Contents

1. Introduction

It is well known that the inverted Collatz sequence can be represented as a graph or a tree. Similarly, it is acknowledged that in order to prove the Collatz conjecture, one must demonstrate that this tree covers all odd natural numbers. A structured reachability analysis is hitherto unavailable. This paper investigates the problem from a graph theory perspective. We define a tree that consists of nodes labeled with Collatz sequence numbers. This tree will be transformed into a sub-tree that only contains odd labeled nodes. Furthermore, we derive and prove several formulas that can be used to traverse the graph. The analysis covers the Collatz problem both in its original form $3x+1$ as well as in the generalized variant $kx+1$. Finally, we transform the Collatz graph into a binary tree, following the approach of Kleinnijenhuis, which could form the basis for a comprehensive proof of the conjecture.

1.1 Motivation

The Collatz conjecture is a number theoretical problem, which has puzzled countless researchers using myriad approaches to solve the problem. Presently, there are scarcely any methodologies to describe and treat the problem from the perspective of the Algebraic Theory of Graphs. Such an approach is promising with respect to facilitating the comprehension of the Collatz sequence's "mechanics."

The current gap in research forms the motivation behind the present contribution. The authors are convinced that exploring the Collatz conjecture in an algebraic manner, relying on the findings and fundamentals of Graph Theory, will contribute to a simplification of the problem.

Key results of this manuscript have been achieved using Data Science techniques. Our main tool was a Python-API, which implements the theorems that will be introduced later and is optimized for processing arbitrarily big integers [1], see chapter "About our approach".

1.2 Related Research

The following literature study is largely based on one given by a similar earlier essay [2] which deals with the Collatz conjecture from the vantage point of automata theory.

The Collatz conjecture is one of the unsolved "Million Dollar Problems" [3]. When Lothar Collatz began his professorship in Hamburg in 1952, he mentioned this problem to his colleague Helmut Hasse. From 1976 to 1980, Collatz wrote several letters but missed referencing that he first proposed the problem in 1937. He introduced a function $g : \mathbb{N} \rightarrow \mathbb{N}$ as follows:

$$g(x) = \begin{cases} 3x+1 & 2 \nmid x \\ x/2 & \text{otherwise} \end{cases} \tag{1.1}$$

This function is surjective, but it is not injective (for example $g(3) = g(20)$) and thus is not reversible. The Collatz conjecture states that for each start number $x_1 > 0$ the sequence $x_1, x_2 = g(x_1), x_3 = g(x_2), \ldots$ will at some point enter the so called trivial cycle $(4,2,1)$. One example is the sequence $(17,52,26,13,40,20,10,5,16,8,4,2,1)$ starting at $x_1 = 17$. The assumption has not yet been proven. The conjecture would be falsified if the sequence either diverges indefinitely for a starting number x_1 or enters a cycle different from the trivial one (a so called non-trivial cycle). In order to specify compressed Collatz sequences containing only the odd members, Bruckman [4] for instance used the more convenient function that opts out all even integers:

$$f(x) = (3x+1) \cdot 2^{-\alpha(x)}, \text{where} \quad 2^{\alpha(x)} \parallel (3x+1) \tag{1.2}$$

Note that $\alpha(x)$ is the largest possible exponent for which $2^{\alpha(x)}$ exactly divides $3x+1$. Especially for prime powers, one often says p^α *divides* the integer x *exactly*, denoted as $p^\alpha \parallel x$, if p^α is the greatest power of the prime p that divides x.

In his book "The Ultimate Challenge: The 3x+1 Problem" [5], along with his annotated bibliographies [6], [7] and other manuscripts like an earlier paper from 1985 [8], Lagarias researched and put together different approaches from various authors intended to describe and solve the Collatz conjecture.

For the integers up to 2,367,363,789,863,971,985,761 the conjecture holds valid. For instance, see the computation history given by Kahermanes [9] that provides a timeline of the results which have already been achieved.

Inverting the Collatz sequence and constructing a Collatz tree is an approach that has been carried out by many researchers. It is well known that inverse sequences [10] arise from all functions $h \in H$, which can be composed of the two mappings $q, r : \mathbb{N} \to \mathbb{N}$ with $q : m \mapsto 2m$ and $r : m \mapsto (m-1)/3$:

$$H = \{h : \mathbb{N} \to \mathbb{N} \mid h = r^{(j)} \circ q^{(i)} \circ \ldots, i, j, h(1) \in \mathbb{N}\}$$

An argumentation that the Collatz Conjecture cannot be formally proved can be found in the work of Craig Alan Feinstein [11], who presents the position that any proof of the Collatz conjecture must have an infinite number of lines and thus no formal proof is possible. However, this statement will not be acknowledged in depth within this study.

Treating Collatz sequences in a binary system can be performed as well. For example, Ethan Akin [12] handles the Collatz sequence with natural numbers written in base 2 (using the Ring $\mathbb{Z}_2$ of two-adic integers), because divisions by 2 are easier to deal with in this method. He uses a shift map σ on $\mathbb{Z}_2$ and a map τ:

$$\sigma(x) = \begin{cases} (x-1)/2 & 2 \nmid x \\ x/2 & \text{otherwise} \end{cases} \qquad \tau(x) = \begin{cases} (3x+1)/2 & 2 \nmid x \\ x/2 & \text{otherwise} \end{cases}$$

The shift map's fundamental property is $\sigma(x)_i = x_{i+1}$, noting that $\sigma(x)_i$ is the i-th digit of $\sigma(x)$. This property can easily be comprehended by an example $x = 5 = 1010000\ldots = x_0 x_1 x_2 \ldots$, containing $\sigma(x) = 2 = 0100000\ldots$

Akin then defines a transformation $Q : \mathbb{Z}_2 \to \mathbb{Z}_2$ by $Q(x)_i = \tau^i(x)_0$ for non-negative integers i which means $Q(x)_i$ is zero if $\tau^i(x)$ is even and then it is one in any other instance. This transformation is a bijective map that defines a conjugacy between τ and σ: $Q \circ \tau = \sigma \circ Q$ and it is equivalent to the map denoted Q_∞ by Lagarias [8] and it is the inverse of the map Φ introduced by Bernstein [13]. Q can be described as follows: Let x be a 2-adic integer. The transformation result $Q(x)$ is a 2-adic integer y, so that $y_n = \tau^{(n)}(x)_0$. This means, the first bit y_0 is the parity of $x = \tau^{(0)}(x)$, which is one, if x is odd and otherwise zero. The next bit y_1 is the parity of $\tau^{(1)}(x)$, and the bit after next y_2 is parity of $\tau \circ \tau(x)$ and so on. The conjugancy $Q \circ \tau = \sigma \circ Q$ can be demonstrated by transforming the expression as follows: $(\sigma \circ Q(x))_i = Q(x)_{i+1} = \tau^{(i+1)}(x)_0 = \tau^{(i)}(\tau(x))_0 = Q(\tau(x))_i$

A simulation of the Collatz function by Turing machines has been presented by Michel [14]. He introduces Turing machines that simulate the iteration of the Collatz function, where he considers them having 3 states and 4 symbols. Michel examines both Turing machines, those that never halt and those that halt on the final loop.

A function-theoretic approach to this problem has been provided by Berg and Meinardus [15], [16] as well as Gerhard Opfer [17], who consistently relies on the Berg's and Meinardus' idea. Opfer tries to prove the Collatz conjecture by determining the kernel intersection of two linear operators U, V that act on complex-valued functions. First he determined the kernel of V, and then he attempted to prove that its image by U is empty. Benne de Weger [18] contradicted Opfer's attempted proof.

At the number of divisions by two Paul S. Bruckman [4] and Koch et al. [19] have taken a deeper look. Bruckmann has attempted to provide an elementary proof by contradiction. He repeatedly applies the Collatz function using a starting value n_0 and defines:

$$\{e_k\} : n_1 = (3n_0 + 1) \cdot 2^{-e_1}, n_2 = (3n_1 + 1) \cdot 2^{-e_2} = (3^2 n_0 + 3 + 2^{e_1}) \cdot 2^{-(e_1+e_2)}, \ldots$$

Denoting the sum of exponents as $E_k = e_1 + e_2 + \ldots + e_k$ Bruckman obtains the following equation:

$$2^{E_k} n_k = 3^k n_0 + \sum_{j=0}^{k-1} 3^{k-1-j} 2^{E_j}$$

Reachability Considerations based on a Collatz tree exist as well. It is well known that the inverted Collatz sequence can be represented as a graph; to be more specific, they can be depicted as a tree [20], [21]. It is acknowledged that in order to prove the Collatz conjecture, one needs to demonstrate that this tree covers all odd natural numbers.

