of a number.

1.1 The $3n+1$ conjecture

We first define some useful functions and concepts to describe behavior of the sequences and starting values in the $3n+1$ problem. First we note that if n is odd, then $3n+1$ is always even. Therefore, a commonly used function is the $3n+1$ *function* below.

Definition 1.1.1 ($3n+1$ function)**.** *The $3n+1$ function $T : \mathbb{N}_+ \to \mathbb{N}_+$ is defined as:*

$$T(n) = \begin{cases} T_0(n) = n/2 & \text{if } n \equiv 0 \pmod 2 \\ T_1(n) = (3n+1)/2 & \text{if } n \equiv 1 \pmod 2 \end{cases}$$

The inverse $3n+1$ mapping $T^{-1} : \mathcal{P}(\mathbb{N}_+) \to \mathcal{P}(\mathbb{N}_+)$ (from sets of positive numbers to sets of positive numbers) is defined as:

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

Furthermore, we define $T^{-1}(A \cup B) = T^{-1}(A) \cup T^{-1}(B)$ for any two sets A, B, and we write $T^{k+1}(n) = T(T^k(n))$ and $T^{-k-1}(n) = T^{-1}(T^{-k}(n))$ for all $k \geq 1$, and $T^0(n) = n$.

With the definition of the $3n+1$ function, we can now easily formalize the $3n+1$ *conjecture* as follows.

Conjecture 1.1.2 ($3n+1$ conjecture)**.** *For every $n \in \mathbb{N}_+$ there exists a $k \in \mathbb{N}$ with $T^k(n) = 1$.*

Note that if the $3n+1$ conjecture is not true, then this can have two different reasons. Either iterations of some number n end in a different cycle than the *trivial cycle* $C_{triv} = (1, 2)$, or there exists some number n such that $T^k(n) \to \infty$ as k goes to infinity. If we seperate these two cases, we get the following "partial" $3n+1$ conjectures.

Conjecture 1.1.3 ($3n+1$ cycle conjecture)**.** *If $n \in \mathbb{N}_+$ and there exists a $k \in \mathbb{N}_+$ with $T^k(n) = n$, then $n = 1$ or $n = 2$.*

Conjecture 1.1.4 ($3n + 1$ divergence conjecture). *For each $n \in \mathbb{N}_+$ there exists some $N \in \mathbb{N}_+$ such that for all $k \in \mathbb{N}_+$, $T^k(n) < N$.*

We can easily verify that the $3n + 1$ conjecture is true if and only if both the $3n + 1$ cycle and divergence conjectures are true.

1.2 $pn + q$ problems

A common generalization of the $3n + 1$ problem, when investigating similar but slightly different problems, is to generalize the 3 and 1 to variables p and q respectively. This gives us the following definition of the *$pn + q$ function.*

Definition 1.2.1 ($pn + q$ function). *The $pn + q$ function $T_{p,q} : \mathbb{N}_+ \to \mathbb{N}_+$ is defined as:*

$$T_{p,q}(n) = \begin{cases} T_{p,q,0}(n) = n/2 & \text{if } n \equiv 0 \pmod 2 \\ T_{p,q,1}(n) = (pn + q)/2 & \text{if } n \equiv 1 \pmod 2 \end{cases}$$

Note that p and q should both be odd, to prevent that $(pn + q)/2$ is not an integer (when one is even) and to prevent that $(pn + q)/2$ can be simplified (when both are even).

It is very likely that if we understand more about these general $pn + q$ problems, or more about specific kinds of $pn+q$ problems, that we also learn more about the $3n+1$ problem. For example, when $p = 5$ and $q = 1$ we expect that there exist numbers n such that $T^k(n) \to \infty$ as k goes to infinity, since the geometric mean of the factors $5/2$ and $1/2$ is $\frac{1}{2}\sqrt{5} \approx 1.12 > 1$. This means that on average (if in the long run a sequence contains as many odd as even numbers) a number roughly increases by a factor 1.12 in each iteration. So maybe if we investigate the $5n + 1$ problem, we learn more about problems with divergent paths in general. This may then be useful for proving the (non-)existence of divergent paths in the $3n + 1$ problem.

1.3 Collatz-like problems

Another further generalization of the $T_{p,q}$ problem is to generalize the 2 cases $T_{p,q,0}$ and $T_{p,q,1}$ to m cases $T_0, \ldots, T_{m-1}$. This leads to so-called *Collatz-like functions* as defined below.

Definition 1.3.1 (Collatz-like functions). *The Collatz-like function $C_m : \mathbb{N}_+ \to \mathbb{N}_+$ is defined as:*

$$C_m(n) = \begin{cases} (a_0 n + b_0)/m & n \equiv 0 \text{ mod } m \\ (a_1 n + b_1)/m & n \equiv 1 \text{ mod } m \\ \vdots & \vdots \\ (a_{m-1} n + b_{m-1})/m & n \equiv m-1 \text{ mod } m \end{cases}$$

Note that the a_i and b_i have to be such that $a_i \cdot (\alpha m + i) + b_i$ is divisible by n for all $\alpha \in \mathbb{Z}$.

This class of problems also has a strong similarity with the $3n + 1$ and $pn + q$ problems. After all, the choice of dividing by 2 and considering only two cases was rather arbitrary. Maybe inspection of these Collatz-like functions could also lead to more insight about the $3n + 1$ conjecture, which is just the Collatz-like problem with $n = 2$ and $a_0 = 1$, $b_0 = 0$, $a_1 = 3$ and $b_1 = 1$. Note that similarly to the $3n + 1$ and $pn + q$ problems, we can estimate the average increase of k in the iterations. If all congruence classes modulo m are assumed to appear in the iterations of a number n in the same amount, then we expect divergent paths if $f = \sqrt[m]{a_0 a_1 a_2 \cdots a_{m-1}} > m$ and we expect no divergent paths if $f < m$.

1.4 General terminology

For convenience, we define some general terminology about the functions T, $T_{p,q}$ and C_m, most of which needs no explanation. We will define the terminology using T, but most of the definitions can analogously be used for $T_{p,q}$ and C_m as well.

- **Trajectory**: The trajectory $O^+(n)$ of n is the ordered set $\{n, T(n), T^2(n), T^3(n), \ldots\}$.
- **Divergent trajectory**: If $|O^+(n)| = \infty$ then $O^+(n)$ is said to be a divergent trajectory.
- **Cycle**: If $|O^+(n)| = k < \infty$ and $T^k(n) = n$ then $O^+(n)$ is said to be a cycle of length k.
- **Infinite convergent path**: An infinite convergent path is an infinite path $I_C = \{\ldots, c_{-1}, c_0, c_1, \ldots, c_{k-1}\}$ ending in the cycle $C = \{c_0, c_1, \ldots, c_{k-1}\}$ with $c_{-1} \notin C$.
- **Infinite divergent path**: An infinite divergent path is an infinite path $I_P = \{\ldots, c_{-1}, c_0, c_1, \ldots\}$ not ending in a cycle.
- **Component**: A component G is a minimal nonempty subset $\{n_1, n_2, \ldots\}$ of $\mathbb{N}_+$ which is invariant under T^{-1}.
- **Root**: If $G = G_C$ is a component with a cycle C, then the root n_0 of G_C is the smallest element in the cycle C. If $G = G_P$ does not contain a cycle, we define the root n_0 as the smallest element of G_P. We also write $r(G) = n_0$.
- **Level**: If $n \in G_C$ and $r(G_C) = n_0$, then the level of n, denoted by $\ell(n)$, is the smallest $k \in \mathbb{N}$ such that $T^k(n) = n_0$. If $n \in G_P$, $r(G_P) = n_0$, and $T^{k_1}(n) = T^{k_2}(n_0)$ for some integers k_1, k_2, then the level $\ell(n)$ is defined as $\ell(n) = k_1 - k_2$. Note that $\ell(T(n)) = \ell(n) - 1$, except when $n = r(G_C)$. Then $\ell(T(n)) = \ell(n) - 1 + k$ where k is the cycle length of C.

The concepts root and level, suggested by De Weger, are a generalization of the more common term total stopping time, which for a number n is the smallest number k such that $T^k(n) = 1$. The stopping time is not well-defined if the problem has more than one cycle or divergent trajectories, while the root and level are well-defined regardless of the number of components in the problem. With the extra terminology we can also easily define several variants of the $3n+1$ (cycle/divergence) conjecture, such as the following.

Theorem 1.4.1 ($3n+1$ conjecture, variant)**.** *The $3n+1$ conjecture is equivalent to each of the following formulations.*

- *The only component is $G = \mathbb{N}_+$.*
- *For every $n \in \mathbb{N}_+$, $1 \in O^+(n)$.*

Theorem 1.4.2 ($3n+1$ cycle conjecture, variant)**.** *The $3n+1$ cycle conjecture is equivalent to each of the following formulations.*

- *The only cycle is C_{triv}.*
- *For every $n \in \mathbb{N}_+$, $T^{\ell(n)} = 1$.*

Theorem 1.4.3 ($3n+1$ divergence conjecture, variant)**.** *The $3n+1$ divergence conjecture is equivalent to each of the following formulations.*

- *There are no divergent trajectories.*
- *For every $n \in \mathbb{N}_+$, $|O^+(n)| < \infty$.*
- *For all $n \in \mathbb{N}_+$ there exists some $N \in \mathbb{N}$ such that $T^k(n) < N$ for all $k \in \mathbb{N}$.*

Using the above terminology, we can now move on to different approaches of the $3n+1$ problem, which are discussed in the next chapters.

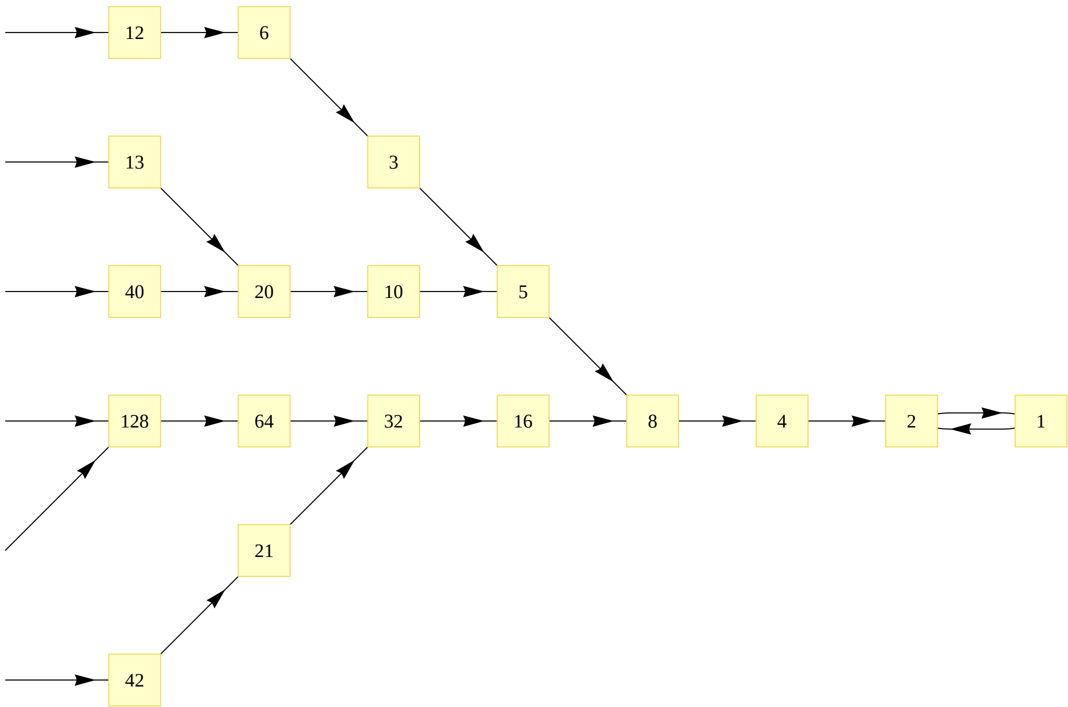

Figure 1.1: Part of the component in the $3n+1$ graph containing the cycle $(1,2)$. Numbers aligned vertically have the same level, and the level decreases when moving right in the graph. Furthermore, $\ell(1) = 0$.

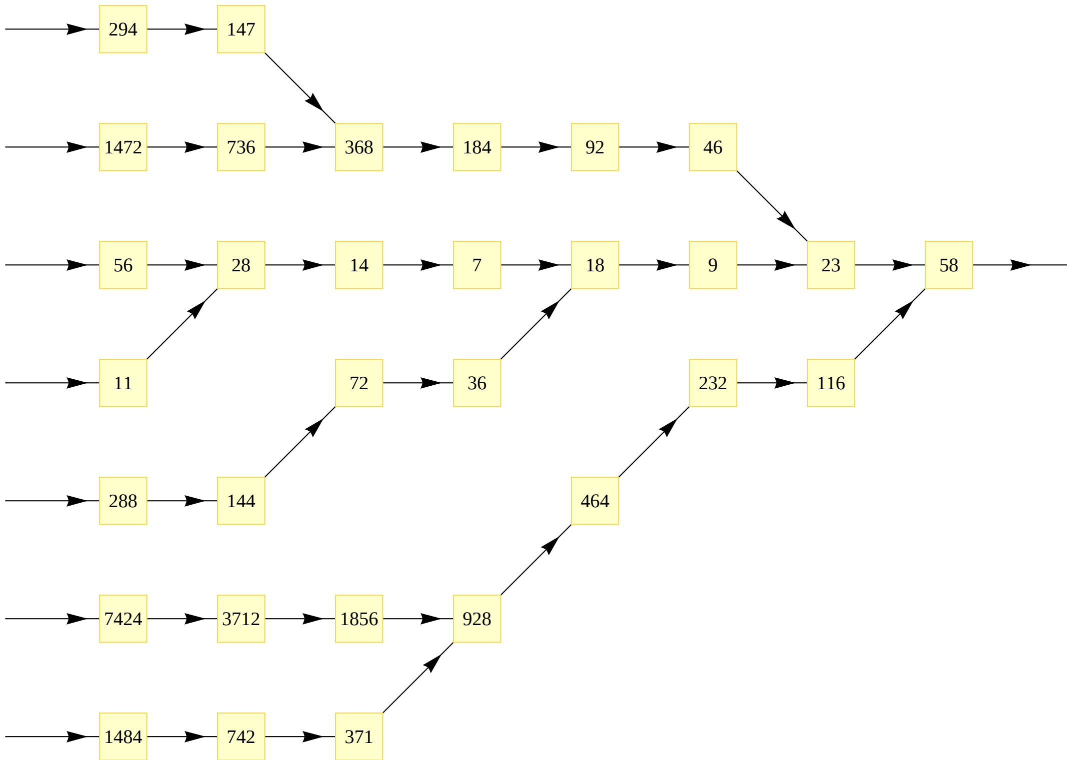

Figure 1.2: The component of the $5n+1$ graph that includes 7. The trajectory starting with $n = 7$ is most likely divergent. Numbers aligned vertically all have the same level, and $\ell(7) = 0$.

Chapter 2

Basic Calculations

2.1 The $3n+1$ conjecture

One obvious approach to the $3n+1$ conjecture is to calculate the form of the iterates for a certain starting number n_0. After all, the $3n+1$ function looks very simple, and so simply calculating the form of iterates might give us more information about the truth of the conjecture. Below we will show why this approach does not work, and why it is hard to find other cycles, should they exist.

First of all, we assume that our starting point n_0 of a cycle is odd. If n_0 is even, one can just divide all the factors 2 in the prime factor decomposition of n_0 to get an odd number, which is obviously in the trajectory of n_0. Secondly, we do not know much about n_0 and which steps will be taken in each iteration (whether $T^k(n_0)$ is odd or even), so therefore we just assume that there are certain numbers $k_1, k_2, \ldots$ and $l_1, l_2, \ldots$ such that $T^{k_1}(n_0) = T_1^{k_1}(n_0) = n_1$, $T^{l_1}(n_1) = T_0^{l_1}(n_1) = n_2$, $T^{k_2}(n_2) = T_1^{k_2}(n_2) = n_3$ and so on. So the first k_1 numbers in the trajectory of n_0 are odd, the l_1 numbers after that are even, the k_2 numbers after that are odd, et cetera. Furthermore, we introduce partial sums of these numbers as:

$$\begin{aligned} K_n &= \sum_{i=1}^{n} k_i \\ L_n &= \sum_{i=1}^{n} l_i \end{aligned}$$

We also write $M_n = K_n + L_n$ and $P_n = K_{n+1} + L_n$ since these numbers will be used alot. Now first we see that for any positive number k and any number m, we have the following result.

Lemma 2.1.1 (Form of $T_1^k(m)$)**.** *For any $k \in \mathbb{N}$ we have:*

$$T_1^k(m) = \frac{3^k m + 3^k - 2^k}{2^k}$$

Proof. We can easily prove this by induction on k. The case $k = 0$ is trivial, while the induction step goes as follows:

$$\begin{aligned} T_1^{k+1}(m) &= T_1(T_1^k(m)) = T_1\left(\frac{3^k m + 3^k - 2^k}{2^k}\right) = \frac{3\left(\frac{3^k m + 3^k - 2^k}{2^k}\right) + 1}{2} \\ &= \frac{3^{k+1} m + 3^{k+1} - 3 \cdot 2^k + 2^k}{2^{k+1}} = \frac{3^{k+1} m + 3^{k+1} - 2^{k+1}}{2^{k+1}} \end{aligned}$$

This is indeed the given expression for $T_1^k(m)$, with k replaced by $k+1$. □

This lemma is now used to prove the following result, about the form of $T^{M_n}(m)$.

Theorem 2.1.2 (Form of $T^{M_n}(m)$)**.** *For any $m \in \mathbb{Z}$ and $n, k_1, \ell_1, k_2, \ell_2, \ldots, k_n, \ell_n \in \mathbb{N}$ such that $T^{M_{i+1}}(m) = T_0^{\ell_{i+1}}(T_1^{k_{i+1}}(T^{M_i}(m)))$ for each $i \in \mathbb{N}$, we have:*

$$T^{M_n}(m) = \frac{3^{K_n} m + \sum_{i=1}^{n} 3^{K_n - K_i} 2^{M_{i-1}} (3^{k_i} - 2^{k_i})}{2^{M_n}}$$

Proof. The proof goes by induction on n. The case $n = 0$ is trivial, and the induction step goes as follows:

$$\begin{aligned}
& T^{M_{n+1}}(m) \\
= \; & T_0^{\ell_{n+1}}\left(T_1^{k_{n+1}}\left(T^{M_n}(m)\right)\right) \\
= \; & \frac{3^{K_{n+1}-K_n}\left(\frac{3^{K_n} m + \sum_{i=1}^{n} 3^{K_n-K_i} 2^{M_{i-1}}(3^{k_i}-2^{k_i})}{2^{M_n}}\right) + (3^{K_{n+1}-K_n} - 2^{K_{n+1}-K_n})}{2^{M_{n+1}-M_n}} \\
= \; & \frac{3^{K_{n+1}} m + \sum_{i=1}^{n} 3^{K_{n+1}-K_i} 2^{M_{i-1}}(3^{k_i} - 2^{k_i}) + 2^{M_n}(3^{K_{n+1}-K_n} - 2^{K_{n+1}-K_n})}{2^{M_{n+1}}} \\
= \; & \frac{3^{K_{n+1}} m + \sum_{i=1}^{n+1} 3^{K_{n+1}-K_i} 2^{M_{i-1}}(3^{k_i} - 2^{k_i})}{2^{M_{n+1}}}
\end{aligned}$$

This is indeed the expression with n replaced by $n+1$, so this concludes the proof. □

Now suppose that there exists a non-trivial cycle in the $3n+1$ conjecture. Then there must also exist a global minimum in that cycle, say m (which must be odd), such that there exist numbers $k_1, k_2, \ldots, k_n$ and $l_1, l_2, \ldots, l_n$ such that $T^{M_n}(m) = m$. So that would mean that in the above formula, we get:

$$T^{M_n}(m) \;=\; \frac{3^{K_n} m + \sum_{i=1}^{n} 3^{K_n-K_i} 2^{M_{i-1}}(3^{k_i} - 2^{k_i})}{2^{M_n}} \;=\; m$$

Rewriting this equation, we get:

$$m \;=\; \frac{\sum_{i=1}^{n} 3^{K_n-K_i} 2^{M_{i-1}}(3^{k_i} - 2^{k_i})}{2^{M_n} - 3^{K_n}} \tag{2.1}$$

So if there exists a cycle with global minimum m, then there must exist nonnegative numbers $\{k_i\}$ and $\{l_i\}$ such that the above holds. This means that for that choice of n, $\{k_i\}$ and $\{l_i\}$, the right hand side must be an integer. We also notice that if this is true, then m is indeed the minimum of a cycle with a period of at most M_n. This is true because divisions in the iterations of T are by a factor 2, while multiplications are with a factor 3. So if m is an integer and for some i, $T^i(m)$ is not, then $T^{i+j}(m)$ is not an integer for any $j = 1, 2, \ldots$. Furthermore, $T_1(2m) = 3m + \frac{1}{2}$, and $T_0(2m+1) = m + \frac{1}{2}$. So if $T^{M_n}(m) = m \in \mathbb{N}_+$ then $T^{M_n}(m)$ is indeed equal to $T_0^{l_n}(T_1^{k_n}(\ldots(T_0^{l_1}(T_1^{k_1}(m)))\ldots))$.

2.1.1 Known cycles

We can use the above results to verify the several known cycles on the positive and negative numbers. The cycle $(1, 2)$, starting with $m = 1$, has $n = k_1 = l_1 = 1$, so $K_1 = L_1 = P_1 = 1$ and

$M_1 = 2$. Using those values in the above formula gives us:

$$m = \frac{3^{1-1}2^0(3^1 - 2^1)}{2^2 - 3^1} = 1$$

So indeed, the formula gives us that for those values of k_i and l_i, we get an integer on the right hand side, and thus a cycle. Similarly, if we look at the negative cycle (-1) we get $n = 1$, $k_1 = 1$ and $l_1 = 0$. So then the formula gives us:

$$m = \frac{3^{1-1}2^0(3^1 - 2^1)}{2^1 - 3^1} = -1$$

And again, the formula gives us $m = -1$. We can also use the formula for the longer cycle starting $m = -17$, which goes $-17 \xrightarrow{T_1^4} -82 \xrightarrow{T_0} -41 \xrightarrow{T_1^3} -136 \xrightarrow{T_0^3} -17$. So we find $n = 2$, $k_1 = 4$, $l_1 = 1$, $k_2 = 3$, $l_2 = 3$ and thus:

$$m = \frac{3^{7-4}2^0(3^4 - 2^4) + 3^0 2^5(3^3 - 2^3)}{2^{11} - 3^7} = (2363) \, / \, (-139) = -17$$

Note that in this case, when the cycle is longer, the absolute value of the denominator has become quite big (139). So from a probabilistic point of view, the chance of getting an integer from this fraction (so that the denominator divides the numerator) is quite small. The cycles starting with $m = \pm 1$ had a denominator of ± 1, so the probability that the right hand side would be a whole number was just 1. For $m = -17$ only 1 out of each 139 possible values for the numerator would make the right hand side an integer. However, probabilistic assessments are not so useful here, since the numerator was indeed one of those 139 numbers divisible by 139. So even though the probability of another cycle of length, say, 10^{37}, is extremely small, there is no reason to assume that there cannot be such a cycle.

2.2 $pn + q$ problems

Analogously to the calculations for the $3n + 1$ conjecture, we can calculate the possible forms of cycles in $pn + q$ problems. For $pn + q$ problems, there can generally be many different cycles and divergent trajectories. Especially when p is big ($p \geq 5$) we expect many divergent trajectories to occur, and when q is big and contains many different prime factors in its prime factorization, we expect many cycles, as we will see later.

If we repeat the calculations we did above for the $3n + 1$ problem, but now for the $pn + q$ generalization, we get the following Theorems.

Theorem 2.2.1 (Calculation of $T^k_{p,q,1}(m)$). *For any $k \in \mathbb{N}$ we have:*

$$T^k_{p,q,1}(m) = \frac{p^k(p-q)m + q(p^k - 2^k)}{2^k(p-2)}$$

The proof is again simply by induction on k, and we will not write it out here. Analogously to the above calculations, we also get the following Theorem for the form of $T^{M_n}_{p,q}(m)$.

Theorem 2.2.2 (Form of $T^{M_n}_{p,q}(m)$). *For any $m \in \mathbb{Z}$ and $n, k_1, \ell_1, k_2, \ell_2, \ldots, k_n, \ell_n \in \mathbb{N}$ such that $T^{M_{i+1}}_{p,q}(m) = T^{\ell_{i+1}}_{p,q,0}(T^{k_{i+1}}_{p,q,1}(T^{M_i}_{p,q}(m)))$ for each $i \in \mathbb{N}$, we have:*

$$T^{M_n}_{p,q}(m) = \frac{p^{K_n} m(p-2) + q \sum_{i=1}^{n} p^{K_n - K_i} 2^{M_i}(p^{k_i} - 2^{k_1})}{2^{M_n}(p-2)}$$

This can again be proven by induction on n easily. This however involves some long and ugly formulas, so we will not write it out here.

As a consequence of the above formula, we can again find the possible starting points m of a cycle of length n, which must have the following form.

$$m = q \left(\frac{\sum_{i=1}^{n} p^{K_m - K_i} 2^{M_i} (p^{k_1} - 2^{k_i})}{(2^{M_n} - p^{K_n})(p-2)} \right)$$

Again, from the formula we can see that if m is an integer, then the numerator must be divisible by the denominator. So given $\{k_i\}$ and $\{l_i\}$, the denominator must at least be divisible by $2^{M_n} - p^{K_n}$. However, this is again a difference between two (high) powers of different numbers. This difference will not be so small when the powers are high, so the probability that there is a long cycle is again quite small.

Another interesting consequence of the formula for m is that on the right hand side, the only dependence on q is the factor q in front of the fraction. This means that if for certain values of p, q, k_i and l_i, the right hand side is not an integer but a fraction, say $\frac{\beta}{\alpha}$, then we can just multiply q by α and look at the $pn+\alpha q$ problem. This problem then does have those extra cycles. In this way we can create $pn + q$ problems with as many cycles as we want. For example, if we want a $pn + q$ problem to have all cycles of length ≤ 5, we can just take $p = 3$ and q such that the right hand side is then always an integer. In this case, we could take $q = 5 \cdot 7^2 \cdot 11 \cdot 13 \cdot 23 \cdot 29 = 23368345$ so that q is the least common multiple of the factors $3^K - 2^{K+L}$, with $K = 1, 2, 3, 4$, $L = 1, 2, 3, 4$ and $K + L = 2, 3, 4, 5$. Then we see that the $pn + q = 3n + 23368345$ problem has the cycles of length ≤ 5 as in Table 2.1. There are more cycles, such as those with parity bits $(0, 0)$ or $(1, 0, 1, 0)$, but those are just repetitions of shorter cycles. Furthermore, the $(0, 1)$ cycle is just a rotation of the cycle $(1, 0)$, so they refer to the same cycle (namely the cycle $(q, 2q)$) but with different starting points.

Starting Point m		Parity bits of $O^+(m)$
0	0	(0)
$-q$	-23368345	(1)
q	23368345	$(1, 0)$
$q/5$	4673669	$(1, 0, 0)$
$-5q$	-116841725	$(1, 1, 0)$
$q/13$	1797565	$(1, 0, 0, 0)$
$5q/7$	16691675	$(1, 1, 0, 0)$
$-19q/11$	-40363505	$(1, 1, 1, 0)$
$q/29$	805805	$(1, 0, 0, 0, 0)$
$5q/23$	5080075	$(1, 1, 0, 0, 0)$
$19q/5$	88799711	$(1, 1, 1, 0, 0)$
$-65q/49$	-30998825	$(1, 1, 1, 1, 0)$
$7q/23$	7112105	$(1, 0, 1, 0, 0)$
$23q/5$	107494387	$(1, 1, 0, 1, 0)$

Table 2.1: Cycles of length ≤ 5 in the $3n + 23368345$ problem.

Also note that if m is the starting point of a cycle of the $pn + 1$ problem, then qm is the starting point of a cycle in the $pn + q$ problem. The converse is not necessarily true at all; m could be a starting point of a cycle in the $pn + q$ problem, but m does not have to be divisible by q, so that m/q is not an integer starting point of a cycle in the $pn+1$ problem. This remark can also be seen in Table 2.1. The left column has only four integer multiples of q, namely $0, 1, -1$ and -5. These are four of the five known cycles of the $3n+1$ problem on the positive/negative integers. The other coefficients, such as $1/13$, $-19/11$ and $23/5$, are rational cycles in the $3n+1$ problem. For example, if we only look at the numerator modulo 2, we could consider the rational cycle of the $3n+1$ problem of the form $1/13 \to 16/13 \to 8/13 \to 4/13 \to 2/13 \to 1/13$ or $-19/11 \to -46/11 \to -23/11 \to -58/11 \to -29/11 \to -76/11 \to -38/11 \to -19/11$.

However, there are certain problems for which the converse is in fact true. We will take a look at certain problems for which we can easily verify this below.

2.2.1 $3n + 3^k$ problems

Here we will concentrate on the problems where $p = 3$ and $q = 3^k$ for some k. Note that the reason for the choice of $q = 3^k$ will appear later on.

First of all, we can easily verify that these problems indeed all have the trivial cycle starting with 3^k, namely the cycle $(3^k, 2 \cdot 3^k)$. Now let the $3n+3^k$ conjecture be defined as follows, with $k \in \mathbb{N}$.

Conjecture 2.2.3 ($3n + 3^k$ conjecture)**.** *The only component in the $3n + 3^k$ problem is the component $G = \mathbb{N}_+$ with $r(G) = 3^k$.*

Now this class of conjectures has an interesting relation with the $3n+1$ problem. It turns out that these $3n + 3^k$ conjectures are either all true or all false. This is proven in the following Theorem, and was also proven in [LL06].

Theorem 2.2.4 (Relation between $3n + 3^k$ problems)**.** *Conjecture 1.1.2 is true if and only if Conjecture 2.2.3 is true for any $k \in \mathbb{N}$.*

Proof. ($\Leftarrow$) Suppose Conjecture 2.2.3 is true for a certain $k \in \mathbb{N}$. For the sake of notation, we will write $T_k(n) = T_{3,3^k}(n)$, so that the function T_k is the $3n + 3^k$ function. First, we note that $T_k(3^k \cdot (2n)) = 3^k n = 3^k T(2n)$ and $T_k(3^k \cdot (2n+1)) = 3^k(3n+2) = 3^k T(2n+1)$. So $T_k(3^k n) = 3^k T(n)$. So also $T_k^q(3^k n) = 3^k T^q(n)$. Since the $3n + 3^k$ conjecture is true, we know that for each n there exists some q_0 with $T_k^{q_0}(3^k n) = 3^k$. That means that $3^k = T_k^{q_0}(3^k n) = 3^k T^{q_0}(n)$, so that $T^{q_0}(n) = 1$. So the $3n+1$ conjecture must also be true.

($\Rightarrow$) Now we assume that the $3n+1$ conjecture is true, and prove that the $3n+3$ conjecture (with the $3n+3$ function $T_1(n) = T_{3,3}(n)$) is also true. The proof can analogously be used to show that also the $3n + 9$ conjecture is true, or generally that the $3n + 3^k$ is true for any $k \in \mathbb{N}$.

Consider a number $n = 2^p(2m + 1) > 0$. Any number can be written like this, with certain integers p and m. Now obviously, $T_1^p(n) = 2m + 1$, and $T_1^{p+1}(n) = 3(m + 1)$. So after $p + 1 < \infty$ iterations, n has become a multiple of 3. Also, $T_1(3(2n)) = 3n$ and $T_1(3(2n + 1)) = 3(3n + 2)$, so a multiple of 3 always iterates to another multiple of 3. So to prove the $3n + 3$ conjecture, it is sufficient to show that all multiples of 3 iterate to 3 in a finite number of steps.

So now consider a number $n = 3m > 0$. Note that we still have that $T_1^q(3m) = 3T^q(m)$ for each m and q. But the $3n + 1$ conjecture is true, so there exists a q_0 with $T^{q_0}(m) = 1$. This means that $T_1^{q_0}(3m) = 3T^{q_0}(m) = 3$, which concludes the proof. □

Although this is an interesting result, which says that instead of proving the $3n + 1$ conjecture we may as well prove the $3n + 3$ conjecture, it is not clear if this result is really useful. Since the conjectures are equivalent, they must be equally hard to prove as well. We will therefore continue with the $3n + 1$ conjecture as the main problem and not the $3n + 3$ or $3n + 9$ problems, although we now know that they are all equivalent.

2.2.2 $pn + p^k q$ problems

Note that the above on $3n + 3^k$ problems can more generally be applied to $pn + p^k q$ problems. The $pn + q$ problems with $p \neq 3$ generally have more cycles and divergent trajectories than the $3n + 1$ problem. But also for the $pn + q$ problems we can just define some cycle set $\mathcal{C}_{p,q} = \{C_1, C_2, C_3, \ldots, C_n\}$, which we can conjecture to be the complete set of cycles for this problem. Then again, we can prove that the $pn + p^k q$ problem will have the same cycles. So if we write the $pn + p^k q$ cycle conjecture as follows:

Conjecture 2.2.5 ($pn + p^k q$ cycle conjecture)**.** *The only cycles in the $pn + p^k q$ problem are the cycles $C \in \mathcal{C}_{p,q}$.*

Then, analogously to the section on $3n + 3^k$ problems, we can prove the following Theorem.

Theorem 2.2.6 (Relation between $pn + p^k q$ problems)**.** *Conjecture 2.2.5 is true for $k = k_0 \in \mathbb{N}$ if and only if Conjecture 2.2.5 is true for any $k \in \mathbb{N}$.*

The proof is again based on the notion that in the $pn + p^k q$ problem, for any $n \in \mathbb{N}_+$ we can find an index $i = i(n)$ such that $T^i_{p,p^k q}(n) \equiv 0$ modulo p^k. Then we again note that $T_{p,p^k q}(\alpha p^k) = p^k T_{p,q}(\alpha)$, so that cycles in the $pn + q$ problem correspond one on one with cycles in the $pn + p^k q$ problems.

2.3 Summary

We can say that although we can find direct formulas for the shape of starting points of cycles, in terms of $\{k_i\}$ and $\{l_i\}$, these formulas are too complex to just "solve". It is not so easy to see if the formula has other integer solutions besides the known cycles. We can see that the probability that other cycles exist is small, but we cannot say with certainty that they do not exist.

Furthermore, we got the interesting result that the $3n + 3^k$ problems are equivalent to the $3n + 1$ conjecture. It is hard to see how this notion can be used to prove or disprove the conjecture. However, this does mean that if some method turns out to work "better" for a different $3n + 3^k$ problem (for example nicer formulas, or a more obvious structure) we could also look at that problem instead, since proving a different $3n + 3^k$ problem also means proving the $3n + 1$ conjecture. However, since the conjectures are equivalent, it is unlikely that certain methods will work much better for, say, the $3n + 3$ problem than the $3n + 1$ problem.

Summarizing, we can say that we got more insight into the $3n+1$ problem and $pn+q$ problems in general, and the formulas gave us an idea why the problem is not so easy to solve. We will probably need other methods to learn more about the problem or to find a proof or counterexample to the conjecture. Therefore we will now move on to different approaches to the problem, starting with the Collatz Digraph in the next chapter.

Chapter 3

The Collatz Digraph and its spectrum

3.1 The $3n + 1$ conjecture

Instead of considering the $3n + 1$ function as a function from $\mathbb{N}_+$ to $\mathbb{N}_+$, we can also look at repeated iterations of $T(n)$ as being paths in a directed graph (digraph) with vertices $V = \mathbb{N}_+$ and edges $E = \{(v_1, v_2) \mid T(v_1) = v_2\}$. Then, instead of saying that $T^{70}(27) = 1$, we can also say that after 70 steps in the Collatz digraph, starting at vertex 27, we are at the vertex labeled 1. Similarly, the $3n + 1$ conjecture can be reformulated as the conjecture that from every vertex $n \in V = \mathbb{N}_+$, there is some $k \in \mathbb{N}$ such that after k transitions in the Collatz graph, starting at vertex n, we arrive at the vertex labeled 1.

3.1.1 Partial and Infinite Collatz Digraphs

To be more specific, we first define the *Partial Collatz Digraph*, which is the Collatz graph mentioned above, but reduced to the first n integers of $\mathbb{N}_+$:

Definition 3.1.1 (Partial Collatz Digraph)**.** *The Partial Collatz Digraph (PCD) up to a given number n, denoted by $\mathcal{G}_n$, is the directed graph $G = (V_n, E_n)$ such that*

$$\begin{aligned} V_n &= \{1, 2, 3, \ldots, n-1, n\} \\ E_n &= \{(i, j) \mid 1 \leq i, j \leq n \text{ and } T(i) = j\}. \end{aligned}$$

Furthermore, we denote the adjacency matrix of $\mathcal{G}_n$ with A_n, which is an $n \times n$ matrix of the form below. Zeroes in the matrix are replaced by dots, to increase the readability and to emphasize the structure.

$$A_n = \begin{pmatrix} . & 1 & . & . & . & . & . & . & \cdots \\ 1 & . & . & . & . & . & . & . & \cdots \\ . & . & . & . & 1 & . & . & . & \cdots \\ . & 1 & . & . & . & . & . & . & \cdots \\ . & . & . & . & . & . & . & 1 & \cdots \\ . & . & 1 & . & . & . & . & . & \ddots \\ . & . & . & . & . & . & . & . & \cdots \\ . & . & . & 1 & . & . & . & . & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Or, more formally, A_n is defined by:

$$(A_n)_{ij} = \begin{cases} 1 & \text{if } T(i) = j; \\ 0 & \text{else.} \end{cases}$$

As an example, we have drawn the PCD for $n = 32$ in Figure 3.1. Note that this graph is not connected, because some numbers 'climb' above 32 before descending back to 1. For example, $T(27) = 41$, but since 41 is not in the graph, there is no outgoing edge from the vertex labeled 27. Similarly, we have drawn the PCD with $n = 5000$ in Figure 3.2, without single vertices and without vertex labeling. This graphic nicely shows the structure of the $3n+1$ problem. Most numbers are already 'sucked up' by the massive component containing the cycle $(1, 2)$, while there are some small other unconnected parts which will soon be sucked up by the big component as well.

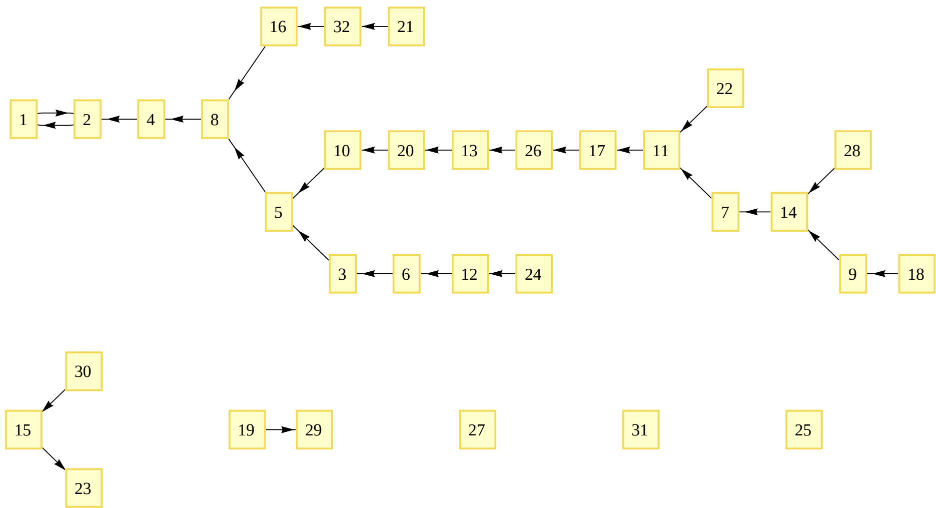

Figure 3.1: The Partial Collatz Digraph $\mathcal{G}_{32}$ which as expected contains exactly one cycle. We can already see one big component arising, containing the trivial cycle.

Now we can also define the *Infinite Collatz Digraph* formally as below.

Definition 3.1.2 (Infinite Collatz Digraph)**.** *The Infinite Collatz Digraph (ICD), denoted by $\mathcal{G}_\infty$, is the infinite graph $G = (V_\infty, E_\infty)$ such that:*

$$\begin{aligned} V_\infty &= \{1, 2, 3, \ldots\} \\ E_\infty &= \{(i, j) \mid 1 \leq i, j \text{ and } T(i) = j\}. \end{aligned}$$

Furthermore, we denote the adjacency matrix of $\mathcal{G}_\infty$ with A, which is an infinite-dimensional $\infty \times \infty$ matrix of the form:

$$A = \begin{pmatrix} . & 1 & . & . & . & . & . & . & \cdots \\ 1 & . & . & . & . & . & . & . & \cdots \\ . & . & . & . & 1 & . & . & . & \cdots \\ . & 1 & . & . & . & . & . & . & \cdots \\ . & . & . & . & . & . & . & 1 & \cdots \\ . & . & 1 & . & . & . & . & . & \ddots \\ . & . & . & . & . & . & . & . & \cdots \\ . & . & . & 1 & . & . & . & . & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

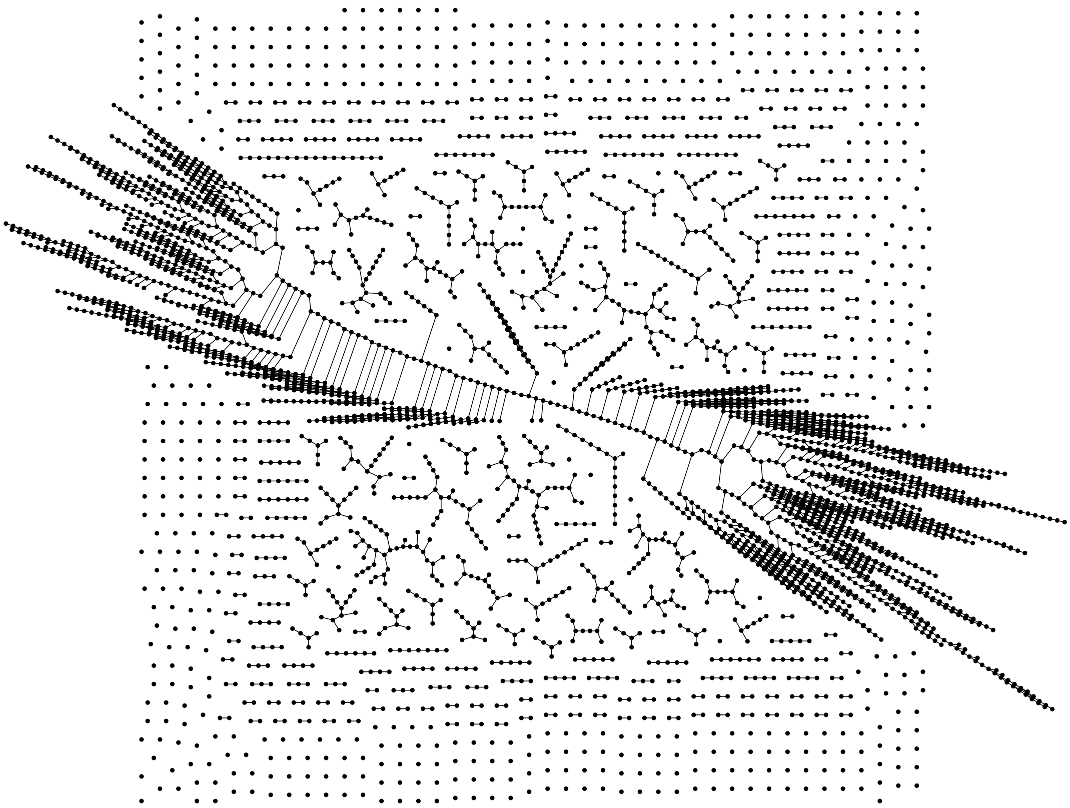

Figure 3.2: The Partial Collatz Digraph $\mathcal{G}_{5000}$.

Or, more formally, A is defined by:

$$A_{ij} = \begin{cases} 1 & \textit{if } T(i) = j; \\ 0 & \textit{else.} \end{cases}$$

We will also use A^T which is the transpose matrix of A. So $(A^T)_{ij} = 1$ means that $T(j) = i$, or equivalently that $j \in T^{-1}(i)$.

Now the $3n+1$ cycle conjecture is equivalent to the conjecture that the graph $\mathcal{G}_\infty$ contains exactly one cycle (namely the trivial cycle $(1, 2)$), and the $3n+1$ divergence conjecture is equivalent to the conjecture that the graph $\mathcal{G}_\infty$ has no components containing no cycles. Thus the $3n+1$ conjecture says that this graph has exactly one connected component with the cycle $(1, 2)$. Note that the previous statement about the divergence conjecture cannot be said about the PCDs, since the PCD of size n has roughly $5n/6$ components; one component containing the $(1, 2)$ cycle, and $n/6$ components where the leaves are odd numbers i bigger than $(2n-1)/3$, such that $T(i) > n$ and thus i has no outgoing edges.

Now, instead of continuing with the Collatz graph, which is just the $3n+1$ conjecture on vertices instead of numbers, we continue with the matrix A and its transpose A^T. These matrices can be seen as the matrices of linear functions from $\mathbb{C}^\infty \to \mathbb{C}^\infty$.

3.1.2 Special vectors

First we define some more notation.

- **0**: The all-zeroes vector $(0, 0, 0, 0, \ldots)$.

- $\mathbf{1}$: The all-ones vector $(1,1,1,1,\ldots)$.
- $\boldsymbol{e}_i$: The ith unit vector $(0,0,\ldots,0,1,0,\ldots)$.

One can now easily verify that $A\boldsymbol{e}_i = \sum_{j\in T^{-1}(i)} \boldsymbol{e}_j$ and $A^T\boldsymbol{e}_i = \boldsymbol{e}_{T(i)}$ for all i. For example, $A\boldsymbol{e}_8 = \boldsymbol{e}_5 + \boldsymbol{e}_{16}$, and $A^T\boldsymbol{e}_8 = \boldsymbol{e}_4$.

We will write G_C and G_P for the sets of numbers in the components containing the cycle C and divergent trajectory P respectively, and we will just assume that C has a certain cycle length k and minimum c_0. Then we get the following special vectors $\boldsymbol{v}$ for the matrix A.

$$\begin{aligned}
\boldsymbol{v}(G) &= \sum_{n\in G} \boldsymbol{e}_n \\
\boldsymbol{v}_i(G_C) &= \sum_{\substack{n\in G_C \\ \ell(n)\equiv i \pmod k}} \boldsymbol{e}_n \\
\boldsymbol{v}(G_C) &= \sum_{i=0}^{k-1} \boldsymbol{v}_i(G_C)
\end{aligned}$$

Similarly, for the matrix A^T we get the following vectors $\boldsymbol{w}$. Below, I_P is one of the infinitely many infinite divergent paths in G_P.

$$\begin{aligned}
\boldsymbol{w}(C) &= \sum_{n\in C} \boldsymbol{e}_n \\
\boldsymbol{w}(I_P) &= \sum_{n\in I_P} \boldsymbol{e}_n \\
\boldsymbol{w}_i(G_C) &= \boldsymbol{e}_{T^i(c_0)} \\
\boldsymbol{w}(G_C) &= \sum_{i=0}^{k-1} \boldsymbol{w}_i(G_C)
\end{aligned}$$

For example, with $C = C_{triv}$ we get:

$$\begin{aligned}
\boldsymbol{v}_0(G_C) &= (1,0,0,1,1,1,0,\ldots) \\
\boldsymbol{v}_1(G_C) &= (0,1,1,0,0,0,1,\ldots) \\
\boldsymbol{w}_0(G_C) &= (1,0,0,0,0,0,0,\ldots) \\
\boldsymbol{w}_1(G_C) &= (0,1,0,0,0,0,0,\ldots)
\end{aligned}$$

Now, we define $\zeta_k = e^{2\pi i/k}$ and we define $R_k = \{1,\zeta_k,\zeta_k^2,\ldots,\zeta_k^{k-1}\}$ as the set of roots of unity. For these $\zeta\in R_k$ and for complex numbers $\omega\in\mathbb{C}^*$ ($\omega\in\mathbb{C}$ and $\omega\neq 0$), we define:

$$\begin{aligned}
\boldsymbol{v}(G_C,\zeta) &= \sum_{n\in G_C} \zeta^{-\ell(n)}\boldsymbol{e}_n \\
\boldsymbol{v}(G_P,\omega) &= \sum_{n\in G_P} \omega^{-\ell(n)}\boldsymbol{e}_n
\end{aligned}$$

For the transpose matrix A^T we get the special vectors:

$$\begin{aligned}
\boldsymbol{w}(C,\zeta) &= \sum_{n\in C} \zeta^{\ell(n)}\boldsymbol{e}_n \\
\boldsymbol{w}(I_P,\omega) &= \sum_{n\in I_P} \omega^{\ell(n)}\boldsymbol{e}_n \\
\boldsymbol{w}(I_C,\omega) &= \sum_{n\in I_C\setminus C} \left(1-\frac{1}{\omega^k}\right)\omega^{\ell(n)}\boldsymbol{e}_n + \sum_{n\in C}\omega^{\ell(n)}\boldsymbol{e}_n
\end{aligned}$$

Note that $\boldsymbol{w}(I_C,\omega) = \boldsymbol{w}(C,\zeta)$ when $\omega\in R_k$, since then $(1-\frac{1}{\omega^k}) = 0$.