The Stopping Time theory has been introduced by Terras [22], it has been taken up and continued, inter alia, by Silva [23] and Idowu [24]. Terras introduces another notation of the Collatz function $T(n) = (3^{X(n)} n + X(n))/2$, where $X(n) = 1$ when n is odd and $X(n) = 0$ when n is even, and defined the stopping time of n, denoted by $\chi(n)$, as the least positive k for which $T^{(k)}(n) < n$, if it exists, or otherwise it reaches infinity. Let L_i be a set of natural numbers, it is observable that the stopping time exhibits the regularity $\chi(n) = i$ for all n fulfilling $n \equiv l(mod 2^i)$, $l \in L_i$, $L_1 = \{4\}$, $L_2 = \{5\}$, $L_4 = \{3\}$, $L_5 = \{11, 23\}$, $L_7 = \{7, 15, 59\}$ and so on. As i increases, the sets L_i, including their elements, become significantly larger. Sets L_i are empty when $i \equiv l(mod 19)$ for $l = 3, 6, 9, 11, 14, 17, 19$. Additionally, the largest element of a non-empty set L_i is always less than 2^i.

Dynamical systems provide a wide basis for examining the Collatz sequence as well [25]. A dynamical system [26, p. 464] is a triple (M, G, Φ) for a set M, a group $(G, +)$ and a map $\Phi : M \times G \to M$ for which $\Phi(\cdot, 0) = id_M(\cdot)$ firstly applies and secondly $\Phi(\Phi(m,s),t) = \Phi(m, s+t)$ for all $m \in M$, $s, t \in G$. The set M is called phase space. Terence Tao [27] considers orbits of the dynamical system generated by the Collatz map (an orbit, also called trajectory, is a subset of the phase space). For an integer function $f : \mathbb{Z} \to \mathbb{Z}$, we denote by $f^i = f \circ f^{i-1}$ the i-fold iterate of f with the convention $f^0 = id_{\mathbb{Z}}$. If $n \in \mathbb{Z}$, the orbit (trajectory) of n under f is the sequence $T_f(n) = (n, f(n), f \circ f(n), f \circ f \circ f(n), \ldots)$, see [25, p. 10]. Tao proved that nearly all of these orbits attain almost bounded values. To achieve this, he advanced the results of Allouche [28] and Korec [29]. Their main idea was to prove that the set of positive integers with finite stopping time has a density one, in this case the term density refers to the concept of *natural density* (also known as *asymptotic density*). It measures how large a subset of the set of natural numbers is. The natural density of a set $M \subseteq \mathbb{N}$ is defined as:

$$\lim_{n \to \infty} \frac{\#\{m \in M : m < n\}}{n}$$

In this context, the authors used the Collatz map as the map Φ. They proved that the set $\{x \in \mathbb{N} : (\exists t \in \mathbb{N})(\Phi(x,t) < x)\}$ has a natural density one.

Many other approaches exist as well. From an algebraic perspective, Trümper [30] analyzes the Collatz problem in the light of an Infinite Free Semigroup. Kohl [31] generalized the problem by introducing residue class-wise affine mappings, in short, rcwa mappings. A polynomial analogue of the Collatz Conjecture has been provided by Hicks et al. [32] [33] and there are also stochastical, statistical and Markov chain-based and permutation-based approaches to proving this elusive theory.

2. The Collatz Tree

2.1 The Connection between Groups and Graphs

Let (a_k) be a numerical sequence with $a_k = g^{(k)}(m)$, then a reversion produces an infinite number of sequences of reversely-written Collatz members [10].

Let S be a set containing two elements q and r, which are bijective functions over $\mathbb{Q}$:

$$\begin{aligned} q(x) &= 2x \\ r(x) &= \tfrac{1}{3}(x-1) \end{aligned} \tag{2.1}$$

Let a binary operation be the right-to-left composition of functions $q \circ r$, where $q \circ r(x) = q(r(x))$. Composing functions is an associative operation. All compositions of the bijections q and r and their inverses q^{-1} and r^{-1} are again bijective. The set, whose elements are all these compositions, is closed under that operation. It forms a free group F of rank 2 with respect to the free generating set S, where the group's binary operation $\circ$ is the function composition and the group's identity element is the identity function $id_{\mathbb{Q}} = e$. We call e an *empty string*. F consists of all expressions (strings) that can be concatenated from the generators q and r. The corresponding Cayley graph $Cay(F,S) = G$ is a regular tree whose vertices have four neighbors [34, p. 66]. A tree is called *regular* or *homogeneous* when every vertex has the same degree, in this case, $d(v) = 4$ for every vertex v in G. The Cayley graph's set of vertices is $V(G) = F$, and its set of edges is $E(G) = \left\{\{f, f \circ s\} \mid f \in F, s \in \left(S \cup S^{-1}\right) \setminus \{e\}\right\}$ [34, p. 57]. More precisely, the vertices are *labeled* by the elements (strings) of F.

In conformance with graph-theoretical precepts [35], [36], [37] we specify a subgraph H of G as a triple $(V(H), E(H), \psi_H)$ consisting of a set $V(H)$ of vertices, a set $E(H)$ of edges and an incidence function ψ_H. The latter is, in our case, the restriction $\psi_G|_{E(H)}$ of the Cayley graph's incidence function to the set of edges that only join vertices, which are labeled by a string over alphabet $\{r, q\}$ without the inverses: $E(H) = \{\{f, f \circ s\} \mid f \in F, s \in S \setminus \{e\}\}$.

This subgraph corresponds to the monoid S^*, which is freely generated by S follows related thoughts [30] that examine the Collatz problem in terms of a free semigroup on the set S^{-1} of inverse generators. Note that this semigroup is not to be confused with an *inverse semigroup* "in which every element has a unique inverse" [38, p. 26], [34, p. 22].

Let $Y^X = \{f \mid f \text{ is a map } X \to Y\}$ be the set of functions, which in category theory is referred to as the *exponential object* for any sets X, Y. The evaluation function $ev : Y^X \times X \to Y$ sends the pair (f, x) to $f(x)$. For a detailed description of this concept, see [39, p. 127], [40, p. 155], [41, p. 54] and [42, p. 188]. We define the evaluation function $ev_{S^*} : S^* \times \{1\} \to \mathbb{Q}$ that assesses an element of S^*, id est a composition of q and r, for the given input value 1. Furthermore we define the corestriction $ev^0_{S^*}$ of ev_{S^*} to $\mathbb{N}$. Since a corestricion of a function restricts the function's codomain [43, p. 3], the function $ev^0_{S^*}$ operates on a subset $T \subset S^*$ that

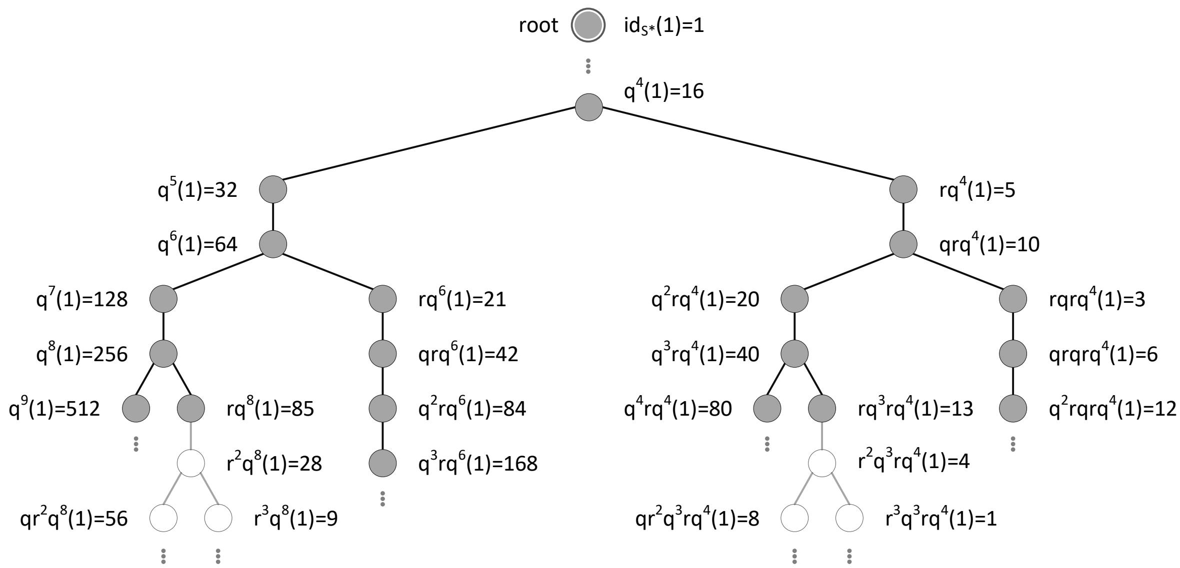

Figure 2.1: Small section of H_T with darkly highlighted subtree H_U

contains only those compositions of q and r, which return a natural number when inputting the value 1.