3.1.3 Properties of the special vectors

First, we look at the vectors $\boldsymbol{v}$, which have special properties when multiplied from the left by A. If $n \in G_C$ and the length of the cycle C is k, then $\ell(T(n)) \equiv \ell(n) - 1 \pmod{k}$ and so $\zeta^{\ell(T(n))} = \zeta^{\ell(n)-1}$ for all $\zeta \in R_k$.

$$\begin{aligned}
A\boldsymbol{v}(G) &= \sum_{n\in G} A\boldsymbol{e}_n = \sum_{n\in G}\sum_{m\in T^{-1}(n)} \boldsymbol{e}_m = \boldsymbol{v}(G) \\
A\boldsymbol{v}_i(G_C) &= \sum_{\substack{n\in G_C\\ \ell(n)\equiv i}} A\boldsymbol{e}_n = \sum_{\substack{n\in G_C\\ \ell(n)\equiv i}}\sum_{m\in T^{-1}(n)} \boldsymbol{e}_m = \sum_{\substack{m\in G_C\\ \ell(m)\equiv i+1}} \boldsymbol{e}_m = \boldsymbol{v}_{i+1}(G_C) \\
A\boldsymbol{v}(G_C,\zeta) &= \sum_{n\in G_C} \zeta^{-\ell(n)} A\boldsymbol{e}_n = \sum_{n\in G_C}\sum_{m\in T^{-1}(n)} \zeta^{-\ell(n)}\boldsymbol{e}_m = \sum_{m\in G_C} \zeta^{1-\ell(m)}\boldsymbol{e}_m = \zeta\boldsymbol{v}(G_C,\zeta) \\
A\boldsymbol{v}(G_P,\omega) &= \sum_{n\in G_P} \omega^{-\ell(n)} A\boldsymbol{e}_n = \sum_{n\in G_P}\sum_{m\in T^{-1}(n)} \omega^{-\ell(n)}\boldsymbol{e}_m = \sum_{m\in G_P} \omega^{1-\ell(m)}\boldsymbol{e}_m = \omega\boldsymbol{v}(G_P,\omega)
\end{aligned}$$

Similarly, for the vectors $\boldsymbol{w}$ we have the following properties when they are multiplied from the right by A (so from the left by A^T).

$$\begin{aligned}
A^T\boldsymbol{w}(C) &= \sum_{n\in C} A^T\boldsymbol{e}_n = \sum_{n\in C} \boldsymbol{e}_{T(n)} = \boldsymbol{w}(C) \\
A^T\boldsymbol{w}(I_P) &= \sum_{n\in I_P} A^T\boldsymbol{e}_n = \sum_{n\in I_P} \boldsymbol{e}_{T(n)} = \boldsymbol{w}(I_P) \\
A^T\boldsymbol{w}_i(G_C) &= A^T\boldsymbol{e}_{T^i(c)} = \boldsymbol{e}_{T(T^i(c))} = \boldsymbol{w}_{i+1}(G_C) \\
A^T\boldsymbol{w}(C,\zeta) &= \sum_{n\in C} \zeta^{\ell(n)} A^T\boldsymbol{e}_n = \sum_{n\in C} \zeta^{\ell(T(n))+1}\boldsymbol{e}_{T(n)} = \zeta\sum_{m\in C}\zeta^{\ell(m)}\boldsymbol{e}_m = \zeta\boldsymbol{w}(C,\zeta) \\
A^T\boldsymbol{w}(I_P,\omega) &= \sum_{n\in I_P} \omega^{\ell(n)} A^T\boldsymbol{e}_n = \sum_{n\in I_P} \omega^{\ell(T(n))+1}\boldsymbol{e}_{T(n)} = \omega\sum_{m\in I_P}\omega^{\ell(m)}\boldsymbol{e}_m = \omega\boldsymbol{w}(I_P,\omega)
\end{aligned}$$

For the following calculation we will denote the point in the cycle where the infinite path I_C first hits the cycle with c_1, and we will take the root of the component containing C the c_0 in the cycle such that $T(c_0) = c_1$.

$$\begin{aligned}
A^T\boldsymbol{w}(I_C,\omega) &= \sum_{n\in I_C\setminus C}\left(1-\frac{1}{\omega^2}\right)\omega^{\ell(n)}\boldsymbol{e}_{T(n)} + \sum_{n\in C}\omega^{\ell(n)}\boldsymbol{e}_{T(n)} \\
&= \omega\sum_{n\in I_C\setminus C}\left(1-\frac{1}{\omega^k}\right)\omega^{\ell(n)}\boldsymbol{e}_n + \left(1-\frac{1}{\omega^2}\right)\omega^2\boldsymbol{e}_{c_1} + \omega\sum_{n\in C\setminus\{c_1\}}\omega^{\ell(n)}\boldsymbol{e}_n + \boldsymbol{e}_{c_1} \\
&= \omega\sum_{n\in I_C\setminus C}\left(1-\frac{1}{\omega^k}\right)\omega^{\ell(n)}\boldsymbol{e}_n + \omega\sum_{n\in C}\omega^{\ell(n)}\boldsymbol{e}_n \\
&= \omega\boldsymbol{w}(I_C,\omega)
\end{aligned}$$

3.1.4 Eigenvalue 0

As each row of A has exactly one 1 and each column has at least one 1, it follows that $A\boldsymbol{v} = \boldsymbol{0}$ implies that $\boldsymbol{v} = \boldsymbol{0}$. Therefore there are no eigenvectors with eigenvalue 0 for the matrix A.

Since there are infinitely many columns in A^T with multiple 1s, we see that there are infinitely many eigenvectors with eigenvalue 0. They are a linear combination of the vectors $\boldsymbol{e}_{2n+1} - \boldsymbol{e}_{6n+4}$, which have $A^T(\boldsymbol{e}_{2n+1} - \boldsymbol{e}_{6n+4}) = \boldsymbol{e}_{3n+2} - \boldsymbol{e}_{3n+2} = \boldsymbol{0}$. These are also all the eigenvectors for the eigenvalue 0, since $A^T\boldsymbol{v} = \boldsymbol{0}$ implies that for each n, $(A^T\boldsymbol{v})_n = 0$, so that $\sum_{m\in T^{-1}(n)} \boldsymbol{e}_m = 0$.

3.1.5 Eigenvalue 1

From the previous calculations, we saw that $A\boldsymbol{v}(G) = \boldsymbol{v}(G)$, so $\boldsymbol{v}(G)$ is an eigenvector for A with eigenvalue 1, for each component G. The $3n+1$ conjecture says that there is only one component on $\mathbb{N}_+$, namely the component containing all positive numbers. So an equivalent formulation of the $3n+1$ conjecture is that the only eigenvector of A with eigenvalue 1 is the vector $\boldsymbol{v}(G) = \boldsymbol{v}(\mathbb{N}_+) = (1, 1, 1, \ldots)$.

Similarly, we saw that $A^T\boldsymbol{w}(C) = \boldsymbol{w}(C)$ for each cycle C, and $A^T\boldsymbol{w}(P) = \boldsymbol{w}(P)$ for each divergent path P. So there is at least one known eigenvector for the eigenvalue 1, namely the vector $\boldsymbol{w}(C_{triv})$. Furthermore, this means that any other cycle will also lead to a new eigenvector of A^T with the eigenvalue 1. The $3n+1$ cycle conjecture is thus equivalent with the statement that the eigenspace of A^T for the value 1 has dimension 1 and contains only all multiples of $\boldsymbol{w}(C_{triv})$.

3.1.6 Eigenvalues $\zeta \in R_k$

From the above calculations we saw that if C has cycle length k and $\zeta \in R_k$, then $A\boldsymbol{v}(G_C, \zeta) = \zeta\boldsymbol{v}(G_C, \zeta)$. So $\boldsymbol{v}(G_C, \zeta)$ is an eigenvector for A with eigenvalue ζ. For example, for $C = C_{triv}$, we get the eigenvector $\boldsymbol{v}(G_C, 1) = \sum_{n\in G_C} 1^{-\ell(n)}\boldsymbol{e}_n = (1, 1, 1, 1, \ldots) = \boldsymbol{v}_0(G_C) + \boldsymbol{v}_1(G_C)$ with eigenvalue 1, and the eigenvector $\boldsymbol{v}(G_C, -1) = \sum_{n\in G_C} (-1)^{-\ell(n)}\boldsymbol{e}_n = (1, -1, -1, 1, \ldots) = \boldsymbol{v}_0(G_C) - \boldsymbol{v}_1(G_C)$ with eigenvalue -1.

For A^T we saw that if C has cycle length k and $\zeta \in R_k$, then $A^T\boldsymbol{w}(C, \zeta) = \zeta\boldsymbol{w}(C, \zeta)$ so that $\boldsymbol{w}(C, \zeta)$ is an eigenvector for A^T with eigenvalue ζ. Again taking the example $C = C_{triv}$, this gives us the eigenvectors $\boldsymbol{w}(C, 1) = \sum_{n\in C} 1^{\ell(n)}\boldsymbol{e}_n = \boldsymbol{e}_1 + \boldsymbol{e}_2$ with eigenvalue 1, and $\boldsymbol{w}(C, -1) = \sum_{n\in C} -1^{\ell(n)}\boldsymbol{e}_n = \boldsymbol{e}_1 - \boldsymbol{e}_2$ with eigenvalue -1.

3.1.7 Eigenvalues $\omega \in \mathbb{C}^*$

Above, we also saw that for any divergent trajectory P and any complex number $\omega \neq 0$ we have $A\boldsymbol{v}(G_P, \omega) = \omega\boldsymbol{v}(G_P, \omega)$. So for any divergent trajectory, we find the set of eigenvalues $\mathbb{C}^*$, each with one eigenvector.
Similarly, for A^T we saw that for any infinite divergent path I_P and complex number $\omega \neq 0$, we have $A^T\boldsymbol{w}(I_P, \omega) = \omega\boldsymbol{w}(I_P, \omega)$. So if a component with divergent trajectories exists, then all complex numbers are eigenvalues with infinite-dimensional eigenspaces. Furthermore, for cycles we found the eigenvectors $\boldsymbol{w}(I_C, \omega)$ with eigenvalues $\omega \in \mathbb{C}^*$. So if a cycle exists, then any $\omega \in \mathbb{C}^*$, $\omega \notin R_k$ is an eigenvalue with an infinite-dimensional eigenspace.

3.1.8 Spectrum of the $3n+1$ problem

If we now apply the above results to the $3n+1$ problem, we see that if the $3n+1$ conjecture is true, then for A we get only one eigenvector and eigenvalue, namely:

- $(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, \ldots)$ with eigenvalue 1.

For A^T we then expect to get eigenvectors as the following:

- $(1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalue 1.
- $(1, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalue -1.
- $(1, \omega, 0, \omega^2 - 1, 0, 0, 0, \omega^3 - \omega, 0, 0, 0, 0, 0, 0, 0, \omega^4 - \omega^2, 0, 0, \ldots)$ with eigenvalues $\omega \in \mathbb{C}^*$.
- $(1, \omega, \omega^5 - \omega^3, \omega^2 - 1, \omega^4 - \omega^2, \omega^6 - \omega^4, 0, \omega^3 - \omega, 0, 0, 0, \omega^7 - \omega^5, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalues $\omega \in \mathbb{C}^*$.
- $\boldsymbol{e}_{2n+1} - \boldsymbol{e}_{6n+4}$ with eigenvalue 0, for all $n \in \mathbb{N}$.

As we can see, 1 is an eigenvalue for A with eigenvector $(1, 1, 1, 1, \ldots)$. As we saw earlier on, the $3n + 1$ conjecture is true if and only if the Collatz digraph has only one component. Since every other component (containing either a divergent trajectory or a cycle) would give rise to at least one new eigenvector with eigenvalue 1 (namely the vector with 1s at the position of numbers in this component), the following Theorem can easily be verified.

Theorem 3.1.3 ($3n+1$ conjecture, variant (1))**.** *The $3n+1$ conjecture is true if and only if the dimension of the eigenspace for the eigenvalue 1 of A is 1.*

Similarly, if another cycle or divergent path exists, we see that we will also get new eigenvectors for A^T for the eigenvalue 1. Therefore, the following theorem obviously holds as well.

Theorem 3.1.4 ($3n+1$ conjecture, variant (2))**.** *The $3n+1$ conjecture is true if and only if the dimension of the eigenspace for the eigenvalue 1 of A^T is 1.*

Note that the two above theorems are not trivially equivalent, since the transpose of an infinite matrix does not necessarily have to have the same spectrum and dimensions of eigenspaces.

3.2 $pn + q$ problems

Analogously to the above approach, we can look at the graph, matrix and eigenvalues of other $pn + q$ problems. First of all, we see that different $pn + q$ problems lead to different graphs with different adjacency matrices. The even rows of the matrix stay the same (because of the division by 2 for even numbers) but the position of the 1 in odd rows changes.

3.2.1 The $n + 1$ problem

One simple example of a $pn+q$ problem is the $n+1$ problem with $p = q = 1$. The graph associated to this problem has the following adjacency matrix B.

$$B = \begin{pmatrix} 1 & . & . & . & . & . & . & . & \cdots \\ 1 & . & . & . & . & . & . & . & \cdots \\ . & 1 & . & . & . & . & . & . & \cdots \\ . & 1 & . & . & . & . & . & . & \cdots \\ . & . & 1 & . & . & . & . & . & \cdots \\ . & . & 1 & . & . & . & . & . & \cdots \\ . & . & . & 1 & . & . & . & . & \cdots \\ . & . & . & 1 & . & . & . & . & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

For this example, we easily see that there are no divergent paths, and that there is only one cycle on the positive integers, namely the cycle (1). For the matrix B we therefore find only one eigenvector, corresponding to the component $\mathbb{N}_+$:

- $(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, \ldots)$ with eigenvalue 1.

For the transpose matrix B^T, we find several eigenvectors, including:

- $(1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalue 1.
- $(1, \omega - 1, \omega^2 - \omega, 0, 0, \omega^3 - \omega^2, 0, 0, 0, 0, \omega^4 - \omega^3, 0, 0, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalues $\omega \in \mathbb{C}^*$, $\omega \notin R_1$.
- $\boldsymbol{e}_{2n+1} - \boldsymbol{e}_{2n+2}$ with eigenvalue 0, for all $n \in \mathbb{N}$.

For B^T we therefore find exactly one eigenvector with eigenvalue 1, and infinitely many eigenvectors for all other complex eigenvalues (including 0).

3.2.2 The $5n + 1$ problem

Things get more interesting when we look at the $5n + 1$ problem, which has multiple cycles and is expected to have many divergent trajectories. The graph of the $5n+1$ problem has the adjacency matrix C given below.

$$C = \begin{pmatrix} . & . & 1 & . & . & . & . & . & \cdots \\ 1 & . & . & . & . & . & . & . & \cdots \\ . & . & . & . & . & . & . & 1 & \cdots \\ . & 1 & . & . & . & . & . & . & \ddots \\ . & . & . & . & . & . & . & . & \cdots \\ . & . & 1 & . & . & . & . & . & \cdots \\ . & . & . & . & . & . & . & . & \cdots \\ . & . & . & 1 & . & . & . & . & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

An interesting comparison between the $3n + 1$ problem and the $5n + 1$ problem can be made using Figure 3.3, the partial digraph on the first 5000 vertices, and Figure 3.2, the same graph for the $3n + 1$ problem. Figure 3.3 nicely shows the structure of the $5n + 1$ problem. There are no really big connected parts, and we expect that most of the unconnected parts will also remain unconnected and form different components in the $5n+1$ problem. The $5n+1$ problem only has 3 known cycles. Probably most of the other connected parts are components arising from divergent trajectories.

Since with the approach for the $3n+1$ problem we did not make any assumptions on the existence of other cycles or divergent trajectories, we already saw general formulas for eigenvalues and eigenvectors there. We know that the $5n+1$ problem contains multiple cycles, such as $(1, 3, 8, 4, 2)$, $(13, 33, 83, 208, 104, 52, 26)$ and $(17, 43, 108, 54, 27, 68, 34)$. We also expect infinitely many divergent trajectories to exist, because values increase on average by a factor $\frac{1}{2}\sqrt{5} > 1$ in each iteration. This leads to the following eigenvectors for C:

- $(1, 1, 1, 1, 0, 1, 0, 1, 0, 0, 0, 1, 0, 0, 1, 1, 0, 0, \ldots)$ with eigenvalue 1.
- $(0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, \ldots)$ with eigenvalue 1.
- $(0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 1, 0, 0, 1, 0, 0, 0, 1, \ldots)$ with eigenvalue 1.
- $(0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, \ldots)$ with eigenvalue 1.
- $(1, \zeta^4, \zeta, \zeta^3, 0, 1, 0, \zeta^2, 0, 0, 0, \zeta^3, 0, 0, \zeta^4, \zeta, 0, 0, \ldots)$ with eigenvalues $\zeta \in R_5$.
- $(0, 0, 0, 0, \zeta, 0, 0, 0, 0, \zeta^2, 0, 0, 1, 0, 0, 0, 0, 0, \ldots)$ with eigenvalues $\zeta \in R_7$.
- $(0, 0, 0, 0, 0, 0, 1, 0, \omega^{-2}, 0, \omega^3, 0, 0, \omega, 0, 0, 0, \omega^{-1}, \ldots)$ with eigenvalues $\omega \in \mathbb{C}^*$.

Similarly, for C^T we get the following eigenvectors:

- $(1, 1, 1, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalue 1.
- $(1, \zeta, \zeta^4, \zeta^2, 0, 0, 0, \zeta^3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalues $\zeta \in R_5$.
- $(1, \omega, \omega^4, \omega^2, 0, \omega^5 - 1, 0, \omega^3, 0, 0, 0, \omega^6 - \omega, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalues $\omega \in \mathbb{C}^*$.
- $(0, 0, 0, 0, 0, 0, 1, 0, \omega^{-2}, 0, 0, 0, 0, \omega, 0, 0, 0, \omega^{-1}, \ldots)$ with eigenvalue $\omega \in \mathbb{C}^*$.
- $\boldsymbol{e}_{10n+6} - \boldsymbol{e}_{2n+1}$ with eigenvalue 0, for all $n \in \mathbb{N}$.

If there are indeed infinitely many components containing divergent trajectories, then all complex numbers are eigenvectors for both C and C^T, each with an associated eigenspace of dimension ∞.

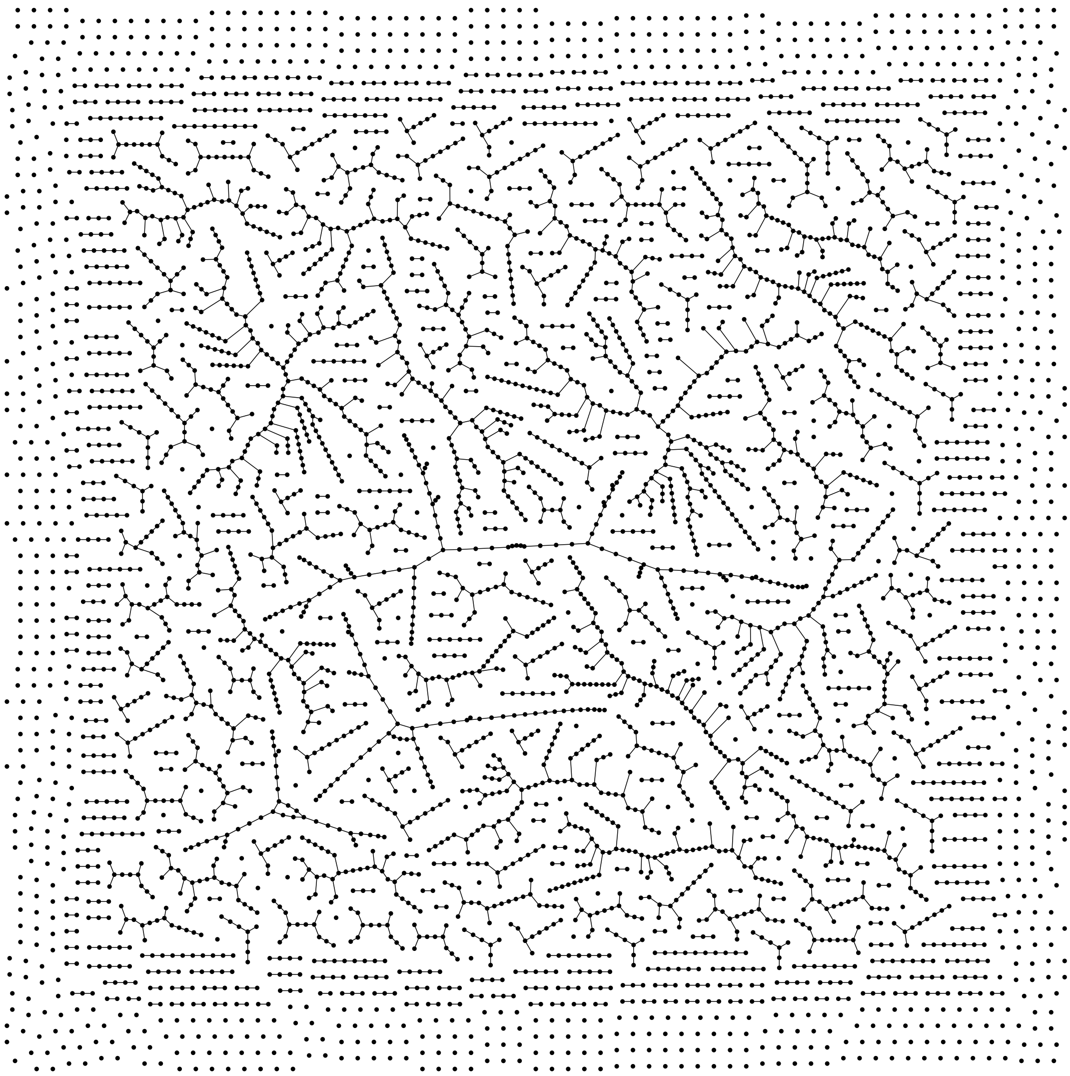

Figure 3.3: The Partial $5n + 1$ Digraph on 5000 vertices.

3.3 Collatz-like problems

The above approach can also be used for Collatz-like problems in general. For example, we can look at the Collatz-like problem $C_3(n)$ defined as below:

$$C_3(n) = \begin{cases} n/3 & n \equiv 0 \bmod 3 \\ (2n+1)/3 & n \equiv 1 \bmod 3 \\ (4n+1)/3 & n \equiv 2 \bmod 3 \end{cases}$$

Note that in this case, the geometric mean of the $\{a_i\}$ is $f = \sqrt[m]{a_0 a_1 a_2} = \sqrt[3]{1 \cdot 2 \cdot 4} = 2 < 3 = m$, so we expect no divergent trajectories to exist. The number of components will therefore probably be equal to the number of cycles in this problem. Generally there are only few cycles in such problems, so we expect only few components. This can also be verified through Figure 3.4. We see two big components coming from the cycles (1) and (5, 7), and only a few other small unconnected parts, which will soon be connected to one of the two bigger components as well, when the 5000 is changed to something bigger.

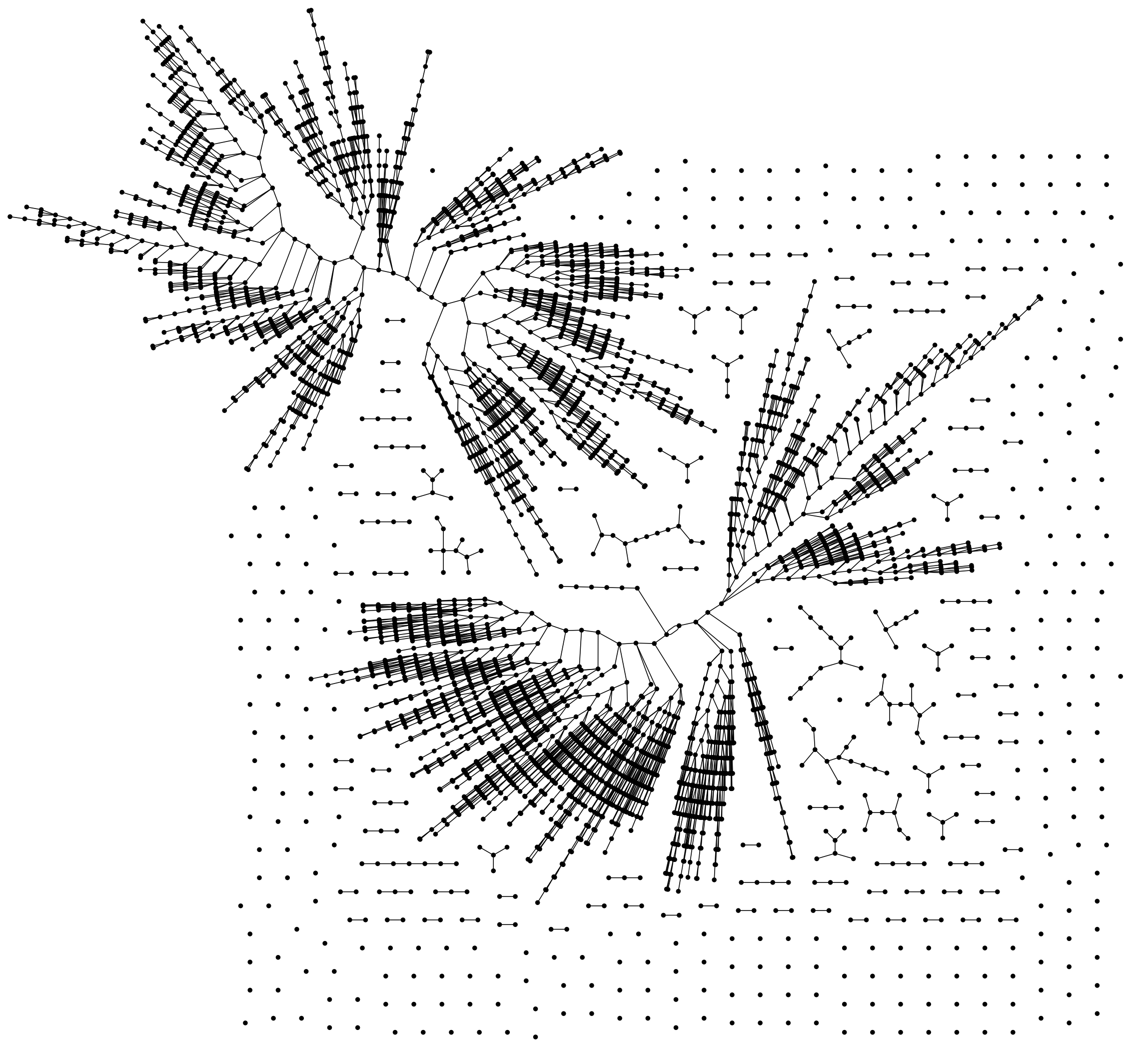

Figure 3.4: The Partial C_3 Digraph on 5000 vertices.

The graph associated with the $C_3(n)$ problem has the following adjacency matrix:

$$D = \begin{pmatrix} 1 & . & . & . & . & . & . & . & \cdots \\ . & . & 1 & . & . & . & . & . & \cdots \\ 1 & . & . & . & . & . & . & . & \cdots \\ . & . & 1 & . & . & . & . & . & \cdots \\ . & . & . & . & . & . & 1 & . & \cdots \\ . & 1 & . & . & . & . & . & . & \ddots \\ . & . & . & . & 1 & . & . & . & \cdots \\ . & . & . & . & . & . & . & . & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \end{pmatrix}$$

If we assume that the cycles (1) and $(5,7)$ are the only cycles, and there are no divergent trajectories, then we only get the following two eigenvectors for D, corresponding to the components containing these two cycles:

- $(1,1,1,1,0,1,0,0,1,0,0,1,1,1,0,0,0,1,\ldots)$ with eigenvalue 1.
- $(0,0,0,0,1,0,1,1,0,1,1,0,0,0,1,1,1,0,\ldots)$ with eigenvalue 1.

For D^T we find the following eigenvectors:

- $(1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalue 1.
- $(1, 0, \omega - 1, 0, 0, 0, 0, 0, \omega^2 - \omega, 0, 0, 0, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalues $\omega \in \mathbb{C}^*$.
- $(0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalue 1.
- $(0, 0, 0, 0, 1, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \ldots)$ with eigenvalue -1.
- $(0, 0, 0, 0, 1, 0, \omega^{-1}, 0, 0, 0, \omega^2 - 1, 0, 0, 0, \omega - \omega^{-1}, \omega^3 - \omega, 0, 0, \ldots)$ with eigenvalue $\omega \in \mathbb{C}^*$.
- $\boldsymbol{e}_{6n+3} - \boldsymbol{e}_{3n+1}$ with eigenvalue 0, for all $n \in \mathbb{N}$
- $\boldsymbol{e}_{12n+9} - \boldsymbol{e}_{3n+2}$ with eigenvalue 0, for all $n \in \mathbb{N}$
- $\boldsymbol{e}_{6n+4} - \boldsymbol{e}_{3n+2}$ with eigenvalue 0, for all $n \in \mathbb{N}$

If the two mentioned cycles are the only cycles and there are no divergent trajectories, then the eigenspace for the eigenvalue 1 is 2 for both D and D^T. For D^T all other numbers are also eigenvalues, with an infinite-dimensional eigenspace.

3.4 Functions $f : \mathbb{N}_+ \longrightarrow \mathbb{N}_+$

Note that we could even apply the above theory to general surjective functions from $\mathbb{N}_+$ to $\mathbb{N}_+$. Repeated iterations of any such function f on a number n will also have to result in either a cycle or a divergent trajectory. So for any such function we can define an associated digraph with an adjacency matrix, and calculate eigenvalues and eigenvectors for that matrix. Above we already saw which eigenvectors are associated to cycles and divergent trajectories. Thus we can also find all the eigenvectors and eigenvalues for any problem generated by any surjective function $f : \mathbb{N}_+ \to \mathbb{N}_+$.

Note that if f is not surjective, i.e. if there exists some n such that there is no m with $f(m) = n$, then things are different. For example, if we look at the function f defined by $f(n) = 2n$, then there exists no $m \in \mathbb{N}_+$ with $f(m) = 1$. So then the component $G_P = \{1, 2, 4, 8, \ldots\}$ has no associated eigenvector(s) for the matrix A^T.

3.5 Summary

Using the Collatz graph and its adjacency matrix, we found a way to express existences of cycles or divergent paths in terms of the eigenvectors and eigenvalues of this adjacency matrix. We saw specifically which eigenvectors and eigenvalues exist when we have components containing cycles, and which eigenvectors exist when there exist components with divergent paths. For a proof that the mentioned eigenvalues also form the complete spectrum of A and A^T, we refer the reader to De Weger's more detailed and extensive analysis of this problem.

Looking at the eigenvectors and eigenvalues, we can also draw some conclusions. For example, the only eigenvectors with a finite support (a finite number of non-zero entries) are the eigenvectors coming from cycles, where the only non-zero entries are on the positions of the numbers in the cycle. This means that we will be able to find these eigenvectors with truncated versions of the matrices A and A^T as well, since those vectors are also eigenvectors for square matrices of size $M \times M$, where M is the maximum value in the cycle. This also corresponds to the fact that we can easily verify the existence of another cycle if it is given, but not the existence of divergent paths, even if the starting point is known.

Although there previously existed some literature about the eigenvectors and -values of the $3n+1$ problem, this chapter forms a more complete analysis of this problem than this other material. We have written out all possible eigenvalues and -vectors, without making any assumptions about the existence of other cycles or divergent paths. This means that the above method can be generalized and used for other $pn+q$ problems as well. We looked at some examples, namely the $n+1$ problem and the $5n+1$ problem, and we saw what eigenvalues and -vectors we get for those problems. Analogously, the theory can be applied to Collatz-like functions such as $C_3(n)$ as well, and even to general surjective functions $f : \mathbb{N}_+ \to \mathbb{N}_+$. In all cases, we can say that the above methods will give us the complete spectrum and the complete set of eigenvectors for those problems.

Chapter 4

Collatz Modular Digraphs and De Bruijn Digraphs

4.1 The $3n+1$ conjecture

Instead of looking at the infinite Collatz digraph, or reductions of the Collatz graph by just leaving out vertices and associated edges, we can also compress the size of the graph by dividing all positive integers into congruence classes. We could for example look at the transitions between congruence classes modulo some integer n. Then we get a graph with n vertices (the n congruence classes) which still covers all positive integers. Although we lose some valuable information in this reduction (the existence of a path from i to 1 no longer implies that the number i iterates to the number 1) there are some advantages to this approach as well. We will find out that a particular class of these Collatz Modular Digraphs has interesting properties, which can be used to get insight about the $3n+1$ problem in general.

4.1.1 Collatz Modular Digraphs

First of all, we will start with giving precise definitions of the modular digraphs and what they look like. Then we will try to analyze properties of these graphs.

Definition 4.1.1 (Collatz Modular Digraph (CMD))**.** *The Collatz Modular Digraph (CMD) with modulus n, denoted by $\mathcal{C}_n$, is the graph $G = (V_n, E_n)$ such that:*

$$\begin{aligned} V_n &= \{0, 1, 2, \dots, n-1\} \\ E_n &= \{(v_1, v_2) \mid v_1, v_2 \in V \textit{ and } \exists\, v_3 \in \mathbb{N} : v_3 \equiv v_1 \pmod{n}, T(v_3) \equiv v_2 \pmod{n}\}. \end{aligned}$$

Furthermore, we denote the adjacency matrix of $\mathcal{C}_n$ with C_n, which is defined by:

$$(C_n)_{ij} = \begin{cases} 1 & \textit{if } (i,j) \in E_n \\ 0 & \textit{else} \end{cases}$$

Figures 4.1, 4.2, 4.3 and 4.4 show the Collatz Modular Digraphs with modulus respectively 2, 4, 6 and 8. Note that $(C_2)_{ij} = 1$ for all i and j, so C_2 is the *Unit Matrix U_2*, with 1's everywhere. The consequence of this is that independent of the starting vertex, after 1 iteration we can be at either vertex 0 or vertex 1 through exactly 1 possible path. Similarly, we note that:

$$(C_4)^2 = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \end{pmatrix}^2 = U_4$$

And:

$$(C_8)^3 = \begin{pmatrix} 1&0&0&0&1&0&0&0\\ 0&0&1&0&0&0&1&0\\ 0&1&0&0&0&1&0&0\\ 0&1&0&0&0&1&0&0\\ 0&0&1&0&0&0&1&0\\ 1&0&0&0&1&0&0&0\\ 0&0&0&1&0&0&0&1\\ 0&0&0&1&0&0&0&1 \end{pmatrix}^3 = U_8$$

However, there is no k such that $C_6^k = U_6$. This can also be seen from the graphs; $\mathcal{C}_2$, $\mathcal{C}_4$ and $\mathcal{C}_8$ share some properties like symmetries, while $\mathcal{C}_6$ is different and ugly.

On further inspection, we see that some special properties only arise in graphs with modulus $n = 2^k$. Therefore, in the next subsection, we will only consider the case where the modulus is a power of 2. This special class of CMDs will turn out to have quite some interesting properties.

4.1.2 Binary Collatz Modular Digraphs

First of all, we start with the definition of *Binary Collatz Modular Digraphs.*

Definition 4.1.2 (Binary Collatz Modular Digraph (BCMD))**.** *The Binary Collatz Modular Digraph (BCMD) with modulus $n = 2^k$, $k \in \mathbb{N}$, denoted by $\mathcal{M}_k$, is the Collatz Modular Digraph $\mathcal{C}_n$. Binary Collatz Modular Digraphs are thus a special case of Collatz Modular Digraphs, namely where the modulus is a power of* 2.

We already saw the BCMDs with moduli 2, 4 and 8, and Figures 4.5 and 4.6 also show the BCMD with moduli 16 and 32 ($k = 4, 5$). Note that $M_4^4 = U_{16}$ and $M_5^5 = U_{32}$, so there is exactly one path of length 4 (5) from every vertex i to j in $\mathcal{M}_4$ ($\mathcal{M}_5$).

From these examples, we get the strong suspicion that for any $k \geq 1$, $M_k^k = U_{2^k}$. Furthermore, we see interesting properties in the graphical representation of the graphs when n is a power of 2. For example, when the graphs are drawn right, there is a certain form of symmetry, and the structure of the graph (two self-cycles, two edges from and to every vertex) does not seem to change drastically when k gets bigger. In the following sections we will therefore only analyze these BCMDs.

Note that when we consider T as a mapping from one congruence class to another, like we did above, then this is not a well-defined function anymore. For example, if we take $n = 4$, then $(0,0) \in E_4$ (since $T(0) = 0$) but also $(0,2) \in E_4$ (since $T(4) = 2$). So $T([0]) = \{[0],[2]\}$ and in fact, as we will prove later for BCMDs, because of the division by 2 in each iteration step, all congruence classes are mapped to two congruence classes. Thus T is not a function, but a mapping, mapping each congruence class to two congruence classes.

4.1.3 Binary De Bruijn Digraphs

First we introduce the so-called Binary De Bruijn Digraphs as below.

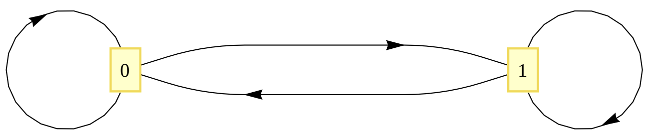

Figure 4.1: The Collatz Modular Digraph $\mathcal{C}_2$.

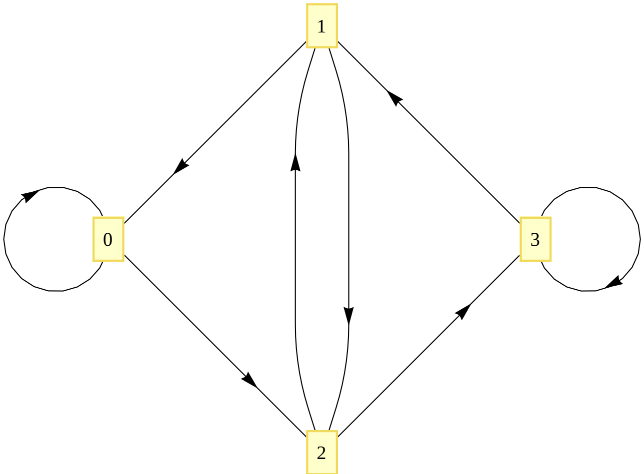

Figure 4.2: The Collatz Modular Digraph $\mathcal{C}_4$.

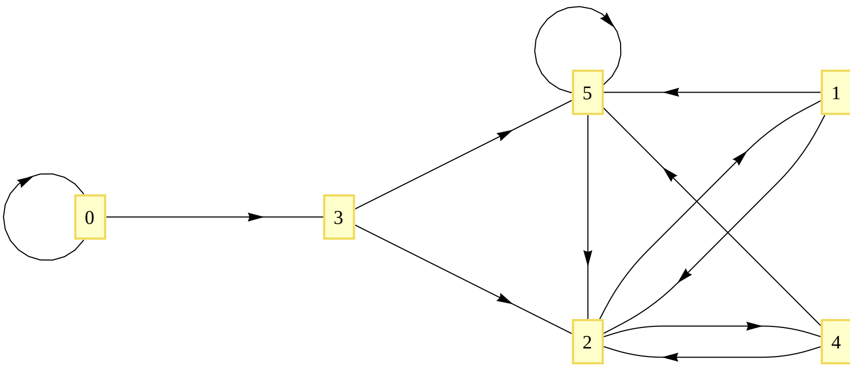

Figure 4.3: The Collatz Modular Digraph $\mathcal{C}_6$.

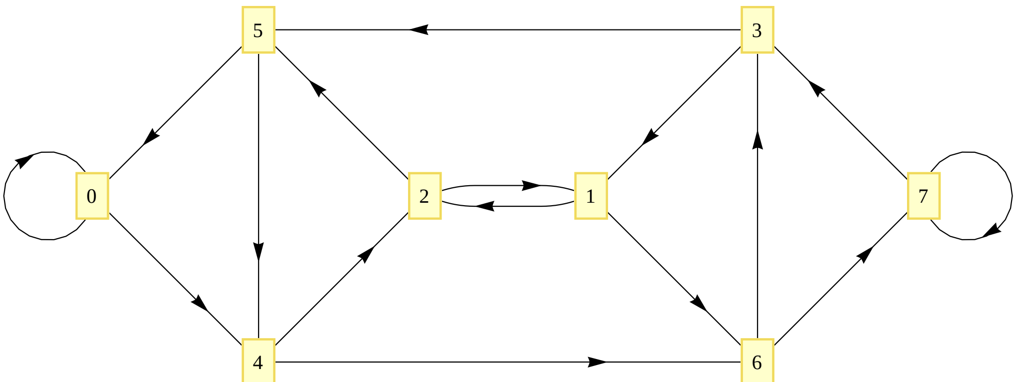

Figure 4.4: The Collatz Modular Digraph $\mathcal{C}_8$.

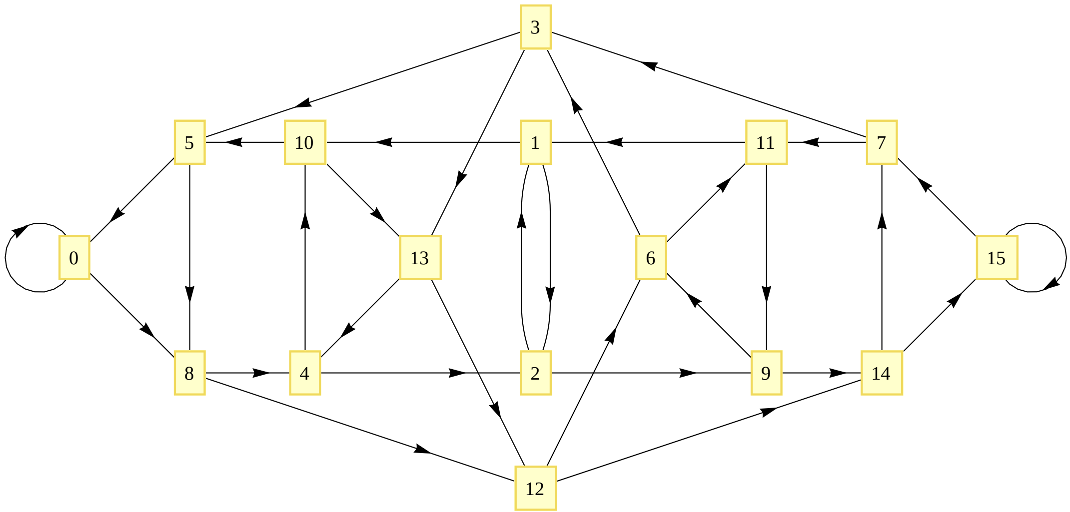

Figure 4.5: The Binary Collatz Modular Digraph $\mathcal{M}_4$.

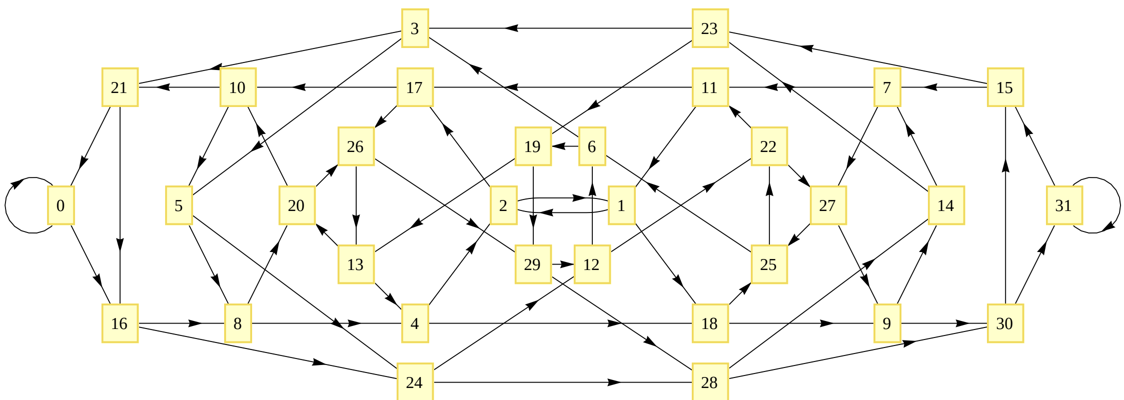

Figure 4.6: The Binary Collatz Modular Digraph $\mathcal{M}_5$.

Definition 4.1.3 (Binary De Bruijn Digraphs [Bru46]). *If $k \geq 1$ and $n = 2^k$, then the k-dimensional Binary De Bruijn Digraph (BDBD), denoted by $\mathcal{B}_k$, is the graph $G = (B_k, S_k)$ with*

$$\begin{aligned} B_k &= \{0,1\}^k \\ S_k &= \{((b_1, b_2, \ldots, b_{k-1}, b_k), (b_2, b_3, \ldots, b_k, b_{k+1})) \mid b_i \in \{0,1\} \; \forall \; i = 1, 2, \ldots, k+1\} \\ &= \{0,1\}^{k+1} \end{aligned}$$

Note that we may use both $((b_1, b_2, \ldots, b_{k-1}, b_k), (b_2, b_3, \ldots, b_k, b_{k+1}))$ and $(b_1, b_2, \ldots, b_{k-1}, b_k, b_{k+1})$ to refer to the same edge.

Some examples of Binary De Bruijn Digraphs are shown in Figures 4.7, 4.8, 4.9, 4.10, and 4.11 which (when drawn as in those figures) show a strong structural similarity with the Binary Collatz Modular Digraphs.

Before we continue with the Central Theorem, we first give some definitions from basic Graph Theory, and then four lemmas. These are then used for the Central Theorem.

Definition 4.1.4 (Indegree and outdegree). *If $G = (V, E)$ is a digraph and $v \in V$, then the in- and outdegree of v, denoted by $d^-(v)$ and $d^+(v)$, are the number of edges of the form (v, w) and (w, v) in E respectively, for some $w \in V$.*

Definition 4.1.5 (Strongly connected). *A digraph $G = (V, E)$ is said to be strongly connected if for each pair of vertices $v_1, v_2 \in V$, there is a path from v_1 to v_2 and a path from v_2 to v_1 in G.*

Definition 4.1.6 (Line Digraph). *If $G = (V, E)$ is a digraph, then the line digraph of G, denoted by $L(G)$, is the graph $L(G) = (E, F)$ such that $(e_1, e_2) \in F$ if and only if the two edges e_1 and e_2 are connected in G.*

Definition 4.1.7 (Transpose Digraph). *If $G = (V, E)$ is a digraph, then the transpose digraph of G, denoted by G^T, is the graph $G^T = (V, F)$ such that $(v_1, v_2) \in F$ if and only if $(v_2, v_1) \in E$.*

Definition 4.1.8 (Isomorphic Digraphs). *If $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are two digraphs, then G_1 and G_2 are said to be isomorphic, denoted by $G_1 \cong G_2$, if and only if there exists a bijection $f : V_1 \to V_2$ such that for all vertices $v, w \in V_1$:*

$$(v, w) \in E_1 \Leftrightarrow (f(v), f(w)) \in E_2$$

The function f is then said to be the isomorphism between G_1 and G_2. Similarly, the inverse of f, $f^{-1} : V_2 \to V_1$ is said to be the isomorphism between G_2 and G_1.

Below are first two lemmas about De Bruijn Digraphs and their known properties, followed by two lemmas which give sufficient conditions for the existence of Eulerian and Hamiltonian paths in digraphs in general.

Lemma 4.1.9 (De Bruijn Digraph Isomorphy (1)). *For each $k = 1, 2, \ldots$, $L(\mathcal{B}_k) \cong \mathcal{B}_{k+1}$ with the isomorphism $\beta_k : L(\mathcal{B}_k) \to \mathcal{B}_{k+1}$ defined as:*

$$\beta_k((b_1, b_2, \ldots, b_k), (b_2, b_3, \ldots b_{k+1})) = (b_1, b_2, b_3, \ldots, b_{k+1})$$

The inverse $\beta_k^{-1} : \mathcal{B}_{k+1} \to L(\mathcal{B}_k)$ is analogously defined as:

$$\beta_k^{-1}(b_1, b_2, b_3, \ldots, b_{k+1}) = ((b_1, b_2, \ldots, b_k), (b_2, b_3, \ldots b_{k+1}))$$

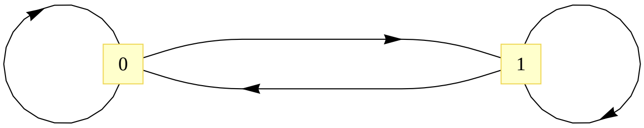

Figure 4.7: The Binary De Bruijn Digraph $\mathcal{B}_1$.

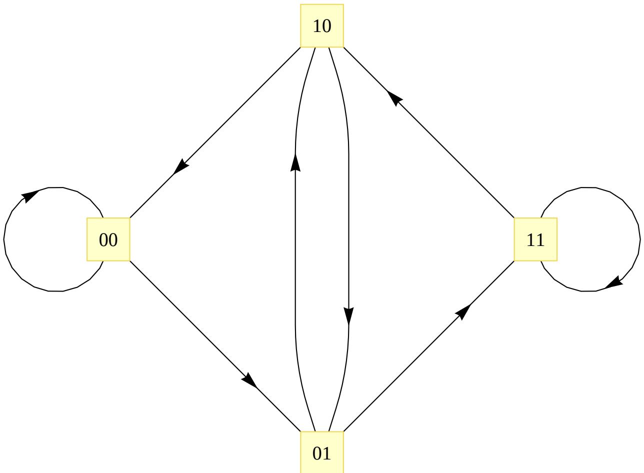

Figure 4.8: The Binary De Bruijn Digraph $\mathcal{B}_2$.

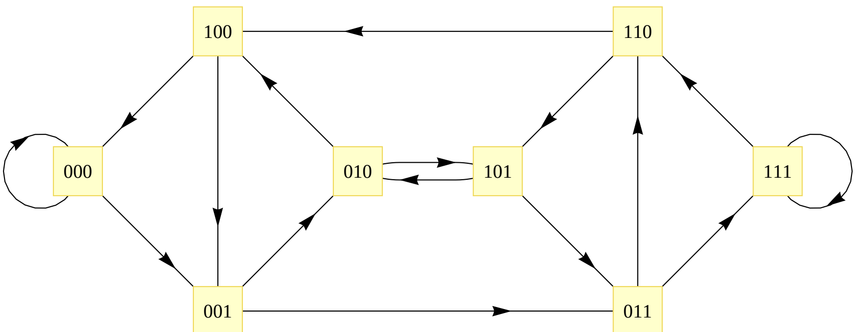

Figure 4.9: The Binary De Bruijn Digraph $\mathcal{B}_3$.