The set T does not form a monoid under function composition, for example $ev_{S^*}(qrq^4, 1) = 10$ and $ev_{S^*}(rq^6, 1) = 21$, but the composition qrq^4rq^6 does not lie in T, because the evaluation $ev_{S^*}(qrq^4rq^6, 1)$ yields a value outside the codomain $\mathbb{N}$. However, each element of this set labels a vertex of a tree $H_T \subset H$, which is a proper subtree of H.

Let $U \subset T$ be a subset of T, which does not contain a reduced word with two or more successive characters r. The corresponding tree $H_U \subset H_T$ reflects Collatz sequences as demonstrated in figure 2.1.

*When talking about trees having a root ("rooted trees"), another important concept should be explained: the **depth of a vertex** in a tree is the length of the path from the root to this vertex [44, p. 226]. In other words, it is the vertex's distance (the number of edges in the path) from the root. The root node has a depth of zero. The **level of a vertex** is its depth plus one $level(v) = depth(v) + 1$. The level of a tree's root is always one. The **height of a vertex** is the number of edges on the longest downward path from that vertex and a leaf. Any leaf node has a height of zero. The **height of a tree** is the height of its root, or equivalently, the depth of its deepest vertex [44, p. 226]. The **size of a tree** is its number of nodes. One has to be careful, because the literature provides varying definitions. According to Rosen [45, p. 804] for example, the level of a vertex is the length of the path from the root to this vertex; and the height of a tree is the largest vertex level in this tree.*

2.2 Defining the Tree

The starting point for specifying our tree is H_U. Due to its significance, we first concertize H_U by the definition 2.1 below, which establishes four essential characteristics.

Definition 2.1 The graph H_U possess the following key properties:

- $\boldsymbol{H_U}$ **is a directed graph (digraph):** Fundamentally, when we consider the more general case, an undirected graph as a triple (V, E, ψ), the incidence function maps an edge to an arbitrary vertex pair $\psi : E \to \{X \subseteq V : |X| = 2\}$. In a digraph, the set $V \times V$ represents ordered vertex pairs. Accordingly the incidence function is more specifically defined, namely as a mapping of the edges to that set $\psi : E \to \{(v, w) \in V \times V : v \neq w\}$, see [46, p. 15].

- $\boldsymbol{H_U}$ **is a rooted tree:** According to Rosen [45, p. 747], a rooted tree is, "a tree in which one vertex has been designated as the root and every edge is directed away from the root." Peculiarly, this definition considers the directionality as an inherent part of rooted trees. Unlike Mehlhorn and Sanders [47, p. 52], for example, who distinguish between an undirected and directed rooted tree.

  Note: As long as we do not stipulate that vertices may collapse, it is absolutely guaranteed that the graph is a tree.

- $\boldsymbol{H_U}$ **is an out-tree:** There is exactly one path from the root to every other node [47, p. 52], which means that edge directions go from parents to children [48, p. 108]. This property is implied in Rosen's definition for a rooted tree as well by saying "every edge is directed away from the root." An out-tree is sometimes designated as *out-arborescence* [48, p. 108].

- $\boldsymbol{H_U}$ **is a labeled tree:** For defining a labeled graph, Ehrig et al. [49, p. 23] use a label alphabet consisting of a vertex label set and an edge label set. Since we only label the vertices, in our case the specification of a vertex label set L_V together with the vertex label function $l_V : V \to L_V$ is sufficient. Originally, we said vertex labels are strings over the alphabet $S = \{q, r\}$, through which the free monoid S^* is generated. We illustrate labeling H_U by defining $l_{V(H_U)}(v) = ev^0_{S^*}(l_{V(G)}(\iota(v)), 1)$, where $\iota : V(H_U) \hookrightarrow V(G)$ is the inclusion map [50, p. 142] from the set of vertices of H_U to the set of vertices from the previously defined Cayley graph G.

We define a tree $H_{C,3}$ by taking the tree H_U as a basis and for every vertex $v \in V(H_U)$ satisfying $2 \mid l_{V(H_U)}(v)$, we contract the incoming edge. We attach the label of the parent of v to the new vertex, which results by replacing (merging) the two overlapping vertices that the contracted edge used to connect with. Visually, we obtain $H_{C,3}$ by contracting all edges in H_U that have an even-labeled target vertex, which (due to contraction) becomes "merged into its parent." Edge contraction is occasionally referred to as *collapsing an edge*. For more details and examples on edge contraction, one can see Voloshin [51, p. 27] and Loehr [52].

The tree $H_{C,3}$ is well known as the so-called *Syracuse tree*, see for example [53], [54], and [55]. It is a *minor of H_U*, since it can be obtained from H_U "by a sequence of any vertex deletions, edge deletions and edge contractions" [51, p. 32]. The sequence of contracting the edges between adjacent (in our case even-labeled) vertices is called *path contraction*.

A small section of the tree $H_{C,3}$, the Syracuse tree, is displayed in figure 2.2. Other definitions of the same tree exist, see for example Conrow [56], Bauer [57, p. 379], Batang [58] or Jan Kleinnijenhuis and Alissa M. Kleinnijenhuis [53], [59].

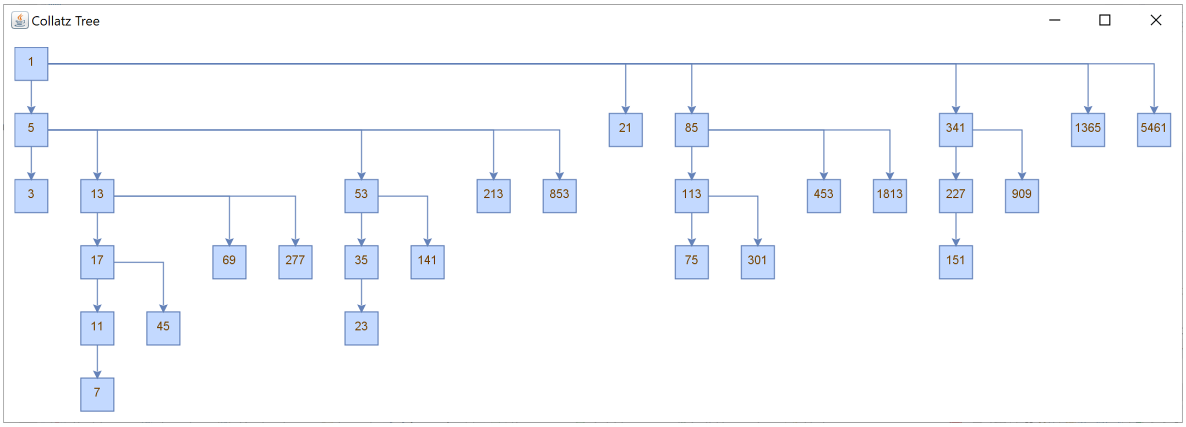

Figure 2.2: Section of the Syracuse tree $H_{C,3}$ (displaying the trivial cycle is waived)

2.3 Relationship of successive nodes in $H_{C,3}$

Let v_1 and v_{n+1} be two vertices of $H_{C,3}$, where v_1 is reachable from v_{n+1} with $depth(v_1) - depth(v_{n+1}) = n$. Hence, a path $(v_{n+1}, \ldots, v_1)$ exists between these two vertices. Theorem 2.1 specifies the following relationship between v_1 and v_{n+1}, empirically identified by Koch [1].

Theorem 2.1 $l_{V(H_{C,3})}(v_{n+1}) = 3^n l_{V(H_{C,3})}(v_1) \prod_{i=1}^{n} \left(1 + \frac{1}{3 l_{V(H_{C,3})}(v_i)}\right) 2^{-\alpha_i}$. In order to simplify readability, we waive writing down the vertex label function and put it shortly: $v_{n+1} = 3^n v_1 \prod_{i=1}^{n} \left(1 + \frac{1}{3v_i}\right) 2^{-\alpha_i}$. The value $\alpha_i \in \mathbb{N}$ is the number of edges which have been contracted between v_i and v_{i+1} in H_U.

In order to demonstrate the construction produced by theorem 2.1 in an illustrative fashion, example 2.1 runs through a concrete path in $H_{C,3}$.

Example 2.1 For example, the two vertices $v_1 = 45$ and $v_{1+3} = v_4 = 5$ are connected via the path $(5, 13, 17, 45)$, see figure 2.2. Furthermore, one can retrace in figure 2.3 the uncontracted path between these two nodes within H_U. When applied to this example, theorem 2.1 produces the following:

$$5 = v_{1+3} = 3^3 \cdot 45 \cdot \left(1 + \frac{1}{3 \cdot 45}\right) \cdot 2^{-3} \cdot \left(1 + \frac{1}{3 \cdot 17}\right) \cdot 2^{-2} \cdot \left(1 + \frac{1}{3 \cdot 13}\right) \cdot 2^{-3}$$

Proof. This relationship of successive nodes can simply be proven inductively. For the base case, we set $n = 1$ and retrieve

$$v_{1+1} = 3v_1 \left(1 + \frac{1}{3v_1}\right) 2^{-\alpha_1} = (3v_1 + 1)\, 2^{-\alpha_1} = v_2$$

The path from v_2 to v_1 can uniformly be expressed by a string $rq\cdots q$ of S^*, because of $v_1 = r \circ q^{\alpha_1}(v_2)$. We set $n = n+1$ for the step case, which leads to

$$\begin{aligned}
v_{n+2} &= 3^{n+1} v_1 \prod_{i=1}^{n+1} \left(1 + \tfrac{1}{3v_i}\right) 2^{-\alpha_i} \\
&= 3^{n+1} v_1 \left(1 + \tfrac{1}{3v_{n+1}}\right) 2^{-\alpha_{n+1}} \prod_{i=1}^{n} \left(1 + \tfrac{1}{3v_i}\right) 2^{-\alpha_i} \\
&= 3\left(1 + \tfrac{1}{3v_{n+1}}\right) 2^{-\alpha_{n+1}} 3^n v_1 \prod_{i=1}^{n} \left(1 + \tfrac{1}{3v_i}\right) 2^{-\alpha_i} \\
&= 3\left(1 + \tfrac{1}{3v_{n+1}}\right) 2^{-\alpha_{n+1}} v_{n+1} \\
&= (3v_{n+1} + 1)\, 2^{-\alpha_{n+1}}
\end{aligned}$$

In this case the path from v_{n+2} to v_{n+1} is correspondingly expressed by a string $rq\cdots q$ of S^* too, since $v_{n+1} = r \circ q^{\alpha_{n+1}}(v_{n+2})$. □

Even though the tree may theoretically contain two or more identically labeled vertices, it is essential to emphasize that we only consider such paths $(v_{n+1}, \ldots, v_1)$ whose vertices are all labeled differently. Later in section 4.1, we even require that identically labeled nodes are one and the same. In order to correctly determine successive nodes using theorem 2.1, we must consider the halting conditions. These are specified in definition 2.2, which was introduced by Koch et al. [19].

Definition 2.2 Being compliant with the Collatz conjecture, the algorithms (that calculate successive nodes for a given one) in theorem 2.1 and equation 2.18 halt if at least one of the following conditions is fulfilled:

1. $v_{n+1} = 1$
2. $v_{n+1} \in \{v_1, v_2, \ldots, v_n\}$

When the first condition applies, the Collatz conjecture is true for a specific sequence. If the second condition is fulfilled, the sequence has led to a cycle. For every starting value, except $v_1 = 1$, the Collatz conjecture is therefore falsified. Let us consider the example $v_1 = 13$ and $n = 2$. Inserting these values into theorem 2.1 yields:

$$v_{n+1} = 3^2 \cdot \left(1 + \frac{1}{3 \cdot 13}\right)\left(1 + \frac{1}{3 \cdot 5}\right) \cdot 2^{-7} = 1$$

In the above example the algorithm halts after two iterations because the first condition is fulfilled. If we examine the case $v_1 = 1$, we realize that the algorithm finishes after the first iteration, since both halting conditions are true:

$$v_{n+1} = v_1 = 3^1 \cdot 1 \cdot \left(1 + \frac{1}{3 \cdot 1}\right) 2^{-2} = 1$$

The sequence stops in the example above due to the result being one. Apart from that, the sequence has led to a cycle.

Theorem 2.1 can be used for specifying the condition of a cycle as follows:

$$\begin{aligned}
v_1 &= 3^n v_1 \prod_{i=1}^{n} \left(1 + \tfrac{1}{3v_i}\right) 2^{-\alpha_i} \\
2^{\alpha_1 + \cdots + \alpha_n} &= \prod_{i=1}^{n} \left(3 + \tfrac{1}{v_i}\right)
\end{aligned} \tag{2.2}$$

A similar condition has been formulated by Hercher [60] and Eric Roosendaal [61]. Taking a first look at equation 2.2, we are able to recognize the trivial cycle for $n = 1$. One might easily come to the false conclusion that the term only results in a natural number for this trivial cycle, since we are multiplying fractions. The following counterexample, starting at $v_1 = 31$, disproves this assumption:

$$20480 = \left(3 + \frac{1}{31}\right)\left(3 + \frac{1}{47}\right)\left(3 + \frac{1}{71}\right)\left(3 + \frac{1}{107}\right)\left(3 + \frac{1}{161}\right)\left(3 + \frac{1}{121}\right)\left(3 + \frac{1}{91}\right)\left(3 + \frac{1}{137}\right)\left(3 + \frac{1}{103}\right)$$

According to OESIS [62], the integer $v_1 = 31$ is called *self-contained*. The term self-contained is based on the fact that the node $v_{n+1} = v_{10} = 155$ is divisible by the starting node $v_1 = 31$. Moreover, v_{10} results from applying one and the same function (in this case the Collatz function) using v_1 as input, see also Guy [63, p. 332]. For such a case equation 2.2 leads to a natural number, but not necessarily to a cycle. A cycle only occurs if the term results in a power of two. One such example is the trivial cycle. We find another case when we choose the factor 5 instead of 3:

$$128 = 2^7 = \left(5 + \tfrac{1}{13}\right)\left(5 + \tfrac{1}{33}\right)\left(5 + \tfrac{1}{83}\right)$$

The above example demonstrates that non-trivial cycles can be found if we generalize the Collatz conjecture by replacing the factor 3 with the variable k. We study this generalized form and the occurrence of cycles in section 4.1. A detailed elaboration of the divisibility and a deeper understanding of the tree $H_{C,3}$ needs to be performed in order to achieve a proof of the Collatz conjecture.

Generally, for any variant $kx + 1$ it applies that if $v_1 \mid v_{n+1}$, the product $\prod_{i=1}^{n} \left(k + {}^{1}/_{v_i}\right)$ is natural.