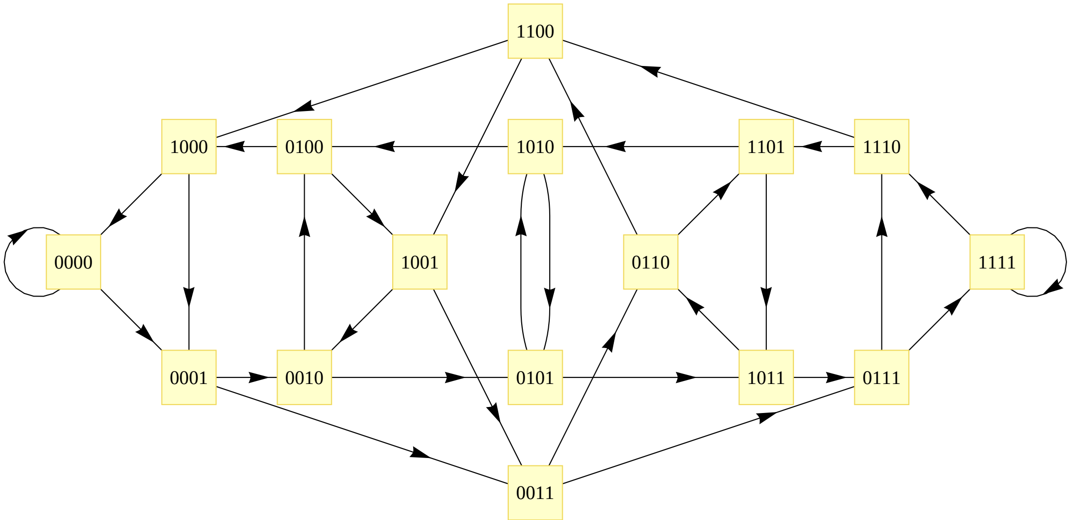

Figure 4.10: The Binary De Bruijn Digraph $\mathcal{B}_4$.

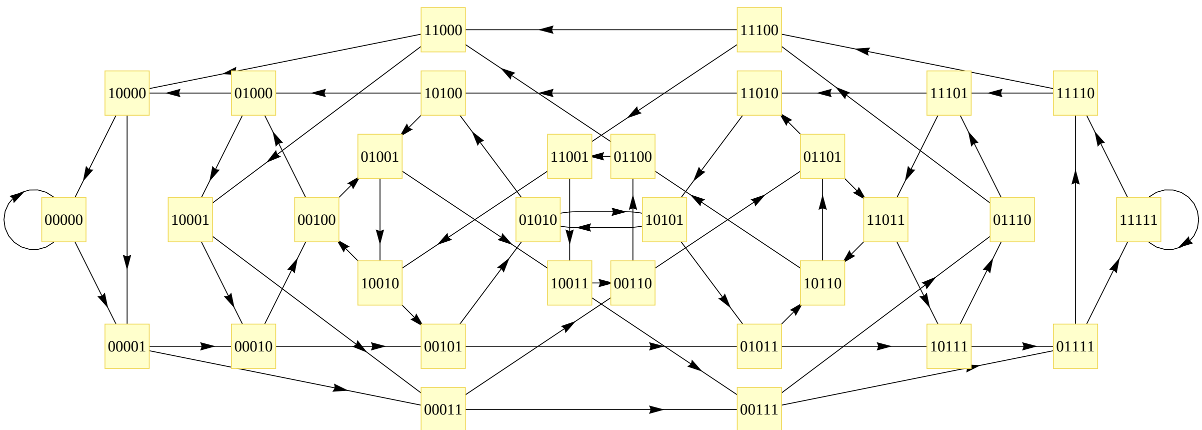

Figure 4.11: The Binary De Bruijn Digraph $\mathcal{B}_5$.

Proof. We can easily verify that all properties of an isomorphism hold. For example, the edges $(b_1, b_2, b_3, \ldots, b_{k+1})$ and $(c_1, c_2, c_3, \ldots, c_{k+1})$ are connected in $\mathcal{B}_k$ if and only if $b_{i+1} = c_i$ for all $i = 1, 2, \ldots, k$. Similarly, the vertices $(b_1, b_2, b_3, \ldots, b_{k+1})$ and $(c_1, c_2, c_3, \ldots, c_{k+1})$ are only connected in $\mathcal{B}_{k+1}$ by an edge when $b_{i+1} = c_i$ for all $i = 1, 2, \ldots, k$. □

Lemma 4.1.10 (De Bruijn Graph Isomorphy (2)). *For each $k = 1, 2, \ldots$, $\mathcal{B}_k \cong \mathcal{B}_k^T$ with the isomorphism $\mu_k : \mathcal{B}_k \to \mathcal{B}_k^T$ defined by:*

$$\mu_k(b_1, b_2, \ldots, b_{k-1}, b_k) = (b_k, b_{k-1}, \ldots, b_2, b_1)$$

For the inverse isomorphism $\mu_k^{-1} : \mathcal{B}_k^T \to \mathcal{B}_k$ we find the same isomorphism:

$$\mu_k^{-1}(b_1, b_2, \ldots, b_{k-1}, b_k) = (b_k, b_{k-1}, \ldots, b_2, b_1)$$

Proof. We know that an edge in $\mathcal{B}_k$ has the form $e = ((b_1, b_2, \ldots, b_k), (b_2, b_3, \ldots, b_{k+1}))$, so that the edges in the transpose graph have the form $e^T = ((b_2, b_3, \ldots, b_{k+1}), (b_1, b_2, \ldots, b_k))$. If we now also reverse the labels on each vertex, so that $(b_1, b_2, \ldots, b_k)$ becomes $(b_k, b_{k-1}, \ldots, b_1)$, then we see that the edge e^T becomes $\mu_k(e^T) = ((b_{k+1}, b_k, \ldots, b_2), (b_k, b_{k-1}, \ldots, b_1))$. If we now say that $c_i = b_{k+2-i}$ then $\mu_k(e^T) = ((c_1, c_2, \ldots, c_k), (c_2, c_3, \ldots, c_{k+1}))$. These are exactly the edges in $\mathcal{B}_k$. So transposing the graph and renaming the vertices as above gives us the same graph again. So indeed, μ_k is an isomorphism from $\mathcal{B}_k$ to $\mathcal{B}_k^T$, and obviously μ_k^{-1} as defined above is then also the isomorphism from $\mathcal{B}_k^T$ to $\mathcal{B}_k$. □

Lemma 4.1.11 (Existence of Hamiltonian paths). *If G is a Eulerian digraph, then $L(G)$ is a Hamiltonian digraph.*

Proof. If $G = (V, E)$ is Eulerian, then there exists a path of edges $(e_1, e_2, \ldots, e_n)$ such that each edge is traversed exactly once. If we then translate the edges of G to vertices of $L(G)$, then $\{e_i\}$ is exactly the set of vertices, and thus the path $(e_1, e_2, \ldots, e_n)$ is a Hamiltonian path in $L(G)$. □

Lemma 4.1.12 (Existence of Eulerian paths [GY06]). *If $G = (V, E)$ is a strongly connected digraph, and for all $v \in V$ we have $d^+(v) = d^-(v) = C > 1$ for some constant C (so the indegree and outdegree of all vertices is equal to C) then G is a Eulerian digraph.*

4.1.4 The Central Theorem

Now we are ready to describe and prove the properties of Binary Collatz Modular Digraphs. The Theorem is up next, followed by the proof and an example of the Theorem, for the graph $\mathcal{M}_3$.

Theorem 4.1.13 (Properties of Binary Collatz Modular Digraphs). *If $k \geq 1$, $\mathcal{M}_k = (V_k, E_k)$ with adjacency matrix M_k, and $\mathcal{M}_k^T = (V_k, F_k)$ is the transpose graph of $\mathcal{M}_k$, then:*

(i) $L(\mathcal{M}_k) \cong \mathcal{M}_{k+1}$

(ii) $(M_k)^k = U_{2^k}$

(iii) $\forall\ v \in V_k : d^+(v) = 2$

(iv) $\forall\ v \in V_k : d^-(v) = 2$

(v) $\mathcal{M}_k$ *is strongly connected*

(vi) $\mathcal{M}_k$ *is Eulerian*

(vii) $\mathcal{M}_k \cong \mathcal{B}_k$

(viii) $\mathcal{M}_k$ *is Hamiltonian*

(ix) $\mathcal{M}_k \cong \mathcal{M}_k^T$

Proof. (i) This follows from the notion that every edge e_i in $\mathcal{M}_k$ corresponds to exactly one congruence class modulo $2n$, and so there is a bijection between the edges in $\mathcal{M}_k$ and the vertices in $\mathcal{M}_{k+1}$. This bijection $\phi_k : L(\mathcal{M}_k) \to \mathcal{M}_{k+1}$ can be given explicitly as below.

$$\phi_k((v_1, v_2)) = \begin{cases} v_1 & \text{if } T(v_1) = v_2 \\ v_1 + 2^{k-1} & \text{if } T(v_1 + 2^{k-1}) = v_2 \end{cases}$$

Furthermore, two edges in $\mathcal{M}_k$ are adjacent if and only if the corresponding two vertices in $\mathcal{M}_{k+1}$ are connected.

(ii) We prove this by proving (by induction on k) that for any i, j, and for any $k \geq 1$, $((M_k)^k)_{ij} = 1$. From this it easily follows that $(M_k)^k = U_n$, for every k.
The base case of the induction is when $k = 1$, when it is easily verified that $(M_k)^k = M_1 = U_2 = U_n$. Now suppose $k \geq 2$, and suppose i and j are given. From (i) it follows that there exist four unique (but not necessarily distinct) vertices v_0, v_1, v_k, v_{k+1} in the graph $\mathcal{M}_{k-1}$ such that $\phi_{k-1}((v_0, v_1)) = i$ and $\phi_{k-1}((v_k, v_{k+1})) = j$. By induction, we know that $((M_{k-1})^{k-1})_{v_1, v_k} = 1$, so by induction we know that there is a unique path of length $k-1$ (containing k vertices) from vertex v_1 to v_k in the graph $\mathcal{M}_{k-1}$. Suppose this path is $(v_1, v_2, v_3, \ldots, v_{k-1}, v_k)$ for certain vertices $v_2, \ldots, v_{k-1}$. Now we add v_0 and v_{k+1} to this path, and we get the path $(v_0, v_1, v_2, v_3, \ldots, v_{k-1}, v_k, v_{k+1})$. We can now translate this path back to a path in $\mathcal{M}_k$, by applying ϕ_{k-1} to the pairs of vertices in this path. So if we say $\phi_{k-1}((v_i, v_{i+1})) = w_i$, for all $i = 0, \ldots, k$, then $(w_0 = i, w_1, w_2, \ldots, w_{k-1}, w_k = j)$ is the translated, unique path from i to j of length k, which was to be shown.

(iii) Suppose $v \in V$. Then $(v, T(v) \pmod n) \in E$. But also $(v, T(v+n) \pmod n) = (v, T(v) + n/2 \pmod n) \in E$. So $d^+(v) \geq 2$. These are also all outgoing edges from v, since for all integers m, we have that $T(v+mn) \equiv T(v) \pmod n$ if m is even, and $T(v+mn) \equiv T(v) + n/2 \pmod n$ if m is odd. So $d^+(v) = 2$.

(iv) Suppose $v \in V$. Then $(2v \pmod n, v) \in E$, since obviously $T(2v) = v$. But we also know that there is one $w \in \{v, v+n, v+2n\}$ with $w \equiv 2 \pmod 3$. Since $(2w-1) \equiv 0 \pmod 3$, and also $(2w-1) \equiv 0 \pmod 2$, we also know that $((2w-1)/3, v) \in E$, because $T((2w-1)/3) = v$. So there are at least two incoming edges in v, for all vertices v. Since the total number of incoming edges must be equal to the total number of outgoing edges, it now follows from (iii) immediately that $d^-(v)$ must also be equal to 2 for all vertices $v \in V$.

(v) This follows directly from (ii), because (ii) says that there is a path from every vertex v to every vertex w of length k.

(vi) From (iii), (iv) and (v) it follows that we can apply Lemma 4.1.12 to this graph to get this result.

(vii) We prove this by induction on k. For $k = 1$ we find the isomorphism $\sigma_1 : \mathcal{M}_1 \to \mathcal{B}_1$ as follows:

$$\begin{aligned} \sigma_1(0) &= 0 \\ \sigma_1(1) &= 1 \end{aligned}$$

For $k \geq 2$, it follows from (i), Lemma 4.1.9, and the remark that if $G_1 \cong G_2$ then $L(G_1) \cong L(G_2)$, that $\mathcal{M}_{k+1} \cong L(\mathcal{M}_k) \cong L(\mathcal{B}_k) \cong \mathcal{B}_{k+1}$, which was to be proven.

(viii) This follows from (i), (vi) and Lemma 4.1.11 for all $k \geq 2$. For $k = 1$ we can verify it by hand by giving the Hamiltonian circuit $(0, 1, 0)$.

(ix) From Lemma 4.1.10 we know that Binary De Bruijn Digraphs are isomorphic to their transpose graphs. Furthermore, we know that if G_1 and G_2 are isomorphic, then G_1^T and G_2^T are obviously isomorphic as well with the same isomorphism as the isomorphism between G_1 and G_2. Therefore $\mathcal{M}_k \cong \mathcal{B}_k \cong \mathcal{B}_k^T \cong \mathcal{M}_k^T$, which concludes the proof.

□

Example 4.1.14 ($\mathcal{M}_3$)**.** *As an example, we look at the above properties for $\mathcal{M}_3$:*

(i) The edges in $\mathcal{M}_3$ correspond one-on-one with numbers modulo 16. For example, the edge $(4,2)$ corresponds to the congruence class $n \equiv 4 \pmod{16}$, while $(4,6)$ corresponds to the class $n \equiv 12 \pmod{16}$. So the bijection ϕ_3 given in the proof above is indeed a bijection from the edges of $\mathcal{M}_3$ to the vertices of $\mathcal{M}_4$. Furthermore, we can verify that if two edges in $\mathcal{M}_3$ share a vertex, then the two corresponding vertices in $\mathcal{M}_4$ are also connected, and vice versa.

(ii) Just calculating $(M_3)^3$ verifies that $(M_3)^3 = U_8$. This result can be interpreted as that from every vertex i in the graph, any (not necessarily other) vertex j can be reached in 3 steps through exactly 1 path.

(iii) We can easily verify that if $0 \leq v \leq 7$ and $T(v) \equiv w \pmod 8$, then the outgoing edges from vertex v are (v,w) and $(v, w+4 \pmod 8)$. So $d^+(v) = 2$.

(iv) We can see that if $0 \leq v \leq 7$ then there is exactly one $w \in \{v, v+8, v+16\}$ with $j \equiv 2 \pmod 3$. So there are two incoming edges in v, namely $(v, 2v \pmod 8)$ and $(v, (2w-1)/3 \pmod 8)$.

(v) This follows from (ii), since $((M_3)^3)_{ij} = 1$ means that there is exactly one path from vertex i to vertex j in 3 steps. So in general, every vertex j is reachable from every vertex i in at most 3 steps.

(vi) We can give an explicit Eulerian circuit. The path:

$$(0,0,4,2,1,2,5,4,6,3,1,6,7,7,3,5,0)$$

traverses every edge exactly once, and begins and ends in vertex 0. So this is an Eulerian circuit for $\mathcal{M}_8$.

(vii) If we compare $\mathcal{M}_3$ from Figure 4.4 with $\mathcal{B}_3$ from Figure 4.9, we find the following bijection for $\sigma_3 : \mathcal{M}_3 \to \mathcal{B}_3$.

$$\begin{aligned}
\sigma_3(0) &= 000 \\
\sigma_3(1) &= 101 \\
\sigma_3(2) &= 010 \\
\sigma_3(3) &= 110 \\
\sigma_3(4) &= 001 \\
\sigma_3(5) &= 100 \\
\sigma_3(6) &= 011 \\
\sigma_3(7) &= 111
\end{aligned}$$

(viii) We can give an explicit Hamiltonian circuit in the graph. One example is:

$$(0,4,6,7,3,1,2,5,0)$$

It can easily be verified that this path visits every vertex once (except for the first and last vertex 0), and that this path is actually an allowed path in $\mathcal{M}_3$.

(ix) From Figure 4.4 it can easily be seen that inverting all edges and then mirroring the vertex labels using the horizontal line from 0 to 7 as a 'mirror' (so $0 \to 0$, $3 \to 6$,

6 → 3 etc.) does not change the graph. So one possibile isomorphism $\rho_3 : \mathcal{M}_3 \to \mathcal{M}_3^T$ *is:*

$$\begin{aligned}
\rho_3(0) &= 0\\
\rho_3(1) &= 1\\
\rho_3(2) &= 2\\
\rho_3(3) &= 6\\
\rho_3(4) &= 5\\
\rho_3(5) &= 4\\
\rho_3(6) &= 3\\
\rho_3(7) &= 7
\end{aligned}$$

Note that in the proofs of the existence of isomorphisms above for (vii) and (ix), we proved the existence of such isomorphisms, but we did not give explicit forms of these isomorphisms. However, we can find more explicit forms for both. If we write $[a]_2 = a \pmod 2$, then the isomorphism $\sigma_k : \mathcal{M}_k \to \mathcal{B}_k$ from (vii) can be given as:

$$\sigma_k(n) = ([n]_2, [T(n)]_2, [T^2(n)]_2, \ldots, [T^{k-1}(n)]_2)$$

We can verify that if an edge goes from n_1 to n_2 in $\mathcal{M}_k$, then $T(n) \equiv m \pmod{2^{k-1}}$, so that $([T(n)]_2, [T^2(n)]_2, \ldots, [T^{k-1}(n)]_2) = ([m]_2, [T(m)]_2, \ldots, [T^{k-2}(m)]_2)$, so that the last $k-1$ bits of $\sigma_k(n)$ and $\sigma_k(m)$ match. So this exactly corresponds to an edge in $\mathcal{B}_k$.

Similarly, we can get a more explicit form for ρ_k as well. Since $\mathcal{M}_k \cong \mathcal{B}_k \cong \mathcal{B}_k^T \cong \mathcal{M}_k^T$ with isomorphisms σ_k, μ_k and σ_k^{-1} respectively, we can write $\rho_k(n) : \mathcal{M}_k \to \mathcal{M}_k^T$ as:

$$\rho_k(n) = \sigma_k^{-1}(\mu_k(\sigma_k(n)))$$

We saw earlier that $\mu_k(b_1, b_2, \ldots, b_k) = (b_k, b_{k-1}, \ldots, b_1)$. So $\rho_k(n_1) = n_2$ if and only if $\sigma_k(n_1)$ is the reverse of $\sigma_k(n_2)$.

4.1.5 Some consequences of the Central Theorem

Theorem 4.1.13 has some interesting consequences. For example, from (ii) it follows that not only every vertex is reachable from every other vertex, but also that all vertices are reachable after k steps from any vertex with the same 'chance'. So if we don't know what exact number n we have, but only know that $n \equiv i \pmod{2^k}$, then after k steps in the graph $\mathcal{M}_k$ starting at vertex i, we could be anywhere with equal probability. This was also investigated by Feix et al. in [FMR94], who investigated the matrices of the form $(1/2)^k M_k$. These are the Markov matrices denoting the probabilities of going from one congruence class to another. Feix et al. derived similar results as in the above Central Theorem, such as $M_k^k = (1/n)^k U_{n^k}$. Maybe because of the coefficients $(1/2)^k$ in their Markov matrices, Feix et al. did not find the relation with De Bruijn Digraphs given above.

Another consequence, which also follows from (ii), is that there are no congruence classes that cannot reach vertex 1 or vertex 2. If the $3n+1$ conjecture is true, then a necessary condition is that vertex 1 is reachable from vertex i for every vertex i in $\mathcal{M}_k$, for every $k \geq 1$. However, this is obviously not a sufficient condition. For example, we can easily verify that the trajectory of 7 contains 1. Therefore, in the graph $\mathcal{M}_3$, the vertex of congruence class 1 is reachable from vertex 7, even though we haven't checked if the number 15 also ends up at 1, or that 23 reaches 1 in a certain number of steps. The fact that $(\mathcal{M}_3^3)_{71} = 1$ only means that there exist n_1, n_2 with $n_1 \equiv 7 \pmod 8$ and $n_2 \equiv 1 \pmod 8$, such that $T^3(n_1) = n_2$. In fact, $\sigma_\infty(7) = 11$ and for every $m > 8$ we know that $T^3(m) > 1$, so there does not even exist an $n \equiv 7 \pmod 8$ such that $T(n) = 1$. In fact, the n_1 and n_2 mentioned above are numbers of the form $n_1 = 47 + 2^6 k_1$, $n_2 = 161 + 2^3 3^3 k_1$

such that $T^3(n_1) = n_2$.

We can also use the graphs to reduce solving the whole problem to solving the conjecture only for certain modulo classes. For example, if we know that the conjecture is true for all $n \equiv 1 \pmod 2$, then we can easily prove that the whole conjecture is true. This can for example be seen easily by deleting the vertex 1 from the modulo-2 graph, and then considering possible cycles or possible divergences. In this simple case, only one vertex and one edge is remaining, which goes from an even vertex to an even vertex, so which 'divides a number' by 2 on every step. So if there was a cycle, it would only contain even numbers and divide by 2 on every step, which is of course impossible. Also, if a divergent trajectory existed, it would also only include even numbers which is also impossible.

But we can also get similar but more sophisticated, less obvious results. An example is given below.

Theorem 4.1.15 (Reduction to one vertex, modulo 8)**.** *The $3n + 1$ conjecture is true if and only if the $3n + 1$ conjecture is true for every number $n \equiv 3 \pmod 8$.*

Proof. For the proof, we use Figure 4.4 of the graph $\mathcal{M}_3$. If we assume that every number equal to 3, modulo 8, converges to 1, then we only have to consider paths in the graph not going through 3. After all, if we do visit 3, then from the assumption we know that $n \to 1$ in a certain number of steps.

So suppose we are at a vertex not equal to 3, and we disregard all edges from and to 3. Now suppose that n is sufficiently large. If n does not converge to 1, then the number of odd numbers in the trajectory of n has to be strictly bigger than the number of even numbers on its path. Therefore, there have to be at least two consecutive numbers n_1, n_2 in the trajectory of n that are odd. Suppose neither of these numbers is equal to 3, modulo 8. From the graph, we see that the only remaining edge from an odd number to an odd number is the edge from 7 to 7, so both these numbers must be equal to 7, modulo 8. So at this point, the trajectory has reached the congruence class 7.

Now we see in the graph that the only other outgoing edge from the vertex 7 is the edge from 7 to 3, which we wanted to disregard. But this means that if we never visit 3, then we will always stay in the congruence class 7 from this point on. However, if $n_2 < 2^k$ for some k (so that $n_2 = 2^k - b$, $1 \leq b \leq 2^k$) then after at most k iterations we will always have encountered at least one even number in the trajectory of n_2. This is true, because:

$$T_1^k(n_2) = T_1^k(2^k - b) = 2^{-k}(3^k(2^k - b) + 3^k - 2^k) = 3^k - 1 - 2^{-k}(3^k(b - 1))$$

On the right hand side, we see that $3^k - 1$ is an integer, but since $(b - 1) < 2^k$, the prime factor decomposition of $3^k(b - 1)$ contains at most $k - 1$ factors 2, while the number is divided by k factors 2, which means that the right hand side is not an integer. Since $T^k(n_2)$ is an integer but $T_1^k(n_2)$ is not, we know that $T^k(n_2) \neq T_1^k(n_2)$ and so there must have been at least one even number in the first k iterations of n_2.

So we know that a number strictly decreases when it does not visit the vertex 3, unless when it ends up at vertex 7, when we know it will eventually leave that vertex and go to 3. So if every number that ever visits the congruence class 3 converges to the number 1, then all numbers converge to 1. □

However, we see that this does not continue to work for bigger n. In $\mathcal{M}_5$ as in Figure 4.6, there are so many paths and cycles in the graph, also containing odd numbers, that we cannot find one vertex such that removing that one vertex makes it impossible to get any cycles in the remaining graph. For example, the simple cycle $(22, 27, 25)$ contains two odd and one even number, so this cycle increases a number when it passes through the whole cycle once. There are more such cycles, such as (31), (23, 19, 29, 28, 14), (7, 27, 9, 14), that we cannot avoid that numbers may still increase if we leave out only one vertex. Therefore we cannot get much better results than Theorem 4.1.15.

Another consequence of Theorem 4.1.13 is the following. From (i) it follows that an edge (v_1, v_2) in $\mathcal{M}_k$ corresponds to a vertex w_1 in $\mathcal{M}_{k+1}$, but also that an edge (v_2, v_3) in $\mathcal{M}_k$ corresponds to a vertex w_2 in $\mathcal{M}_{2n}$. But this also means that a path (v_1, v_2, v_3) in $\mathcal{M}_k$ corresponds to the edge (w_1, w_2) in $\mathcal{M}_{2n}$, which in turn corresponds to some vertex x_1 in $\mathcal{M}_{k+2}$. Repeating this gives us that there is a bijection between paths $(v_1, v_2, \ldots, v_i)$ in $\mathcal{M}_k$ and single vertices in $\mathcal{M}_{k-i+1}$. This is now formalized in the following theorem.