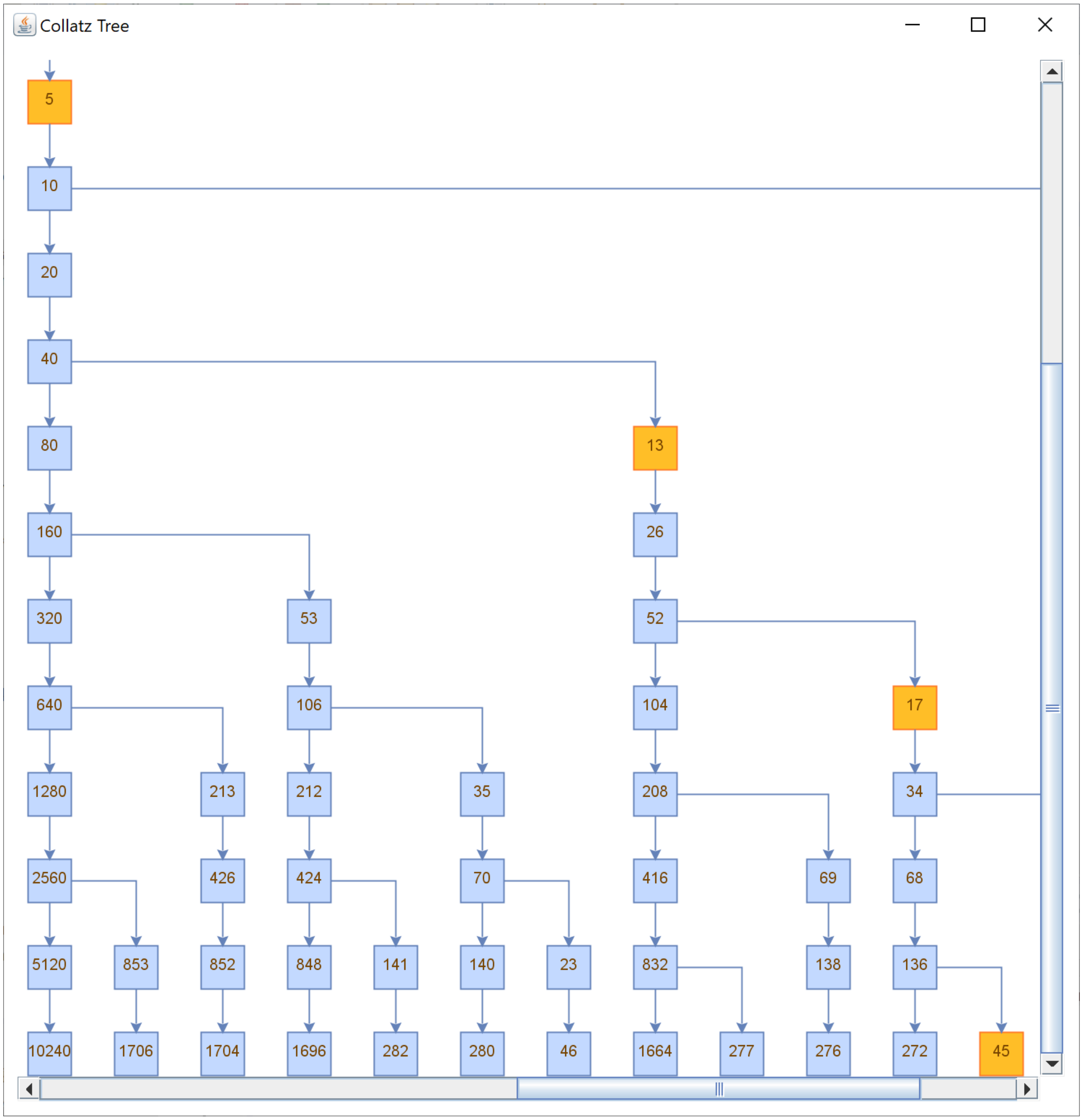

Figure 2.3: Section of H_U containing the path from 5 to 45

2.4 A note on the functions left-child and right-sibling

Referring to the "left-child, right-sibling representation" of rooted trees [64, p. 246], the function *left-child* : $V \to V$ returns the leftmost child of a vertex v. Nesting this function n times leads to the definition of a vertex's n-fold left-child, which is given by $\textit{left-child}^n(v)$. As delineated in figure 2.2, for example $\textit{left-child}^3(13) = 7$.

The function *right-sibling* : $V \to V$ points to the sibling of a vertex v immediately to its right [64, p. 246]. If this function is nested n times, we get a vertex's n-fold right-sibling defined by $\textit{right-sibling}^n(v)$. One example is $\textit{right-sibling}^2(113) = 1813$ which has been demonstrated in figure 2.2 too.

2.5 Relationship of sibling nodes in $H_{C,3}$

In a rooted tree, vertices which have the same parent are called "siblings" [39, p. 702], [45, p. 747]. Sibling vertices accordingly have the same depth and thus the same level.

Let w be a vertex, from which a path exists to the vertex v_1. Let v_2 be the immediate right-sibling of v_1, then $l_{V(H_{C,3})}(v_2) = 4 \cdot l_{V(H_{C,3})}(v_1) + 1$. This fact has been expressed differently by Kak [21] as follows: "If an odd number a leads to another odd number (after several applications of the Collatz transformation) b, then $4a + 1$ also leads to b."

Applied to our approach, consider w as the parent of v_1 and v_2. Suppose, in H_U, a path consisting of $n+1$ edges goes from w to v_1. Then we can straightforwardly show that n edges in H_U have been contracted between both nodes w and v_1 and $n+2$ edges between w and v_2 (for simplicity we again omit writing the label function):

$$\begin{aligned} v_1 &= \tfrac{w \cdot 2^n - 1}{3} \\ v_2 &= \tfrac{w \cdot 2^{n+2} - 1}{3} = 4 \cdot v_1 + 1 \end{aligned} \tag{2.3}$$

For example, $n = 3$ edges in H_U have been contracted between $w = 5$ and $v_1 = 13$ and $n + 2 = 5$ edges between w and $v_2 = 53$, whereby in $H_{C,3}$, the vertex v_2 is the right-sibling of v_1 and these two sibling vertices are immediate children of w.

Batang [58] demonstrated that using the geometric series $s_n = 1 + 4 + 4^2 + \ldots + 4^{n-1} = {}^{4^n-1}/_3$ we are able to directly calculate the sibling nodes (see [65, p. 191-192] for more details on geometric series). Let us consider the sibling nodes $\{5, 21, 85, 341\}$. The first sibling of 5 is calculated by $s_1 + 4^1 \cdot 5 = 21$, the second sibling is $s_2 + 4^2 \cdot 5 = 85$, and the third is $s_3 + 4^3 \cdot 5 = 341$.

The same principle applies to the siblings $\{13, 53, 213, 853\}$. The first sibling of 13 is calculated by $s_1 + 4^1 \cdot 13 = 53$, the next one is $s_2 + 4^2 \cdot 13 = 213$, and the third is $s_3 + 4^3 \cdot 13 = 853$.

2.6 A vertex's left-child, n-fold right-sibling in $H_{C,3}$

Let w be a vertex in $H_{C,3}$ and v_0 the left-child of w. Using techniques of data science [1], we have found out empirically that the n-fold right-sibling of v_0 can be calculated as follows:

$$v_n = \textit{right-sibling}^n(v_0) = \frac{1}{3}\left(w \cdot 2^{2n + \pi_3(w \bmod 3)} - 1\right) \tag{2.4}$$

Here the function π_3, which appears in the exponent, is the self-inverse permutation (involution):

$$\pi_3 = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \tag{2.5}$$

We consider permutations of the set $\{1, 2\}$ and not of $\{0, 1, 2\}$, due to the fact that $w \bmod 3$ cannot be zero. A node w in $H_{C,3}$, which is labeled by an integer divisible by 3 is a leaf; and therefore such node has no left-child. More specifically, it has no children at all. When setting $n = 0$, we trivially retrieve the vertex's w left-child:

$$v_0 = \textit{left-child}(w) = \tfrac{1}{3}\left(w \cdot 2^{\pi_3(w \bmod 3)} - 1\right)$$

Example 2.2 Let us refer to figure 2.2 again and pick out $w = 5$. Then the vertex's w left-child is $v_0 = 3$ and the threefold right-sibling $v_3 = 213$:

$$v_0 = \frac{1}{3}\left(5 \cdot 2^{\pi_3(5 \bmod 3)} - 1\right) = 3$$
$$v_3 = \frac{1}{3}\left(5 \cdot 2^{2\cdot 3+\pi_3(5 \bmod 3)} - 1\right) = 213$$

We will now explain the reasons that are underlying this behavior. Essentially, two integers a and b are congruent modulo n if their difference $a-b$ is divisible by n or, to put it differently, if a and b have the same remainder when divided by n [66, p. 15], [67, p. 44], [68, p. 19], [69, p. 142]:

$$n|(a-b) \leftrightarrow a \equiv b \pmod{n} \tag{2.6}$$

In modular arithmetic we are allowed to interpret integers as names, or to be more specific as *representatives*, for their equivalence class and therefore reduce (or expand) a congruence as follows:

$$(a+n) \equiv b \pmod{n} \leftrightarrow a \equiv b \pmod{n} \tag{2.7}$$

This means, that in modular arithmetic both operations – addition and multiplication – are independent from the choice of representatives in the residue classes [66, p. 16].

The residue class (also termed congruence class) of the integers for a modulus n is the set $[a]_n = \{a+k\cdot n | k \in \mathbb{Z}\}$ and sometimes denoted by $\bar{a}_n$ or by $a+n\mathbb{Z}$, see [66, p. 15], [70, p. 122], [68, p. 25], [69, p. 141]. Let us put all possible remainders that arise from the division modulo n together into a new set – the set of all residue classes $[a]_n$. This set is known as the ring of integers modulo n and denoted by $\mathbb{Z}/n\mathbb{Z} = \{[a]_n | a \in \mathbb{Z}\}$ and trivially $\mathbb{Z}/0\mathbb{Z} = \mathbb{Z}$ and for all $n \neq 0$ we have $\mathbb{Z}/n\mathbb{Z} = \{[0],[1],\ldots,[n-1]\}$, see [66, p. 15], [68, p. 25], [65, p. 81].

Now there is one more tool that we will make use of later, and that is the *Congruence Power Rule (CPR)*. It states that we are allowed to raise both sides of a congruence to the m-th power [68, p. 19], [71, p. 117]:

$$a \equiv b \pmod{n} \leftrightarrow a^m \equiv b^m \pmod{n} \tag{2.8}$$

Let G be a group and $a \in G$. If there exists an integer $d > 0$ with $a^d = e$, then the smallest such d is called the *order* of a, written $d = \mathrm{ord}(a)$ [66, p. 35], [67, p. 50], [72, p. 240]. If no such d exists, we formally write $\mathrm{ord}(a) = \infty$. The number of elements of G is called the *order* of G, written $\mathrm{ord}(G)$ [66, p. 26], [67, p. 50].

Let G be a group and $a \in G$ an element of G. We consider the set of all elements $a^n \in G$ with $n \in \mathbb{Z}$. Since $a^n a^m = a^{n+m} = a^m a^n$ and $(a^n)^{-1} = a^{-n}$, this set forms an abelian subgroup H_a of G. This subgroup H_a is also written $\langle a \rangle$ and called the subgroup of G *generated* by a [67, p. 50]. A group G is called *cyclic*, if an $a \in G$ exists so that G consists only of powers of a (with exponents in $\mathbb{Z}$), thus if $G = \langle a \rangle$ [66, p. 34], [67, p. 50], [72, p. 240]. In this case $\mathrm{ord}(a) = \mathrm{ord}(G)$, id est the order of an element $a \in G$ is equal to the order of the cyclic subgroup $\langle a \rangle$ [67, p. 50].

Let us consider the cyclic group $\langle a \rangle = \{e, a, a^2, \ldots, a^{n-1}\}$ and an element $b \in \langle a \rangle$. Now let us face the question, "How do we find the unique integer $0 \leq j \leq n-1$, such that $a^j = b$?" This integer j is denoted by $j = log_a b$ and it is called the *discrete logarithm* of b [73, p. 255-256]. To make it more clear that we are talking about the discrete logarithm we write $j = \mathrm{dlog}_a\, b$ or more specifically $j = \mathrm{dlog}_{a,k}\, b$ if we solve the congruence $a^j \equiv b \pmod{k}$ which means we solve the equation $a^j \bmod k = b$, see [74].

The multiplicative group of integers modulo n, denoted as $(\mathbb{Z}/n\mathbb{Z})^{\times}$ or briefly as $\mathbb{Z}_n^*$ contains non-negative elements from $\mathbb{Z}/n\mathbb{Z}$ whose representatives are coprime to n [65, p. 87]:

$$Z_n^* = \{a \in \mathbb{Z}/n\mathbb{Z} | \gcd(a,n) = 1\} \tag{2.9}$$

This group $\mathbb{Z}_n^*$ is a finite abelian group, which contains only the elements from the ring $\mathbb{Z}/n\mathbb{Z}$ that are invertible with respect to multiplication – the units of $\mathbb{Z}/n\mathbb{Z}$. That is why the group $\mathbb{Z}_n^*$ is often denoted by $U(n)$, where U stands for units. Within the ring $\mathbb{Z}/n\mathbb{Z}$ an element a is invertible exactly if there exists an element b such that $a * b \equiv 1 \pmod{n}$. An element inverse to a exists exactly if $\gcd(a,n) = 1$.

The *multiplicative order* $\mathrm{ord}(a)$ of an element $a \in \mathbb{Z}_n^*$ is the smallest natural exponent d which satisfies $a^d = 1$. In other words, for a positive integer n we say that an integer a has multiplicative order d modulo n if $a^d \equiv 1 \pmod{n}$ where again d is the smallest possible exponent [75, p. 76], [76, p. 32]. To indicate that the order of a refers to the modulus n, it is also often written $d = \mathrm{ord}_n(a)$. Recall that $\gcd(a,n) = 1$, since $a \in \mathbb{Z}_n^*$

We remember that groups also have an order. The order of a multiplicative group of integers modulo n is given precisely by *Euler's totient function*, see [66, p. 27]:

$$\mathrm{ord}(\mathbb{Z}_n^*) = \phi(n) \tag{2.10}$$

Euler's totient function $\phi(n)$ counts the positive integers up to a given integer n that are coprime to n [67, p. 49]. The fact that equation 2.10 is correct follows directly from the definition of $\phi(n)$ – we include into $\mathbb{Z}_n^*$ exactly those integers (representatives) from $\mathbb{Z}/n\mathbb{Z}$ that are coprime to n.

The elements of the ring of integers modulo n do not form a group with respect to multiplication, because the element 0 can not be inverted. But also $\mathbb{Z}/n\mathbb{Z} \setminus \{0\}$ does not form a group for a composite n, since there are always products of elements $a \neq 0, b \neq 0$ with $a * b = 0$, which means that the "closure" property is not given [77].

An important theorem related to Euler's totient function, which we will use at a later stage, is Euler's theorem. Euler's theorem states that for an integer $a \geq 2$ coprime to the modulus n the following congruence holds [68, p. 37], [67, p. 56], [65, p. 104]:

$$a^{\phi(n)} \equiv 1 \pmod{n} \tag{2.11}$$

This means that given $\langle a \rangle = \mathbb{Z}_n^*$, for any generator a coprime to the modulus n the congruence $a^{\phi(n)} \equiv 1 \pmod{n}$ becomes true, where again $\phi(n)$ is the order of $\mathbb{Z}_n^*$ and thus the order of a (see 2.10). If $\phi(n) \equiv 2 \pmod{4}$ then the group $\mathbb{Z}_n^*$ is cyclic. Consequently the multiplicative group of integers modulo n is cyclic for $n \in \{1, 2, 4, p^j, 2p^j\}$, where p being an odd prime and $j \geq 1$ [77], [78, p. 172], [79].

At this point it is appropriate that we explain the mapping (permutation) given by 2.5 in more detail. A helpful tool that we can use as a point of departure is the multiplicative group of integers modulo 3. The element 2 is a generator $\langle 2 \rangle = \{1, 2\} = \mathbb{Z}_3^*$, since $2 \equiv \mathbf{2} \pmod{3}$ and $2^2 \equiv 4 \equiv \mathbf{1} \pmod{3}$. The order of 2 is 2, since $2^2 \equiv 1 \pmod{3}$. Now we use the CPR given by 2.8 and obtain $(2^2)^{n+1} \equiv 1^{n+1} \pmod{3}$ and the following generic congruence:

$$2^j 2^{2n+2-j} \equiv 1 \pmod{3} \tag{2.12}$$

Setting $j = 0, 1$ leads to the following behavior, which explains the formula 2.4 and the mapping 2.5:

j	**congruence** 2.12	**node** w	**setting** w **as per** 2.7	**divisibility as per** 2.6
0	$1 \cdot 2^{2n+2} \equiv 1$	$w \in [1]_3$	$w \cdot 2^{2n+\pi_3(w \bmod 3)} \equiv 1$	$3 \mid (w \cdot 2^{2n+\pi_3(w \bmod 3)} - 1)$
1	$2 \cdot 2^{2n+1} \equiv 1$	$w \in [2]_3$		

If addition is the group operation, as it is the case for example with the additive group of integers modulo 3, denoted as $(\mathbb{Z}/3\mathbb{Z},+)$ or as $(\mathbb{Z}_3,+)$, then for an element a the term a^n means add (and not multiply) a to itself n times. In this specific case the group contains three elements $\mathbb{Z}_3 = \{0,1,2\}$ and the identity element is $e = 0$. The element 2 is a generator $\langle 2 \rangle = \{0,1,2\} = \mathbb{Z}_3$, since $2 \equiv \mathbf{2} \pmod 3$ and $2+2 \equiv 4 \equiv \mathbf{1} \pmod 3$ and $2+2+2 \equiv 6 \equiv \mathbf{0} \pmod 3$. The order of 2 is 3, because $2^3 \equiv 0 \pmod 3$.