Theorem 4.1.16. *If $i, j, k \geq 1$, then there is a bijection between paths $(v_1, v_2, \ldots, v_i)$ in the graph $\mathcal{M}_k$ and paths $(w_1, w_2, \ldots, w_j)$ in the graph $\mathcal{M}_{k-i+j}$.*

As a special case of Theorem 4.1.16, taking $j = 1$, we see that there is a bijection between paths $(v_1, v_2, \ldots, v_i)$ in the graph $\mathcal{M}_k$ and vertices w in the graph $\mathcal{M}_{k-i+1}$. If we then also take $k = 1$, so that $n = 2$, then we see that there is a bijection between sequences of bits $(b_1, b_2, b_3, \ldots, b_n)$ with $b_m \in \{0, 1\}$ for every m, and vertices w in the graph $\mathcal{M}_k$. This bijection also immediately follows from the isomorphism $\sigma_k(n) : \mathcal{M}_k \to \mathcal{B}_k$. This relation with bits can be interpreted as follows. If we have a certain number m, with binary representation $b_1 b_2 b_3 b_4 b_5 \ldots$, and we only know the first i bits of this binary representation, so that we only know the value of m modulo 2^i, then after i iterations, the last i bits of $T^i(m)$ could be any string of i bits, with equal probability. This also shows how little we know about the iterates of numbers m, because we cannot only look at the first i bits of m. We need to know all bits of the binary representation of m to know what the trajectory of m looks like in the long term, or even only know what the last bits of the numbers in the trajectory of m are. After all, we are very much interested in the parity bit of numbers in a trajectory, which says if a number is odd or even. If we knew that all numbers contain as many odd as even numbers in their trajectories, then we could easily prove the $3n + 1$ divergence conjecture. But to know how many numbers of the first 500 iterates of m have a parity bit of 1, we would have to know all the first 500 bits of the binary representation of m.

4.1.6 The sequences $\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3, \ldots$ and $\mathcal{B}_1, \mathcal{B}_2, \mathcal{B}_3, \ldots$

As we saw earlier, there is an isomorphic relation between $\mathcal{M}_k$ and $\mathcal{B}_k$, with isomorphism $\sigma_k(n) = ([n]_2, [T(n)]_2, [T^2(n)]_2, \ldots, [T^{k-1}(n)]_2)$. If the $3n + 1$ conjecture is true, then for all $n \in \mathbb{N}_+$ there exists some q with $T^q(n) = 1$. After this we will then find $T^{q+2m}(n) = 1$ and $T^{q+2m+1}(n) = 2$. This means that the last m bits in $\sigma_{q+m}(n)$ form the alternating pattern $(\ldots, 1, 0, 1, 0, 1, 0, \ldots, (1/0))$. If m is even then the last bit will be a 0, if m is odd then the last bit is a 1. But also, if there exists a number n that does not end in the repeated pattern $(1, 0)$ after a certain number of steps, then the $3n+1$ conjecture is not true. We can therefore get an obvious reformulation of the $3n+1$ conjecture as follows:

Theorem 4.1.17 (The $3n + 1$ conjecture, variant)**.** *The $3n + 1$ conjecture is true if and only if for every $n \in \mathbb{N}_+$, there exists some $q \in \mathbb{N}_+$ such that the last m bits in $\sigma_{q+m}(n)$ follow the pattern $(\ldots, 1, 0, 1, 0, \ldots, (1/0))$.*

Perhaps further research could be to investigate these sequences $\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3, \ldots$ and $\mathcal{B}_1, \mathcal{B}_2, \mathcal{B}_3, \ldots$, and the corresponding isomorphisms $\sigma_1, \sigma_2, \sigma_3, \ldots$. We can see that other cycles in the $3n + 1$ problem would correspond to other patterns in the sequence $\sigma_1(n), \sigma_2(n), \sigma_3(n), \ldots$. But what happens when divergent trajectories exist? Can they also end in repeated patterns, or can the parity bits of divergent trajectories not be periodic? Also, if we extend the problem to rational numbers, we see that all patterns of parity bits correspond to certain rational cycles. Does this mean that if a number repeats such a pattern, it must therefore be a rational number ending in that cycle? And is it possible at all that two different rational numbers have the same sequence of parity bits in their trajectories?

4.1.7 An infinite Binary Collatz Modular Digraph

Another way to try to make a connection with the $3n + 1$ conjecture, is by defining an infinite Binary Collatz Modular Digraph which should correspond to the normal infinite Collatz digraph. For this, we first define *stable* and *unstable* edges.

Definition 4.1.18 (Stable and unstable edges)**.** *If $e = (v_1, v_2)$ is an edge in a BCMD $\mathcal{M}_k$, then we say e is stable if and only if there exist infinitely many BCMDs $\mathcal{M}_i = (V_i, E_i)$, $i = 1, 2, \ldots$ such that $e \in E_i$. An edge e is called unstable if it is not stable, so e is unstable if there are only finitely many BCMDs $\mathcal{M}_i = (V_i, E_i)$ with $e \in E_i$. Furthermore, we denote the set of all stable edges with $\mathcal{S}$ and the set of all unstable edges with $\mathcal{U}$.*

In Figure 4.12 the unstable edges of $\mathcal{M}_5$ are greyed out, and the stable edges are shown. As one can see in the Figure, the subset of stable edges is chaotically spread out over the graph. The normal Collatz Graph is of course quite chaotic and unordered, while the BCMDs all have nice structural properties. So it was also expected that any transition from BCMDs to the Collatz Graph would disturb the order and restore the chaos, which indeed happens. Note that the graph $\mathcal{M}_5$ with only stable edges is equivalent to the partial Collatz graph on the vertices 0 to 31, which was discussed in the previous section.

Now, to complete the relation with the regular Collatz graph, we define the infinite Collatz Modular Digraph as follows. Note that this definition is not simply an extension of BCMDs to an infinite one. Such an infinite graph can not be defined easily, since it would have an infinite number of congruence classes.

Definition 4.1.19 (Infinite Collatz Modular Digraph (ICMD))**.** *The Infinite Collatz Modular Digraph (ICMD) $\mathcal{M}_\infty$ is defined as the graph $G = (V_\infty, E_\infty)$ with*

$$\begin{aligned} V_\infty &= \{0, 1, 2, \ldots\} \\ E_\infty &= \mathcal{S}. \end{aligned}$$

The corresponding adjacency matrix satisfies

$$(M_\infty)_{ij} = \begin{cases} 1 & \text{if } (i, j) \text{ is a stable edge,} \\ 0 & \text{else.} \end{cases}$$

Using the infinite graph, we can now establish a connection with the regular Collatz Digraphs. If $\mathbf{0} = (0, 0, \ldots)$ is again an infinite vector of all-zeroes, and if the matrix M_∞ is written as

$$M_\infty = \left(\begin{array}{c|c} 1 & \mathbf{0} \\ \hline \mathbf{0}^T & F \end{array} \right),$$

where F is an infinite-dimensional submatrix of E, then, with the matrix A as in the previous section, we have

$$F = A$$

A consequence of this is that the Infinite Collatz Digraph is actually a subgraph of the infinite Binary Collatz Modular Digraph, or, similarly, isomorphic to a subgraph of the infinite Binary De Bruijn Digraph. However, as mentioned above, since this subgraph of the infinite Binary De Bruijn Graph is so chaotic (with the stable and unstable edges randomly spread out over the graph) it is hard to see if this formal relation is very useful.

4.2 $pn + q$ problems

The whole approach above is based on the $3n + 1$ problem. But of course we can also try to apply the above methods of using Modular Digraphs to general $pn + q$ problems. For these functions we can also look at the corresponding $pn + q$ Modular Digraphs and see what they look like.

4.2.1 Binary Modular Digraphs and Binary De Bruijn Digraphs

For these problems, it turns out we had also better look at the Binary Modular Digraphs. We then see that they are also isomorphic with Binary De Bruijn Digraphs, albeit with different isomorphisms. For example, if we take $p = q = 1$ we get the simple $n+1$ recursion:

$$T_{1,1}(n) = \begin{cases} n/2 & \text{if } n \text{ is even} \\ (n+1)/2 & \text{if } n \text{ is odd} \end{cases}$$

In this case, it can easily be verified and proven that, starting with a positive integer, this sequence always converges to the cycle (1), and starting with any non-positive number, we always end in the 1-cycle (0). If we draw the corresponding Binary $n+1$ Modular Digraph, denoted by $\mathcal{M}^*$, with and without unstable edges, we get Figures 4.13 and 4.14. Similarly, for the $5n+1$ problem with $p = 5$ and $q = 1$ we get Figures 4.15 and 4.16. The fact that there may exist divergent paths in the $5n+1$ is irrelevant to these Modular Digraphs; in these graphs you won't notice such divergent trajectories anyway.

4.2.2 The infinite Binary De Bruijn Digraph and the maximum number of cycles of length k

Above we saw that all $pn+q$ problems have Binary Collatz Modular Digraphs isomorphic to the corresponding Binary De Bruijn Digraph. Furthermore, we saw that the infinite Collatz Digraph is a subgraph of the infinite Collatz Modular Digraph. So it is not hard to see that all the infinite $pn+q$ Digraphs are isomorphic to a subgraph of the Infinite Binary De Bruijn Digraph, which is defined as below.

Definition 4.2.1 (Infinite Binary De Bruijn Digraph)**.** *The Infinite Binary De Bruijn Digraph (IBDBD) $\mathcal{B}_\infty$ is defined as the graph $G = (B_\infty, S_\infty)$ with*

$$\begin{aligned} B_\infty &= \{0,1\}^\infty \\ S_\infty &= \{((b_1, b_2, \ldots), (b_2, b_3, \ldots) \mid b_i \in \{0,1\} \; \forall \; i = 1, 2, \ldots\} \\ &= \{0,1\}^\infty \end{aligned}$$

Since these $pn+q$ graphs are subgraphs of the infinite Binary De Bruijn Digraph with only a fraction of the edges in the De Bruijn Digraphs, we cannot draw strong conclusions about the cycles of $pn+q$ graphs from the cycles of the De Bruijn graphs. However, since the graphs are subgraphs of the Binary De Bruijn Graphs, we know that the $pn+q$ graphs do not have more edges, and do not have more cycles of a certain length than the Binary De Bruijn Digraphs. And since we know alot more about the structure of De Bruijn graphs than about $pn+q$ graphs, we can easily get some upper bounds for the number of cycles of length k in the $pn+q$ graphs.

First, we notice that if there exists a 1-cycle in the IBDBD, then there has to be an edge from one vertex to itself. This means that the edge $(b_1, b_2, \ldots), (b_2, b_3, \ldots)$ is such that $b_1 = b_2$, $b_2 = b_3$, ..., so that when b_1 is known, the whole edge is determined. So there are two 1-cycles in the IBDBD, namely the vertex with $b_1 = b_2 = \ldots = 1$ with an edge to itself, and the vertex $b_1 = b_2 = \ldots = 0$ with an edge to itself. Note that this can also easily be seen from Figures 4.8, 4.9 and 4.10, which all have two 1-cycles.

Now, if we look at 2-cycles in the IBDBD, we see that we have at least two (trivial) 2-cycles, namely the two repetitions of the 1-cycles. If we only look at "real" 2-cycles, where the two vertices are distinct, we get that there have to be two edges $(b_1, b_2, \ldots), (b_2, b_3, \ldots)$ and $(b_2, b_3, \ldots), (b_3, b_4, \ldots)$ such that $(b_1, b_2, \ldots) = (b_3, b_4, \ldots)$, so that $b_i = b_{i+2}$ for each $i = 1, 2, \ldots$. There are thus four possible cycles, namely $b_1 = b_2 = 1, b_1 = b_2 = 0, b_1 \neq b_2 = 1$ and $b_1 \neq b_2 = 0$. The first two are

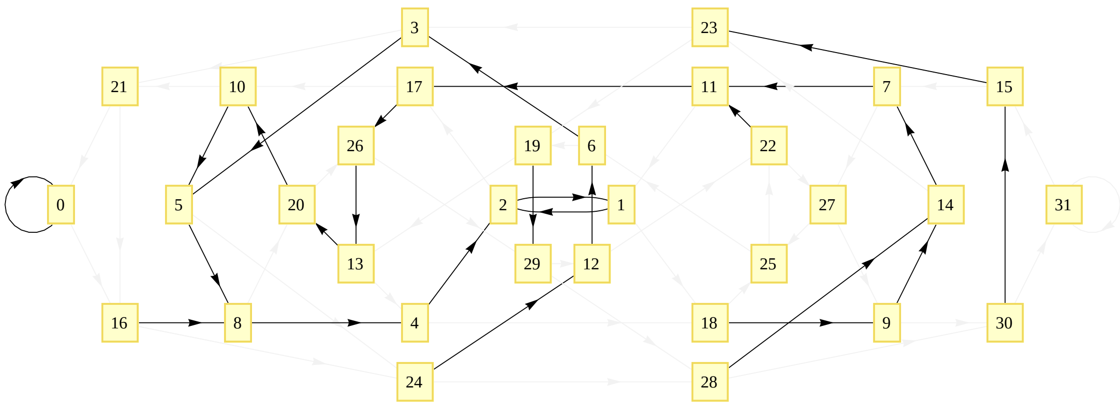

Figure 4.12: The Binary Collatz Modular Digraph $\mathcal{M}_5$ with only stable edges.

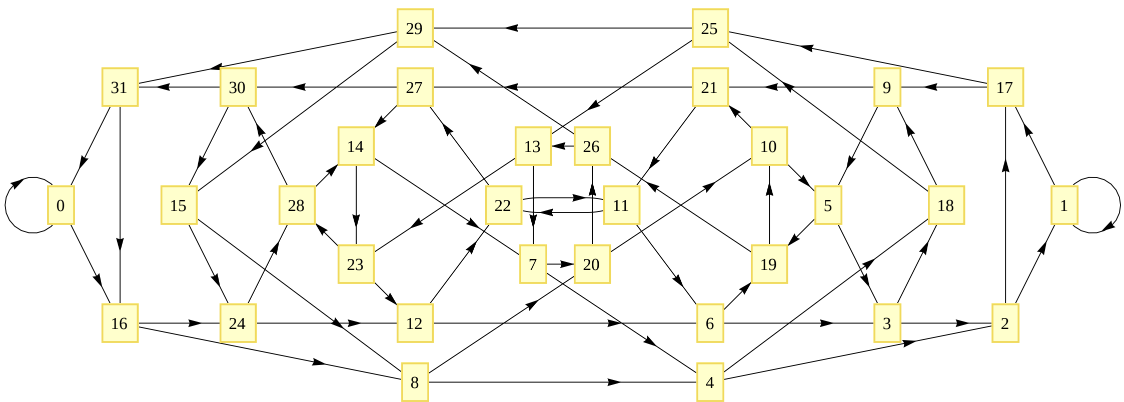

Figure 4.13: The Binary $n + 1$ Modular Digraph $\mathcal{M}_5^*$.

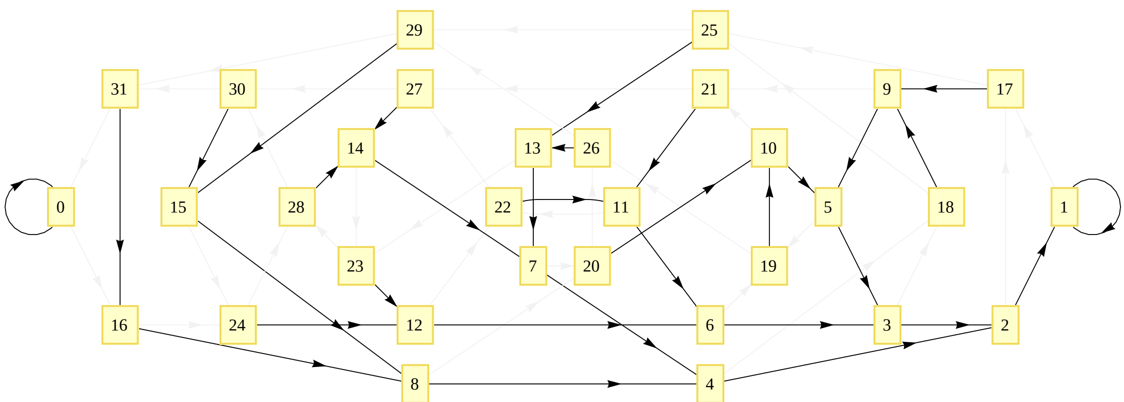

Figure 4.14: The Binary $n + 1$ Modular Digraph $\mathcal{M}_5^*$, with only stable edges. The only cycles of the $n + 1$ function are the trivial cycles (0) and (1), which can also be seen in the graph. In this graph there are two connected components, namely the single vertex 0 and the component with all the other vertices. Note that every vertex has one outgoing edge, since $(n + 1)/2 \leq n$ for every $n \geq 1$.

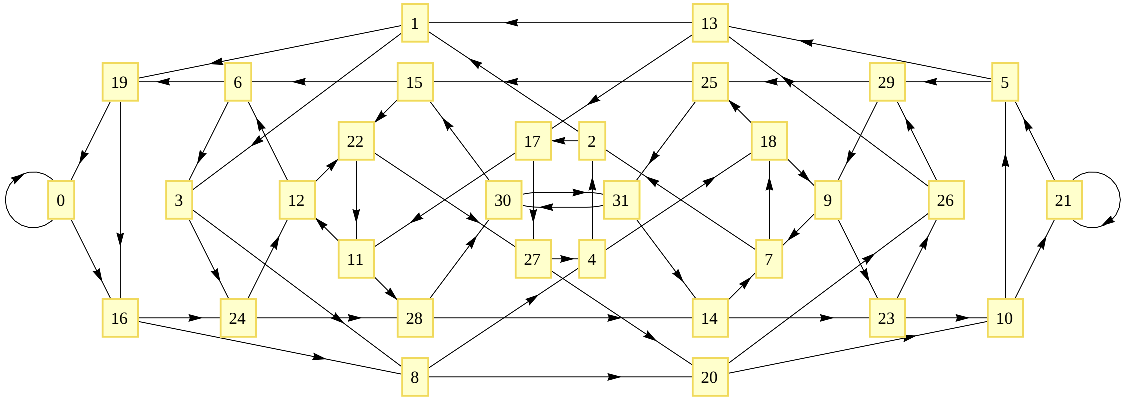

Figure 4.15: The Binary $5n + 1$ Modular Digraph $\mathcal{M}_5^*$.

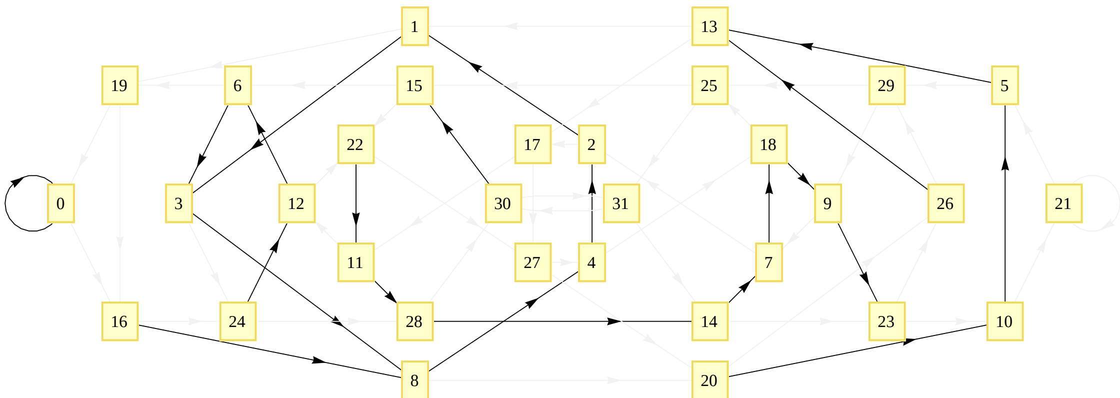

Figure 4.16: The Binary $5n + 1$ Modular Digraph $\mathcal{M}_5^*$, without unstable edges. Note that we can already see the stable cycle $(1, 3, 8, 4, 2)$ which is indeed a cycle in the $5n + 1$ problem. Also note that again, the stable edges are chaotically spread out over the graph.

the two trivial 2-cycles, while the other two are the same cycle, with a different starting point. Therefore, there is only 1 real 2-cycle in the IBDBD (the case $(b_1, b_2) = (1, 0)$) which can again be seen in Figures 4.8, 4.9 and 4.10.

When we look at 3-cycles, we see the same happening again. When b_1, b_2 and b_3 are determined, the whole cycle is determined. Therefore there are at most $2^3 = 8$ 3-cycles. However, the cases $b_1 = b_2 = b_3$ are again repetitions of the 1-cycles, while the other 6 cases are only 2 different cycles with 3 different starting points. Therefore, there are 2 real 3-cycles in the IBDBD, namely the permutations of $(b_1, b_2, b_3) = (1, 0, 0)$ and $(b_1, b_2, b_3) = (1, 1, 0)$.

Repeating this, we see that there are at most $2^4 = 16$ possible real 4-cycles. Two of them are repetitions of the one-cycles, two of them are permutations of the repetitions of the 2-cycle $(1, 0)$, which leaves 12 possible values for (b_1, b_2, b_3, b_4), which are the 4 permutations of the 3 cycles with $(b_1, b_2, b_3, b_4) = \{(1, 0, 0, 0), (1, 1, 0, 0), (1, 1, 1, 0)\}$.

If we repeat this process a little more, we get $(2^5 - 2)/5 = 6$ 5-cycles, $(2^6 - 2 - 2 - 6)/6 = 9$ 6-cycles, and $(2^7 - 2)/7 = 18$ 7-cycles which we will not write out. From this we see a general way of calculating the number of cycles arising. If we write U_k for the number of "real" cycles of length k (so that it's not a repetition of smaller cycles, or a rotation of the same cycle), and $P_k = k$ for the number of rotations of these real cycles (which is equal to k because each starting point gives a different sequence), then we get:

$$U_k = \frac{1}{P_k}(2^k - \sum_{\substack{d|k \\ 1 \le d < k}} U_d P_d)$$

Or, similarly, if we write $Q_k = U_k \cdot P_k$ and we include the divisor $d = k$ in the above summation, we get:

$$Q_k = 2^k - \sum_{d|k} Q_d + Q_k$$

Eliminating the Q_k, bringing the summation to the other side and applying Möbius inversion then gives us

$$Q_k = \sum_{d|k} \mu(d) 2^{k/d}$$

where $\mu(n)$ is the Möbius function. So for U_k we get:

$$U_k = \frac{1}{k} \sum_{d|k} \mu(d) 2^{k/d}$$

For example, for U_6 we find:

$$\begin{aligned} U_6 &= \frac{1}{6}\left(\mu(1)2^6 + \mu(2)2^3 + \mu(3)2^2 + \mu(6)2\right) \\ &= \frac{1}{6}(64 - 8 - 4 + 2) \\ &= 9 \end{aligned}$$

And for U_7:

$$\begin{aligned} U_7 &= \frac{1}{7}\left(\mu(1)2^7 - \mu(7)2\right) \\ &= \frac{1}{7}(128 - 2) \\ &= 18 \end{aligned}$$

Generally, for any prime number p we find:

$$\begin{aligned} U_p &= \frac{1}{p}\left(\mu(1)2^p + \mu(p)2\right) \\ &= \frac{1}{p}\left(2^p + 2\right) \\ &= \frac{2}{p}\left(2^{p-1} - 1\right) \end{aligned}$$

Note that Fermat's little theorem says that for any a, so in particular for $a = 2$, we have $a^{p-1} \equiv 1 \pmod{p}$. So the right hand side of the above equation is indeed an integer for each p.

This sequence U_k is also known in literature for several other purposes. One of the most similar applications is that U_k is the number of binary Lyndon words of length k, where binary Lyndon words are aperiodic words of bits. [Slo09] The sequences of parity bits are in fact Lyndon words, and so U_k is obviously equal to the number of binary Lyndon words of length k.

From the previous calculations, we can now draw the following conclusion.

Theorem 4.2.2 (Maximum number of cycles of length k in $pn+q$ problems)**.** *The number of cycles $(n_1, n_2, n_3, \ldots, n_k)$ of the function $T_{p,q}$ with all n_i distinct of length at most k, denoted by $R_{p,q,k}$, is for every $k \geq 1$ bounded by:*

$$R_{p,q,k} \leq U_k$$

Note that this bound is very high. We always have that $|\mu(n)| \leq 1$, and we have that $\mu(1) = 1$. The term of the sum that will thus dominate is the term with $d = 1$, namely the term $\mu(1)2^k = 2^k$. Other terms are at most as big as the square root of this first term, since the exponent of 2 is divided by some divisor of k for all other terms. So the bound U_k is roughly as big as $2^k/k$, which would also be a first rough guess of the number of cycles in $pn + q$ problems of length k (namely the number of bitsequences of length k, divided by the number of rotations of each cycle).