2.7 A vertex's left-child, n-fold right-sibling in $H_{C,5}$

In the following we take a look at the tree $H_{C,5}$ – the $5x+1$ variant of H_C. We must note that it is not a tree and moreover that not all of its vertices are reachable from the root, which makes it particularly interesting as a counterexample. We define the permutation π_5 as follows:

$$\pi_5 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 4 & 3 & 1 & 2 \end{pmatrix}$$

Next, by letting w be a vertex in $H_{C,5}$ and v_0 the left-child of w we obtain the n-fold right-sibling of v_0 by the function that is slightly different to the one defined by 2.4:

$$v_n = \textit{right-sibling}^n(v_0) = \frac{1}{5}\left(w \cdot 2^{4n+\pi_5(w \bmod 5)} - 1\right) \tag{2.13}$$

Analogous to 2.5 only permutations on the set without zero {1,2,3,4} need to be considered, since $w \bmod 5$ cannot be zero. Otherwise, if $w \equiv 0 (\bmod 5)$ which means that w would be labeled by an integer divisible by 5, then the node w has no successor in $H_{C,5}$.
By setting $n = 0$, the function (above given by 2.13) returns the left child of w:

$$v_0 = \textit{left-child}(w) = \tfrac{1}{5}\left(w \cdot 2^{\pi_5(w \bmod 5)} - 1\right)$$

Equation 2.13 has been identified empirically as well and can be explained using the cyclic group $\langle 2 \rangle = \{1,2,3,4\} = \mathbb{Z}_5^*$. First of all, it is obvious that 2 generates this group, since $2 \equiv \mathbf{2} \pmod 5$ and $2^2 \equiv \mathbf{4} \pmod 5$ and $2^3 \equiv 8 \equiv \mathbf{3} \pmod 5$ and $2^4 \equiv 16 \equiv \mathbf{1} \pmod 5$. The order is 4 and according to 2.11 and 2.10 we have $2^{\operatorname{ord}(\mathbb{Z}_5^*)} \equiv 2^{\phi(5)} \equiv 2^4 \equiv 1 \pmod 5$. Again we use the CPR given by 2.8 and obtain $(2^4)^{n+1} \equiv 1^{n+1} \pmod 5$ and the following generic congruence:

$$2^j 2^{4n+4-j} \equiv 1 \pmod 5 \tag{2.14}$$

Setting $j = 0,1,2,3$ leads to the following behavior, which explains the formula 2.13 and the mapping 2.7:

j	**congruence** 2.14	**node** w	**setting** w **as per** 2.7	**divisibility as per** 2.6
0	$1 \cdot 2^{4n+4} \equiv 1$	$w \in [1]_5$	$w \cdot 2^{4n+\pi_5(w \bmod 5)} \equiv 1$	$5 \mid (w \cdot 2^{4n+\pi_5(w \bmod 5)} - 1)$
1	$2 \cdot 2^{4n+3} \equiv 1$	$w \in [2]_5$		
2	$4 \cdot 2^{4n+2} \equiv 1$	$w \in [4]_5$		
3	$8 \cdot 2^{4n+1} \equiv 1$	$w \in [3]_5$		

Figure 2.4 illustrates a small section of $H_{C,5}$ starting at its root. The particularly interesting thing about the graph $H_{C,5}$ is that it contains three cycles, the trivial cycle starting from the root $(1,3)$ and two non-trivial cycles $(43,17,27)$ and $(83,33,13)$. To be precise, three cycles are known (as it will become apparent later in section 4.2), and on the basis of present knowledge it cannot be ruled out with any certainty that other cycles exist.

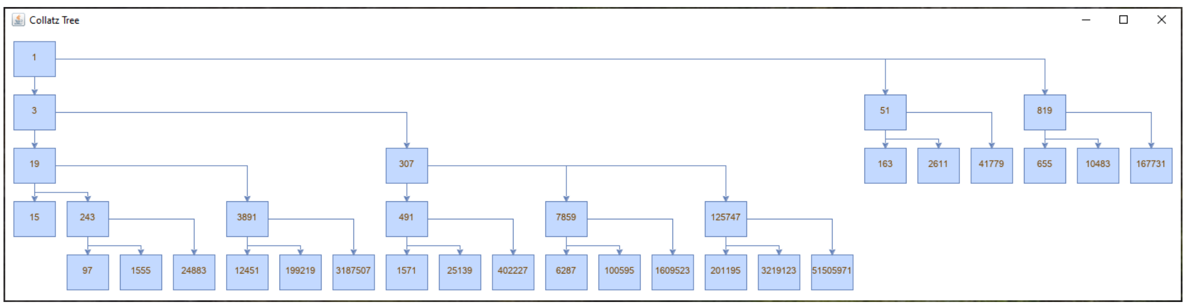

Figure 2.4: Section of the graph $H_{C,5}$ starting at its root (without branches that reflect a subsequence containing the trivial cycle)

2.8 A vertex's left-child, n-fold right-sibling in $H_{C,7}$

Now we are able to develop the formula deductively that calculates for a given node w the left-child and right-sibling in $H_{C,7}$. We refer to the cyclic group $\mathbb{Z}_7^* = \{1,2,3,4,5,6\}$. Note that in this case 2 is not a generator of this group. But nevertheless $\mathbb{Z}_7^*$ is cyclic and $\text{ord}(2) = 3$ which gives $2^3 \equiv 1 \pmod 7$. Again we use the CPR given by 2.8 and obtain $(2^3)^{n+1} \equiv 1^{n+1} \pmod 7$ and the following generic congruence:

$$2^j 2^{3n+3-j} \equiv 1 \pmod 7 \tag{2.15}$$

Setting $j = 0,1,2$ leads to the following behavior, which produces formula 2.16 and the mapping 2.17:

j	**congruence** 2.15	**node** w	**setting** w **as per** 2.7	**divisibility as per** 2.6
0	$1 \cdot 2^{3n+3} \equiv 1$	$w \in [1]_7$	$w \cdot 2^{3n+\pi_7(w \bmod 7)} \equiv 1$	$7 \mid (w \cdot 2^{3n+\pi_7(w \bmod 7)} - 1)$
1	$2 \cdot 2^{3n+2} \equiv 1$	$w \in [2]_7$		
2	$4 \cdot 2^{3n+1} \equiv 1$	$w \in [4]_7$		

$$v_n = right\text{-}sibling^n(v_0) = \frac{1}{7}\left(w \cdot 2^{3n+\pi_7(w \bmod 7)} - 1\right) \tag{2.16}$$

The mapping 2.17 is not a permutation as in the case of π_3 and π_5, it is defined as follows:

$$\pi_7(n) = \begin{cases} 3 & n = 1 \\ 2 & n = 2 \\ 1 & n = 4 \end{cases} \tag{2.17}$$

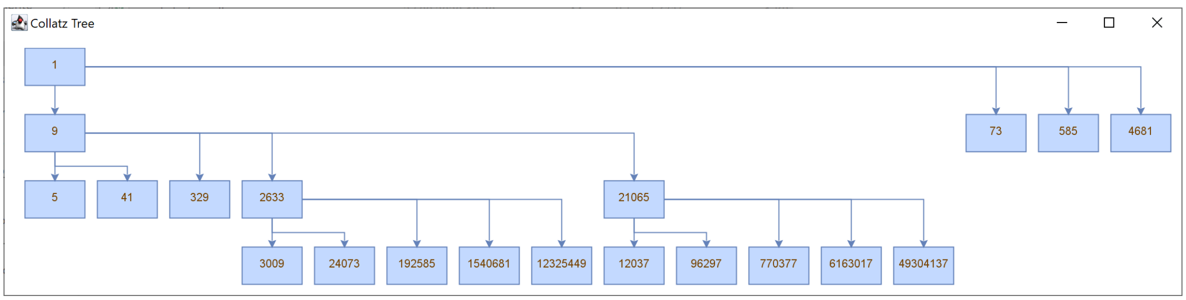

Figure 2.5: Section of the graph $H_{C,7}$ starting at its root (without branches that reflect a subsequence containing the trivial cycle)

2.9 Generalizing the relationship of successive nodes for $H_{C,k}$

Let us refer to $H_{C,k}$. By having introduced and proven theorem 2.1 we already started an assertion about the reachability of successive nodes in $H_{C,3}$. This reachability relationship can be generalized for any graph $H_{C,k}$ as follows:

$$v_{n+1} = k^n v_1 \prod_{i=1}^{n} \left(1 + \frac{1}{kv_i}\right) 2^{-\alpha_i} \tag{2.18}$$

This generalization will be later utilized in chapter 4 for closer observations of cycles in various $kx+1$ variants of the graph H_C.