However, for $pn + q$ problems in general, this bound cannot be made sharper. For any n we can construct p and q such that $R_{p,q,k} = U_k$ for each $k = 1, \ldots, n$. For example, if $n = 5$, we can take $p = 3$, $q = 5 \cdot 7^2 \cdot 11 \cdot 13 \cdot 23 \cdot 29$ and we get all possible cycles of length ≤ 5, as in Table 2.1. This leads to the following Theorem.

Theorem 4.2.3 (U_k is sharp)**.** *The bound U_k in Theorem 4.2.2 is sharp for $pn+q$ problems in general. More specifically, if $p > 3$ is odd and we take*

$$q = \mathrm{lcm}\{2^i - p^j \mid i = 1 \ldots k, j = 1 \ldots i\}$$

then the number of cycles of length at most k of the $pn + q$ problem, denoted by $R_{p,q,k}$, is:

$$R_{p,q,k} = U_k$$

This follows from the formula in the chapter about basic calculations, where we could put q before the complicated fraction. If q just divided the denominator $(2^M - p^K)$ for each M and K, then the value for m would be an integer. So taking q the least common multiple of these factors makes sure that these values for m will always be integers. Concluding, we can say that the bound U_k is sharp for $pn + q$ problems in general, but for most p and q this bound is of course far off.

4.3 Collatz-like problems

Besides the $pn + q$ problems discussed above, we can also look at Collatz-like functions, and see how the above theory then works out. For example, consider the Collatz-like function C_3 defined earlier and also given again below.

$$C_3(n) = \begin{cases} n/3 & n \equiv 0 \bmod 3 \\ (2n+1)/3 & n \equiv 1 \bmod 3 \\ (4n+1)/3 & n \equiv 2 \bmod 3 \end{cases}$$

We can try to apply the theory of Collatz Modular Digraphs to this function as well, and it turns out we had better look at Ternary Modular Digraphs this time, where the modulus is a power of 3 instead of 2. Unsurprisingly, the 2 became a 3 because we considered 3 cases and divide by 3 on each iteration. Therefore, we define the generalizations of Binary Collatz Modular Digraphs and Binary De Bruijn Digraphs as below, where the 2 is replaced by any positive number n.

4.3.1 m-ary Collatz-like Modular Digraphs

Below are the definitions of m-ary Collatz-like Modular Digraphs and n-ary De Bruijn Digraphs.

Definition 4.3.1 (m-ary Collatz-like Modular Digraphs). *The m-ary Collatz-Like Modular Digraph (mCLMD) with modulus m^p for the Collatz-like function C_m, denoted by $\mathcal{M}_{m,p}$, is the graph $G = (V, E)$ such that:*

$$\begin{aligned} V &= \{0, 1, 2, \ldots, n^p - 1\} \\ E &= \{(v_1, v_2) \mid v_1, v_2 \in V \textit{ and } \exists\ v_3 \equiv v_1 \pmod{m^p} : C(v_3) \equiv v_2 \pmod{m^p}\}. \end{aligned}$$

Furthermore, we denote the adjacency matrix of $\mathcal{M}_{m,p}$ with M, which is defined by:

$$(C)_{ij} := \begin{cases} 1 & \textit{if } (i,j) \in E \\ 0 & \textit{else} \end{cases}$$

Definition 4.3.2 (n-ary De Bruijn Digraphs). *If $p \geq 1$ and $q = m^p$, then the q-dimensional m-ary De Bruijn Digraph (mDBD), denoted by $\mathcal{B}_{m,p}$, is the graph $G = (V, E)$ with*

$$\begin{aligned} V &= \{0, 1, 2, \ldots, m-1\}^p \\ E &= \{((b_1, b_2, \ldots, b_{m-1}, b_m), (b_2, b_3, \ldots, b_m, b_{m+1})) \mid b_i \in \{0, 1, 2, \ldots, m-1\}\ \forall\ i = 1, 2, \ldots, p+1\} \\ &= \{0, 1, 2, \ldots, m-1\}^{p+1} \end{aligned}$$

For example, with the previous example $C_3(n)$ we get the Ternary Modular Digraphs $\mathcal{M}_{3,i}$ as in Figures 4.17, 4.18, 4.19 and 4.20. The corresponding Ternary De Bruijn Digraph on 27 vertices is shown in Figure 4.21.

4.3.2 A modified Central Theorem

We can verify that indeed, these Collatz-like graphs are isomorphic to Ternary De Bruijn Digraphs. In fact, all properties of Theorem 4.1.13 are analogously true for these Collatz-like Digraphs. Therefore, we get the generalized version of Theorem 4.1.13 as below. No proof is given, since the proof is completely analogous to the proof of the Central Theorem.

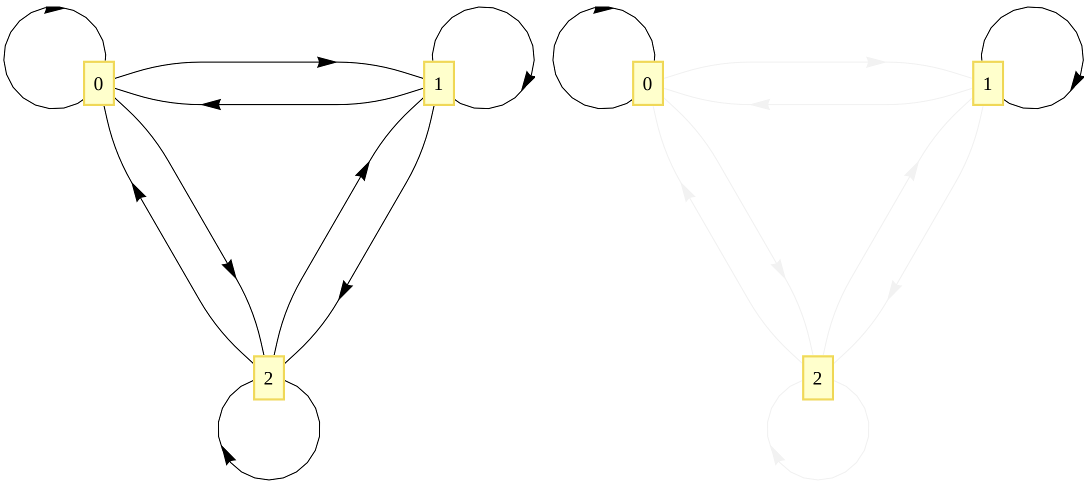

Figure 4.17: The Ternary Modular Digraph $\mathcal{M}_{3,1}$, with and without unstable edges. Note that the graph with all edges is the complete digraph on 3 vertices.

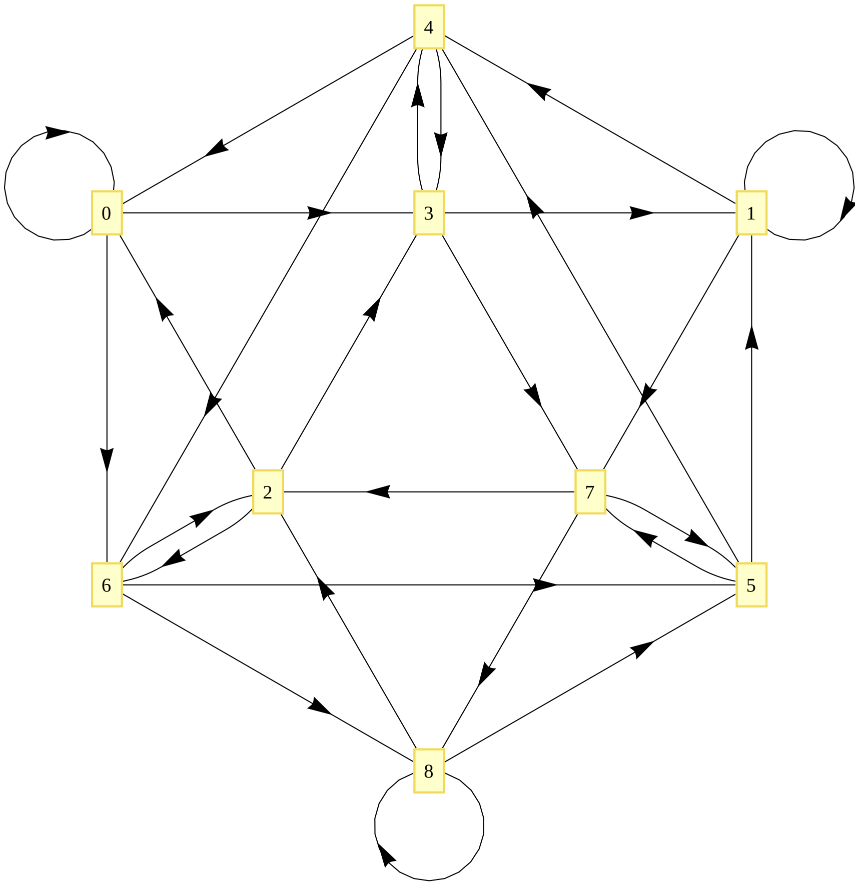

Figure 4.18: The Ternary Modular Digraph $\mathcal{M}_{3,2}$. Note that the graph is the line graph of $\mathcal{M}_{3,1}$ as in Figure 4.17.

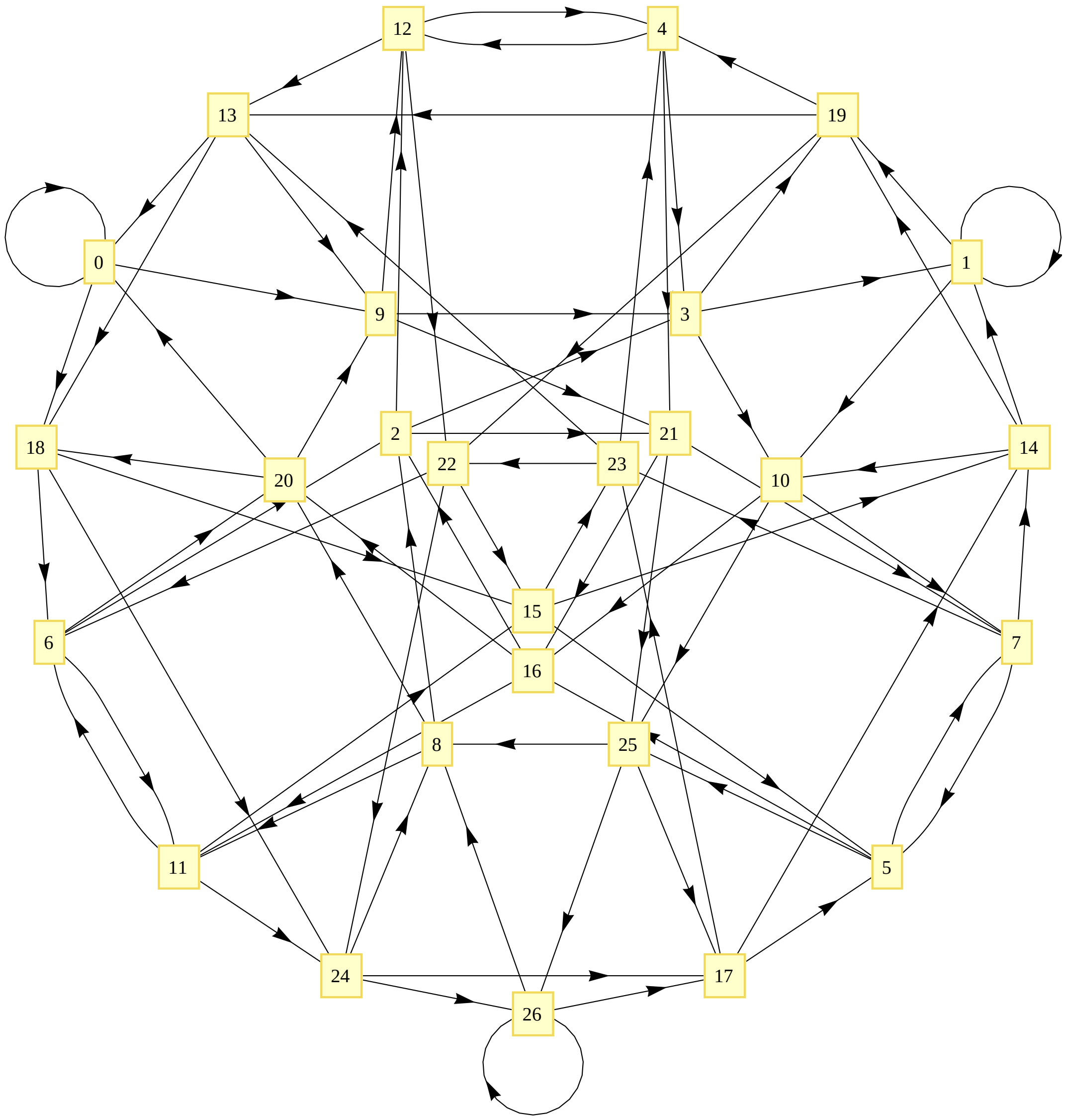

Figure 4.19: The Ternary Modular Digraph $\mathcal{M}_{3,3}$.

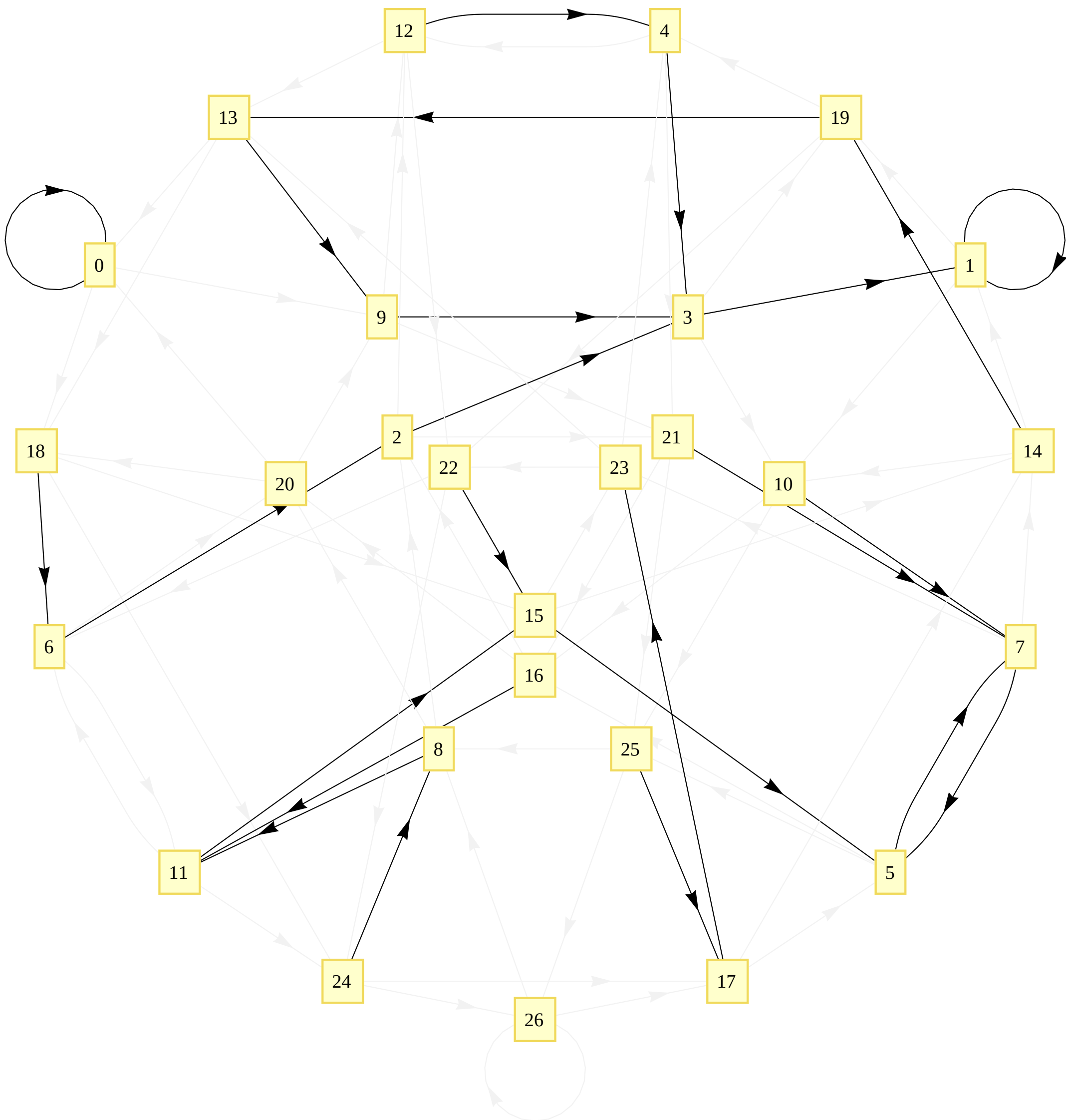

Figure 4.20: The Ternary Modular Digraph $\mathcal{M}_{3,3}$, with only stable edges. We can already see the cycles (0), (1) and $(5,7)$ which are easily verified to be cycles in the iterations of C_3.

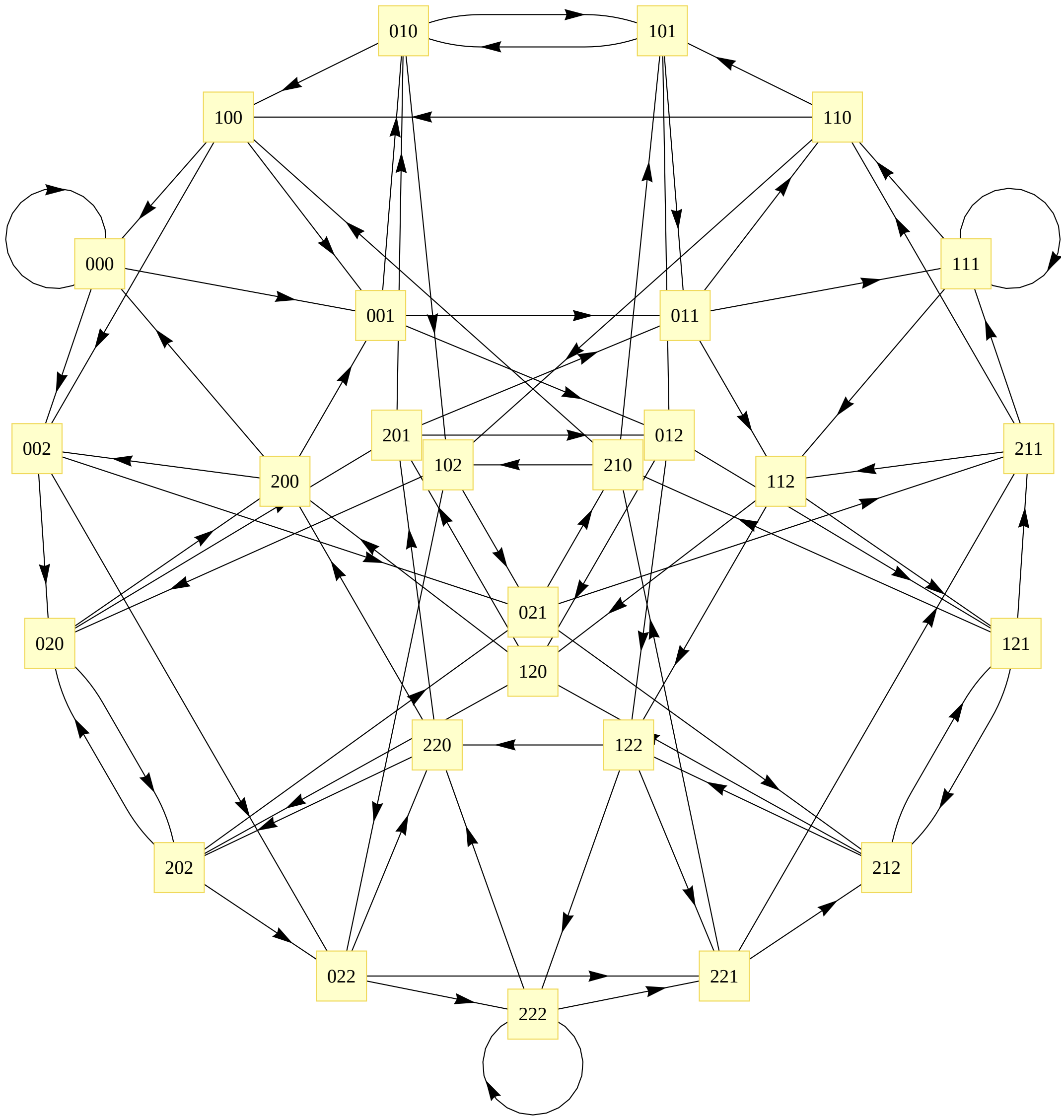

Figure 4.21: The Ternary De Bruijn Digraph $\mathcal{B}_{3,4}$. As we can see, this graph is isomorphic to $\mathcal{M}_{3,3}$ in Figure 4.19. Note that the vertices in the top part of the chart have only zeroes and ones, the bottom left part only zeroes and twos, and the bottom right part only ones and twos. If we remove all vertices containing a 2 and all corresponding edges, we would get the Binary De Bruijn Digraph $\mathcal{B}_{2,4}$.

Theorem 4.3.3 (Properties of m-ary Collatz-like Modular Digraphs)**.** *If $m, p \geq 1$, C_m is a Collatz-like function with m-ary Collatz-like Modular Digraph $\mathcal{M}_{m,p} = (V, E)$ with adjacency matrix M_p, then:*

(i) $L(\mathcal{M}_{m,p}) \cong \mathcal{M}_{m,p+1,C}$

(ii) $M_p^p = U_{m^p}$

(iii) $\forall\, v \in V : d^+(v) = m$

(iv) $\forall\, v \in V : d^-(v) = m$

(v) $\mathcal{M}_{m,p}$ *is strongly connected*

(vi) $\mathcal{M}_{m,p}$ *is Eulerian*

(vii) $\mathcal{M}_{m,p} \cong \mathcal{B}_{m,p}$

(viii) $\mathcal{M}_{m,p}$ *is Hamiltonian*

(ix) $\mathcal{M}_{m,p} \cong (\mathcal{M}_{m,p})^T$

This analogy shows that there exists a strong relation between $pn + q$ problems (including the $3n+1$ conjecture) and the Collatz-like problems. When looking at the Modular Digraphs of both these types of problems, we see that they are both isomorphic to certain De Bruijn Digraphs, from which we can derive some interesting properties of these graphs. The consequence noted for the $3n+1$ problem, that when writing the numbers in their binary form, after k steps the information about the last k bits is lost, analogously applies to the Collatz-like problems. For example, if we have a Collatz-like function C_{10} so that $n = 10$, then we can use the decimal representation of the numbers m, and see that after 3 iterations, the value of $C_{10}^3(m) \pmod{1000}$ could be anything between 0 and 999.

Similar to the subsection about Infinite Binary De Bruijn Digraphs, we can again get upper bounds for the maximum number of cycles in Collatz-like functions. For example, for a function C_3, there are 3 possible cycles of length 1, namely $(b_1) = \{(0), (1), (2)\}$. One can easily verify there are 3 possible cycles of length 2, 8 cycles of length 3, etcetera. In this case, if we write $U_{m,k}$ for the number of real cycles of m-ary Collatz-like functions of length k, then we get the formula:

$$U_{m,k} = \frac{1}{P_{m,k}}(m^k - \sum_{\substack{d|k \\ 1 \leq d < k}} P_{m,d} U_{m,d})$$

where and $P_{m,i} = i$ is the number of permutations of a real cycle of length i. Thus, using Möbius inversion, we get:

$$U_{m,k} = \frac{1}{k} \sum_{d|k} \mu(d) m^{k/d}$$

Note again that by Fermat's little theorem, when k is prime, the right hand side becomes $(n/k) \cdot (n^{k-1} - 1)$ and is an integer for any n. Thus, we get the following Theorem for Collatz-like functions:

Theorem 4.3.4 (Maximum number of real cycles of length k in Collatz-like problems)**.** *The number of cycles $(n_1, n_2, n_3, \ldots, n_k)$ of length at most k of the Collatz-like function C_m with all n_i distinct, denoted by $R_{m,k}$, is for every $k \geq 1$ bounded by:*

$$R_{m,k} \leq U_{m,k}$$

For example, if p is a prime, then the maximum number of "real" cycles of lengths 1, 2 and p for a Collatz-like function C_m are m, $\frac{m}{2}(m-1)$ and $\frac{m}{p}(m^{p-1} - 1)$ respectively. Note again that we can theoretically calculate the possible values of starting points of cycles, for any m and $\{a_i\}$, $\{b_i\}$. We can then adjust the b_i such that the cycles all become integer cycles. So again, the bound is sharp for Collatz-like problems in general, although we give no explicit proof here.

4.4 Summary

Concluding, we can first say that we found an interesting relation between the Collatz Modular Digraphs and Binary De Bruijn Digraphs, a relation which to the knowledge of the author has not been established before by others. This isomorphic relation immediately resulted in some properties which hold for these De Bruijn Graphs, which were mentioned in the Central Theorem. As most of the useful properties in this Theorem were already discovered by others, such as in [FMR94], most of the consequences of the Central Theorem mentioned in this chapter are not new to the literature.

Another interesting result from this chapter is that these Binary De Bruijn Digraphs do not only appear for the $3n + 1$ problem, but for all $pn + q$ problems. In fact, the further generalization to Collatz-like functions resulted in an isomorphy with n-ary De Bruijn Digraphs. This also shows that the structures of the $3n + 1$ problem, $pn + q$ problems and Collatz-like problems are very similar, as we also saw in the previous chapter.

Furthermore, when we restricted the Binary Collatz Modular Digraphs to only those edges which were 'stable' (such that $T(i) = j$ for those vertices i and j), we saw that the regular (partial) Collatz Digraph is isomorphic to this subgraph of the Collatz Modular Digraph. However, these 'stable' and 'unstable' edges turned out to be chaotically spread out over the graph. This also follows from the fact that the Collatz Modular Digraphs are very structured, while the normal Collatz Graph is quite chaotic. So this transition had to result in chaos. Therefore it is likely that this restriction to stable edges will not give us new leads in our search for the truth behind the $3n + 1$ conjecture.

A last result from this chapter is that we found an upper bound U_k for the number of cycles of at most length k for all $pn + q$ problems, and also that this upper bound can indeed be reached with the given right choice of q, for any $p > 3$ odd. Therefore the bound U_k is in fact sharp. So although the value of U_k grows exponentially in k, we cannot get a general sharper bound for the number of cycles of $pn + q$ problems, without knowing which values p and q have.

A point of further research could be to investigate the sequences $\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3, \ldots$ and $\mathcal{B}_1, \mathcal{B}_2, \mathcal{B}_3, \ldots$ and their isomorphisms $\sigma_1, \sigma_2, \sigma_3, \ldots$. In the long term, we can see from these isomorphisms σ_k if a number ends in the cycle $(1, 2)$, so it would be of interest to know more about this sequence. However, since discovering things about the sequence $\sigma_1(n), \sigma_2(n), \sigma_3(n), \ldots$ means discovering things about the $3n + 1$ conjecture, this will probably be hard as well.

Chapter 5

Generating Functions

We can try to analyze the $3n+1$ conjecture, using generating functions, where the coefficients of the power series satisfy the recursion from the $3n+1$ conjecture. We can then analyze these power series, and try to prove that these functions have only one solution, which would then prove that the $3n+1$ conjecture is true. Note that this approach to the $3n+1$ problem was also investigated by Burckel in [Bur94] and by Berg and Meinardus in [BM94] and [BM95].

The same approach can also be used for other $pn+q$ problems, which is discussed as well.

5.1 The $3n+1$ conjecture

If we assume the $3n+1$ conjecture is true, then the recurrence relation defined by

$$a_n = a_{T(n)}$$

or, more specifically,

$$\begin{aligned} a_{2n} &= a_n \\ a_{2n+1} &= a_{3n+2} \end{aligned}$$

with $n \in \mathbb{N}$ has only two linearly independent distinct solutions. Namely the sequence $(1, 0, 0, 0, \ldots)$ belonging to the component containing only 0, and the sequence $(0, 1, 1, 1, \ldots)$, belonging to the component $\mathbb{N}_+$. Now we define the generating function $a(x)$ as follows.

$$a(x) = \sum_{n=0}^{\infty} a_n x^n$$

We also define $a_{3,2}(x)$ as:

$$a_{3,2}(x) = \sum_{n=0}^{\infty} a_{3n+2} x^{3n+2}$$

Furthermore, similarly to the chapter about the Collatz graph, we introduce the complex variables $\zeta_3 = e^{2\pi i/3}$ and the set $R_3 = \{1, \zeta_3, \zeta_3^2\}$. We notice that with n any integer, we have:

$$\begin{aligned} \frac{1}{3}\sum_{r=0}^{2}(\zeta_3)^{(n-2)r} &= \frac{1}{3}\sum_{r=0}^{2} e^{2\pi i(n-2)r/3} \\ &= \begin{cases} 1 & \text{if } n \equiv 2 \pmod 3 \\ 0 & \text{if } n \not\equiv 2 \pmod 3 \end{cases} \\ &=: \mathbb{I}_{3,2,n} \end{aligned}$$

Using this, we get:

$$\begin{aligned}
a_{3,2}(x) &= \sum_{n=0}^{\infty} a_{3n+2}x^{3n+2} = \sum_{n=0}^{\infty} \mathbb{I}_{3,2,n} a_n x^n = \sum_{n=0}^{\infty} \left(\frac{1}{3} \sum_{r=0}^{2} (\zeta_3)^{(n-2)r} \right) a_n x^n \\
&= \frac{1}{3} \sum_{n=0}^{\infty} \sum_{r=0}^{2} (\zeta_3)^{(n-2)r} a_n x^n = \frac{1}{3} \sum_{r=0}^{2} \sum_{n=0}^{\infty} (\zeta_3)^{nr} (\zeta_3)^{-2r} a_n x^n \\
&= \frac{1}{3} \sum_{r=0}^{2} (\zeta_3)^{-2r} \sum_{n=0}^{\infty} (\zeta_3)^{nr} a_n x^n = \frac{1}{3} \sum_{r=0}^{2} (\zeta_3^r)^{-2} \sum_{n=0}^{\infty} a_n (\zeta_3^r x)^n \\
&= \frac{1}{3} \sum_{r=0}^{2} (\zeta_3^r) a(\zeta_p^r x)
\end{aligned}$$

So we can express $a_{3,2}(x)$ in terms of $a(x)$ as:

$$\tilde{a}(x) = a_{3,2}(x) = \frac{1}{3} \sum_{r=0}^{2} \zeta_3^r a(\zeta_p^r x) \tag{5.1}$$

By splitting up the infinite sum of the generating function $a(x)$ in even and odd terms, and then using the recurrence relations, we get:

$$\begin{aligned}
a(x) &= \sum_{n=0}^{\infty} a_n x^n = \sum_{n=0}^{\infty} a_{2n} x^{2n} + \sum_{n=0}^{\infty} a_{2n+1} x^{2n+1} = \sum_{n=0}^{\infty} a_n x^{2n} + \sum_{n=0}^{\infty} a_{3n+2} x^{2n+1} \\
&= \sum_{n=0}^{\infty} a_n (x^2)^n + \frac{1}{x^{1/3}} \sum_{n=0}^{\infty} a_{3n+2} (x^{2/3})^{3n+2} = a(x^2) + \frac{1}{x^{1/3}} \tilde{a}(x^{2/3}) \\
&= a(x^2) + \frac{1}{3x^{1/3}} \left(a(x^{2/3}) + \zeta_3 a(\zeta_3 x^{2/3}) + \zeta_3^2 a(\zeta_3^2 x^{2/3}) \right)
\end{aligned}$$

So if we substitute x^3 for x, we get the functional equation:

$$a(x^3) - a(x^6) - \frac{1}{3x} \left(a(x^2) + \zeta_3 a(\zeta_3 x^2) + \zeta_3^2 a(\zeta_3^2 x^2) \right) = 0$$

If we define $a_0(x)$ and $a_1(x)$ as:

$$\begin{aligned}
a_0(x) &= 1 \\
a_1(x) &= \frac{x}{1-x} = x + x^2 + x^3 + \dots
\end{aligned}$$

Then the $3n+1$ conjecture now says that the only solutions to the functional equation for $a(x)$ are the functions of the following form, where A_0 and A_1 are constants.

$$a^*(x) = A_0 a_0(x) + A_1 a_1(x) = A_0 + \frac{A_1 x}{1-x}$$

Indeed, we can easily verify that $a_0(x)$ is a solution to the functional equation. We can also verify that $a_1(x)$ is a solution. For this we mainly use that $1+\zeta_3+\zeta_3^2=0$. Writing it out, we get:

$$\begin{aligned}
& a_1(x^3)-a_1(x^6)-\frac{1}{3x}\left(a_1(x^2)+\zeta_3 a_1(\zeta_3 x^2)+\zeta_3^2 a_1(\zeta_3^2 x^2)\right) \\
= \; & \frac{x^3}{1-x^3}-\frac{x^6}{1-x^6}-\frac{1}{3x}\left(\frac{x^2}{1-x^2}+\frac{\zeta_3^2 x^2}{1-\zeta_3 x^2}+\frac{\zeta_3 x^2}{1-\zeta_3^2 x^2}\right) \\
= \; & \frac{x^3}{1-x^6}-\frac{x^2(1-\zeta_3 x^2)(1-\zeta_3^2 x^2)+\zeta_3^2 x^2(1-x^2)(1-\zeta_3^2 x^2)+\zeta_3 x^2(1-x^2)(1-\zeta_3 x^2)}{3x(1-x^2)(1-\zeta_3 x^2)(1-\zeta_3^2 x^2)} \\
= \; & \frac{x^3}{1-x^6}-\frac{x^2(1+\zeta_3+\zeta_3^2)-x^4(3\zeta_3+3\zeta_3^2)+x^6(\zeta_3^3+\zeta_3^4+\zeta_3^2)}{3x(1-x^2(1+\zeta_3+\zeta_3^2)+x^4(\zeta_3+\zeta_3^2+1)-x^6)} \\
= \; & \frac{x^3}{1-x^6}-\frac{3x^4}{3x(1-x^6)} \\
= \; & 0
\end{aligned}$$

So we can easily verify that this function satisfies the equation, but it is not easy to verify that these $a^*(x)$ are the only solutions to the equation. Note that the functions $a_0(x)$ and $a_1(x)$ correspond exactly to the two (conjectured) components of the $3n+1$ problem, namely the components $\{0\}$ and $\mathbb{N}_+$, respectively.

5.2 $pn+q$ problems

Using the above approach, we can also get functional equations for $pn+q$ problems in general. First we define the sequence based on a $pn+q$ recursion:

$$b_n = b_{T_{p,q}(n)}$$

Seperating the cases where n is even and odd gives us:

$$\begin{aligned}
b_{2n} &= b_n \\
b_{2n+1} &= b_{pn+(p+q)/2}
\end{aligned}$$

If we follow the same approach as above, we get the generating functions:

$$\begin{aligned}
b(x) &= \sum_{n=0}^{\infty} b_n x^n \\
b_{p,(p+q)/2}(x) &= \sum_{n=0}^{\infty} b_{pn+(p+q)/2} x^{pn+(p+q)/2}
\end{aligned}$$

We similarly introduce the complex variables $\zeta_p = e^{2\pi i/p}$ and the set $R_p = \{1, \zeta_p, \zeta_p^2, \zeta_p^3, \ldots, \zeta_p^{p-1}\}$ which forms the set of solutions to the complex equation $z^p = 1$. We notice that with p, q, n any integers, we have:

$$\begin{aligned}
\frac{1}{p}\sum_{r=0}^{p-1}(\zeta_p)^{(n-q)r} &= \frac{1}{p}\sum_{r=0}^{p-1} e^{2\pi i(n-q)r/p} \\
&= \begin{cases} 1 & \text{if } n \equiv q \pmod p \\ 0 & \text{if } n \not\equiv q \pmod p \end{cases} \\
&=: \mathbb{I}_{p,q,n}
\end{aligned}$$

Using this, we get:

$$\begin{aligned}
b_{p,(p+q)/2}(x) &= \sum_{n=0}^{\infty} b_{pn+(p+q)/2}x^{pn+q} = \sum_{n=0}^{\infty} \mathbb{I}_{p,(p+q)/2,n} b_n x^n \\
&= \sum_{n=0}^{\infty}\left(\frac{1}{p}\sum_{r=0}^{p-1}(\zeta_p)^{(n-(p+q)/2)r}\right) b_n x^n = \frac{1}{p}\sum_{n=0}^{\infty}\sum_{r=0}^{p-1}(\zeta_p)^{(n-(p+q)/2)r} b_n x^n \\
&= \frac{1}{p}\sum_{r=0}^{p-1}\sum_{n=0}^{\infty}(\zeta_p)^{nr}(\zeta_p)^{-(p+q)/2r} b_n x^n = \frac{1}{p}\sum_{r=0}^{p-1}(\zeta_p)^{-(p+q)/2r}\sum_{n=0}^{\infty}(\zeta_p)^{nr} b_n x^n \\
&= \frac{1}{p}\sum_{r=0}^{p-1}(\zeta_p^r)^{-(p+q)/2}\sum_{n=0}^{\infty} b_n(\zeta_p^r x)^n = \frac{1}{p}\sum_{r=0}^{p-1}(\zeta_p^r)^{(p-q)/2} b(\zeta_p^r x)
\end{aligned}$$

So we can express $b_{p,(p+q)/2}(x)$ in terms of $b(x)$ as:

$$\tilde{b}(x) = b_{p,(p+q)/2}(x) = \frac{1}{p}\sum_{r=0}^{p-1}(\zeta_p^r)^{(p-q)/2} b(\zeta_p^r x)$$

Using the new recurrence relation, we now get:

$$\begin{aligned}
b(x) &= \sum_{n=0}^{\infty} b_n x^k \\
&= \sum_{n=0}^{\infty} b_{2n}x^{2n} + \sum_{n=0}^{\infty} b_{2n+1}x^{2n+1} \\
&= \sum_{n=0}^{\infty} b_n x^{2n} + \sum_{n=0}^{\infty} b_{pn+(p+q)/2}x^{2n+1} \\
&= \sum_{n=0}^{\infty} b_n (x^2)^n + x^{-q/p}\sum_{n=0}^{\infty} b_{pn+(p+q)/2}(x^{2/p})^{pn+(p+q)/2} \\
&= b(x^2) + x^{-q/p}\tilde{b}(x^{2/p}) \\
&= b(x^2) + \frac{1}{px^{q/p}}\sum_{r=0}^{p-1}(\zeta_p^r)^{(p-q)/2} b(\zeta_p^r x^{2/p})
\end{aligned}$$

So if we substitute x^p for x, we can write for $b(x)$:

$$b(x^p) - b(x^{2p}) = \frac{1}{px^q}\sum_{r=0}^{p-1}(\zeta_p^r)^{(p-q)/2} b(\zeta_p^r x^2)$$

Now if $p+q>0$, then we have at least two solutions to the above equation, namely:

$$\begin{aligned}
b_0(x) &= B_0 \\
b_1(x) &= \frac{B_1 x}{1-x} = B_1\left(x + x^2 + x^3 + \ldots\right)
\end{aligned}$$

The solution b_0 corresponds to the component $\{0\}$, while the solution b_1 corresponds to the union of components on the positive integers. If $p+q=0$, then $T(1)=0$, so that b_0 and b_1 are not solutions (but $b_0(x)+b_1(x)$ with $B_0=B_1$ is). And if $p+q<0$, then $T(1)<0$ such that the only solutions to the functional equation are those arising from components with cycles on the positive integers.

Furthermore, we see that the $(p-q)/2$ in the exponent of ζ_p^r can be taken modulo p, since $\zeta_p^p=1$. So it also follows that if $(p-q)/2$ is divisable by p, then the coefficient $(\zeta_p^r)^{(p-q)/2}$ drops out. As an example we will look at the $3n+3$ problem below, which as mentioned before is equivalent to the $3n+1$ problem, but which also has that $p-q=0$.

5.2.1 The $3n + 3$ problem

Using the above calculations, we can easily find a functional equation for the $3n+3$ problem. Let the sequence c_i with $i \in \mathbb{N}$ be defined as follows.

$$\begin{aligned} c_{2n} &= c_n \\ c_{2n+1} &= c_{3n+3} \end{aligned}$$

Furthermore, let the generating function $c(x)$ be defined as:

$$c(x) = \sum_{n=0}^{\infty} c_n x^n$$

The functional equation for $c(x)$ then becomes:

$$\begin{aligned} c(x^3) - c(x^6) &= \frac{1}{3x} \sum_{r=0}^{2} c(\zeta_p^r x) \\ &= \frac{1}{3x^3} \left(c(x^2) + c(\zeta_3 x^2) + c(\zeta_3^2 x^2) \right) \end{aligned}$$

If we now look at the function $\tilde{c} := c_{3,3}$ and use (5.1) with $p = 3$ and $q = 3$ we get:

$$\tilde{c}(x) = c_{3,3}(x) = \frac{1}{3} \left(c(x) + c(\zeta_3 x) + c(\zeta_3^2 x) \right)$$

Using the new recurrence relation, we now get:

$$\begin{aligned} c(x) &= \sum_{n=0}^{\infty} c_n x^n \\ &= \sum_{n=0}^{\infty} c_{2n} x^{2n} + \sum_{n=0}^{\infty} c_{2n+1} x^{2n+1} \\ &= \sum_{n=0}^{\infty} c_n x^{2n} + \sum_{n=0}^{\infty} c_{3n+3} x^{2n+1} \\ &= \sum_{n=0}^{\infty} c_n (x^2)^n + \frac{1}{x} \sum_{n=0}^{\infty} c_{3n+3} (x^{2/3})^{3n+3} \\ &= c(x^2) + \frac{1}{x} \tilde{c}(x^{2/3}) \\ &= c(x^2) + \frac{1}{3x} \left(c(x^{2/3}) + c(\zeta_3 x^{2/3}) + c(\overline{\zeta_3} x^{2/3}) \right) \end{aligned}$$

So for $c(x)$ we can write:

$$c(x^3) - c(x^6) = \frac{1}{3x^3} \left(c(x^2) + c(\zeta_3 x^2) + c(\zeta_3^2 x^2) \right)$$

Not let $c_0(x)$ and $c_1(x)$ be defined as follows.

$$\begin{aligned} c_0(x) &= 1 \\ c_1(x) &= \frac{x}{1-x} \end{aligned}$$

Since the $3n + 1$ and $3n + 3$ conjecture are equivalent, an equivalent formulation of the $3n + 1$ conjecture is that the only solutions to the functional equation for $c(x)$ are the solutions of the following form, where C_0 and C_1 are constants.

$$c(x) = C_0 c_0(x) + C_1 c_1(x) = C_0 + C_1 \left(x + x^2 + x^3 + \ldots \right)$$

We can again verify that these solutions satisfy the equation, but it is still hard to see if these solutions are the only solutions. Maybe for some reason certain calculations will turn out to work better with the functional equation for $c(x)$, since the coefficients ζ_3 are gone. But at the moment we don't see how one should prove the proposed solutions $c_0(x)$ and $c_1(x)$ are the only solutions. And after all, since the conjectures are equivalent, proving that $a(x)$ or $c(x)$ only has the mentioned solutions will also be equally hard.

5.2.2 The $5n + 1$ problem

As another example, we look at the $5n+1$ problem. The $5n+1$ problem gives rise to the following recurrence relation:

$$\begin{aligned} d_{2n} &= d_n \\ d_{2n+1} &= d_{5n+3} \end{aligned}$$

The corresponding generating function is defined below.

$$d(x) = \sum_{n=0}^{\infty} d_n x^n$$

For this function we then get the following functional equation, where $\zeta_5 = e^{2\pi i/5}$ is the fifth root of unity.

$$\begin{aligned} d(x^5) - d(x^{10}) &= \frac{1}{5x^3} \sum_{r=0}^{4} (\zeta_5^r)^2 d(\zeta_5^r x^2) \\ &= \frac{1}{5x^3} \left(d(x^2) + \zeta_5^2 d(\zeta_5^1 x^2) + \zeta_5^2 d(\zeta_5^2 x^2) + \zeta_5^4 d(\zeta_5^3 x^2) + \zeta_5^3 d(\zeta_5^4 x^2) \right) \end{aligned}$$

We note that again we see the complex roots of unity coming up. It is interesting that the totally different method of looking at Collatz graphs gives the same complex roots of unity as this methods. Apparently there is a relation between these problems and roots of unity. However, we have to note that for the functional equations, the k in ζ_k is equal to the p in $pn+q$, while for the Collatz graph, the k in ζ_k depended on the cycle length of a cycle.

Note that using our knowledge about the cycles and probable divergent paths in the $5n+1$ problem, we can write down some functions that are likely solutions to the above problem:

$$\begin{aligned} d_0(x) &= D_0 \\ d_1(x) &= D_1 \left(x + x^2 + x^3 + x^4 + x^6 + x^8 + x^{12} + x^{15} + x^{16} + x^{19} + \ldots \right) \\ d_2(x) &= D_2 \left(x^5 + x^{10} + x^{13} + x^{20} + x^{26} + x^{33} + x^{40} + x^{52} + x^{66} + x^{80} + \ldots \right) \\ d_3(x) &= D_3 \left(x^7 + x^9 + x^{11} + x^{14} + x^{18} + x^{22} + x^{23} + x^{28} + x^{29} + x^{35} + \ldots \right) \\ d_4(x) &= D_4 \left(x^{17} + x^{27} + x^{34} + x^{43} + x^{54} + x^{68} + x^{86} + x^{108} + x^{136} + x^{172} + \ldots \right) \\ d_5(x) &= D_5 \left(x^{21} + x^{42} + x^{53} + x^{61} + x^{67} + x^{84} + x^{106} + x^{122} + x^{134} + x^{168} + \ldots \right) \\ d_6(x) &= D_6 \left(x^{25} + x^{31} + x^{39} + x^{49} + x^{50} + x^{62} + x^{63} + x^{77} + x^{78} + x^{79} + \ldots \right) \end{aligned}$$

If there are infinitely many divergent paths (which is highly probable), then there are also infinitely many independent solutions to the functional equation.

5.3 Summary

Although we can derive interesting functional equations for the $3n + 1$ and $pn + q$ problems in general, these functional equations seem very hard to solve. For example, if we try to simply fill in a power series for $a(x)$, the result will just be that the coefficients of the power series have to satisfy the recurrence, which define the generating functions.

One interesting result is that if the $3n+1$ problem has only one cycle and no divergent paths, and the $5n + 1$ problem has infinitely many divergent paths, then the functional equation for $a(x)$ has only two independent solutions, while the functional equation for $d(x)$ has infinitely many. This is not a trivial result at all; why do the two equations, which structurally look similar, differ so much in the number of independent solutions to the equation? We cannot give an answer to this question, and this is perhaps an area for further research.

So although the functional equations look interesting and simple enough, it is hard to see if this approach can give us results about the truth of the $3n + 1$ conjecture. We know too little about solving such equations to draw any conclusions about the $3n + 1$ conjecture or other $pn + q$ problems. For now, the only use of this method has been that we found an elegant and equivalent variant of the $3n+1$ conjecture, namely that the given functional equations for $a(x)$ and $c(x)$ have only two independent solutions.

Perhaps a point of further research could be to include negative numbers in the recursion, and use generating functions with negative powers as well. Then the $3n + 1$ problem will have more solutions, since there are multiple components on the negative integers. Maybe this leads to nothing, but it could be worth looking into.

Conclusion

As was mentioned in the introduction, the aim of this report was not to prove the $3n+1$ conjecture, but to understand more about the conjecture. A part of the material in this report can be found in other literature on the $3n+1$ conjecture as well, while part of the material in this report is new. A short summary about the different chapters is below.

Basic Calculations

This chapter served mainly as an introduction to the $3n+1$ problem, to see why we cannot just calculate the forms of cycles in the $3n+1$ problem or related $pn+q$ problems. The form of the formulas for cycles showed why this is so hard. We also connected the $3n+3^k$ problems to the $3n+1$ conjecture as being equivalent, as was previously described in [LL06]. This chapter does not contain any really new material about the $3n+1$ problem.

The Collatz Digraph and its spectrum

In this chapter we investigated the Collatz Digraph, its adjacency matrix, and the spectrum of this matrix and its transpose. Using some basic linear algebra we managed to find all eigenvalues and -vectors of this infinite matrix and its transpose. Not all the material in this chapter is new, but a complete overview of all eigenvalues and eigenvectors of the infinite adjacency matrix has not been given before. Further research could be to investigate if this complete overview can be used in any way to learn more about the $3n+1$ conjecture, or to investigate what is known in literature about infinite matrices and infinite eigenvectors.

Collatz Modular Digraphs and De Bruijn Digraphs

In this chapter we looked at the Collatz iterations on congruence classes instead of numbers. This was also done in Feix et al. in [FMR94], with some similar results. However, the isomorphic relation between these graphs and De Bruijn Digraphs has not been described before, and this also resulted in some other properties about these graphs which are automatically true, because they hold for De Bruijn Digraphs. This therefore lead to some new results as well. The isomorphic relation to De Bruijn Digraphs also turned out to apply to $pn+q$ problems in general, and even to Collatz-like functions. It could be interesting to investigate if this isomorphic relation with De Bruijn Digraphs has any other consequences not mentioned in this chapter.

Generating Functions

In the chapter about generating functions we did not get any new results for the $3n+1$ problem. The functional equations for the $3n+1$ problem were already described by Berg and Meinardus in [BM94] and [BM95], and by Burckel in [Bur94]. We also derived functional equations for $pn+q$ problems in general, which among others lead to an interesting equation for the $5n+1$ problem.

It would be interesting to investigate why the equation for the $5n+1$ problem has infinitely many independent solutions, while the equation for the $3n+1$ problem probably only has two.

Summarizing, we hope that the reader can say he did get more insight into the $3n+1$ problem and related problems, after reading this report. Maybe some of the new results in this report could lead to new investigations in these areas of the $3n+1$ problem.

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