2.10 Generalizing the relationship of sibling nodes for $H_{C,k}$

In section 2.5 we have taken a closer look at the relationship of sibling nodes in $H_{C,3}$. But what is the formula for calculating the n-fold right-sibling of a given node v_0 generalized to the $kx+1$ variant of H_C? We remember that the multiplicative order $d = \mathrm{ord}_k(2)$ is the smallest natural exponent d such that $2^d \equiv 1 \pmod{k}$. In the case $k=3$ we can calculate the next sibling v_1 of a given node v_0 as follows: $v_1 = v_0 \cdot 4 + 1$, see 2.3. Within $H_{C,7}$, the next sibling of v_0 is given by $v_1 = v_0 \cdot 8 + 1$. In the case of $k=5$, we calculate the next sibling $v_1 = v_0 \cdot 16 + 3$ and for $k=9$ we obtain the next sibling v_1 of a given node v_0 by $v_1 = v_0 \cdot 64 + 7$. The general formula for calculating a given node's v_0 immediate right sibling is:

$$v_1 = v_0 \cdot 2^{\mathrm{ord}_k(2)} + \frac{1}{k}\left(2^{\mathrm{ord}_k(2)} - 1\right) \tag{2.19}$$

For example the node $v_0 = 243$ in $H_{C,5}$ has the right sibling $v_1 = 243 \cdot 2^4 + (2^4 - 1)/5 = 3891$ (see figure 2.4). In order to calculate the n-fold right sibling of a given node v_0, we need to repeatedly nest n times the (linear) function 2.19. For the sake of simplicity, let us substitute $a = 2^{\mathrm{ord}_k(2)}$ and $b = \frac{1}{k}(2^{\mathrm{ord}_k(2)} - 1)$. Then the n-fold right sibling of v_0 is obtained by the following structure:

$$\begin{aligned} v_n = \textit{right-sibling}^n(v_0) &= (((v_0 \cdot a + b) \cdot a + b) \cdot a + b) \cdots \\ &= v_0 \cdot a^n + b(a^{n-1} + \ldots + a^2 + a + 1) = v_0 \cdot a^n + b\frac{a^n - 1}{a - 1} \end{aligned}$$

Note that the term $b(a^{n-1} + \ldots + a^2 + a + 1)$ can be simplified using the n-th partial sum of a geometric series ([65, p. 192]). The resubstitution of both coefficients a and b leads us to the final generalized formula that calculates the n-fold right sibling of a node v_0 in $H_{C,k}$ for a natural $n \geq 0$:

$$v_n = \textit{right-sibling}^n(v_0) = v_0 \cdot 2^{n \cdot \mathrm{ord}_k(2)} + \frac{1}{k}\left(2^{\mathrm{ord}_k(2)} - 1\right) \cdot \frac{2^{n \cdot \mathrm{ord}_k(2)} - 1}{2^{\mathrm{ord}_k(2)} - 1} \tag{2.20}$$

This can be verified by inserting $n=0$ and $n=1$ into formula 2.21 that calculates the a vertex's left-child, n-fold right-sibling of $H_{C,k}$:

$$\begin{aligned} v_0 &= \tfrac{1}{k}\left(w \cdot 2^{\mathrm{ord}_k(2) - \mathrm{dlog}_{2,k} w} - 1\right) & kv_0 + 1 &= w \cdot 2^{\mathrm{ord}_k(2) - \mathrm{dlog}_{2,k} w} \\ v_1 &= \tfrac{1}{k}\left(w \cdot 2^{2\,\mathrm{ord}_k(2) - \mathrm{dlog}_{2,k} w} - 1\right) & kv_1 + 1 &= w \cdot 2^{2\,\mathrm{ord}_k(2) - \mathrm{dlog}_{2,k} w} \end{aligned}$$

This brings us to the following quotient leading to the basic relationship between two sibling nodes that is given by equation 2.19 in the form of $v_1 = v_0 \cdot a + b$:

$$\frac{kv_1 + 1}{kv_0 + 1} = \frac{2^{2\,\mathrm{ord}_k(2) - \mathrm{dlog}_{2,k} w}}{2^{\mathrm{ord}_k(2) - \mathrm{dlog}_{2,k} w}} = 2^{\mathrm{ord}_k(2)}$$

Here we point out that the equation 2.20 of course only works for such k, where the order of two is not infinity $\mathrm{ord}_k(2) \neq \infty$. This means that, for instance, it does not work for $k=1$, id est for the $1x+1$ variant of H_C. This variant is very instructive due to its simple nature and for the sake of completeness we have added a picture including some few words about $H_{C,1}$ in appendix A.1.

2.11 Generalizing a vertex's left-child, n-fold right-sibling for $H_{C,k}$

Let $n \geq 0$ be an integer. We generalize the formulas, which have been developed in sections 2.6 - 2.8 to calculate the left-child, n-fold right-sibling for a given node w that is the direct parent node of v_0 as follows:

$$v_n = \textit{right-sibling}^n(v_0) = \frac{1}{k}\left(w \cdot 2^{\operatorname{ord}_k(2)\cdot n + \operatorname{ord}_k(2) - \operatorname{dlog}_{2,k} w} - 1\right) \tag{2.21}$$

To put the procedure of computation a bit simpler: We start at an arbitrary parent node w, calculate its left-child v_0 and then determine the n-fold right-sibling (the n-th neighbor from the right) of v_0. Let us choose for example the node $w = 2633$ from $H_{C,7}$, whose left child is $v_0 = 3009$. The fourth right-sibling of this left-child is $v_4 = (2633 \cdot 2^{3\cdot 4+3-0} - 1)/7 = 12325449$ (see figure 2.5).

Recall that the discrete logarithm $\operatorname{dlog}_{2,k} w = j$ finds the smallest exponent j such that $2^j \equiv w \pmod{k}$ respectively solves the equation $2^j \bmod k = w$.

3. Binary Collatz Tree

3.1 Some essentials on binary trees

A binary tree is a rooted tree, where each node has at most two immediate successors. Those nodes, from which no edge goes out downward, are called leaves, the others are called internal nodes. In a full binary tree, all internal nodes have exactly two children [80, p. 102]. Full binary trees have an odd number $2n+1$ of nodes. Of these $n+1$ are leaves and n are inner nodes [81, p. 134]. Each node in a binary tree has a left subtree and a right subtree, which is why a binary tree is inherently recursive, since the left and right subtrees of the root are themselves binary trees [82, p. 246-247]. As it often pops up in combinatorial problems, the famous n-th Catalan number, named after the Belgian mathematician Eugène Catalan, comes in connection with binary trees into play. For $n \geq 1$ it specifies the number of binary trees on n vertices [82, p. 247]:

$$B_n = \sum_{i=0}^{n-1} B_i B_{n-1-i} = \sum_{i=1}^{n} B_{i-1} B_{n-i} = \frac{1}{n+1}\binom{2n}{n}$$

There is an interesting property that trees exhibit regarding abstract algebra. Let's have a look at the algebraic structure of magmas. Consider an element x of a magma $(M,*)$ which is an iterated product of other elements in M. Such an element can be described by a planar (no edges cross each other) rooted binary tree whose n leaves are labelled by these other elements $x_1,\ldots,x_n \in M$ [83, p. 96].

Binary trees make well-suited data structures for storing information. With about 2^m data points (nodes), a search of a binary tree takes only about m steps, compared to about 2^{m-1} steps which are required to search a simple list [71, p. 84].

3.2 Transforming the Collatz tree into a binary tree

Jan Kleinnijenhuis and Alissa M. Kleinnijenhuis [53] introduced a binary tree $T_{\geq 0}$ by transforming the original Collatz tree H_U into the Syracuse tree $H_{C,3}$, which in turn is transformed into the binary tree $T_{\geq 0}$ as described next. The edges are changed according to the following procedure: whenever a parent node w has edges to its child nodes $v_0, v_1, \ldots, v_n$, on the tree $H_{C,3}$, we draw an edge from w to v_0, and edges from v_i to v_{i+1} for each $i = 1,\ldots,n-1$, in the binary new tree. Note that the nodes $v_1, v_2, \ldots, v_n$ are sorted in increasing order of label $v_0 < v_1 < \ldots < v_n$, which is already given by 2.20. Figure 3.1 and 3.2 display that tree – once in our standard layout and once reversed (from bottom to top).

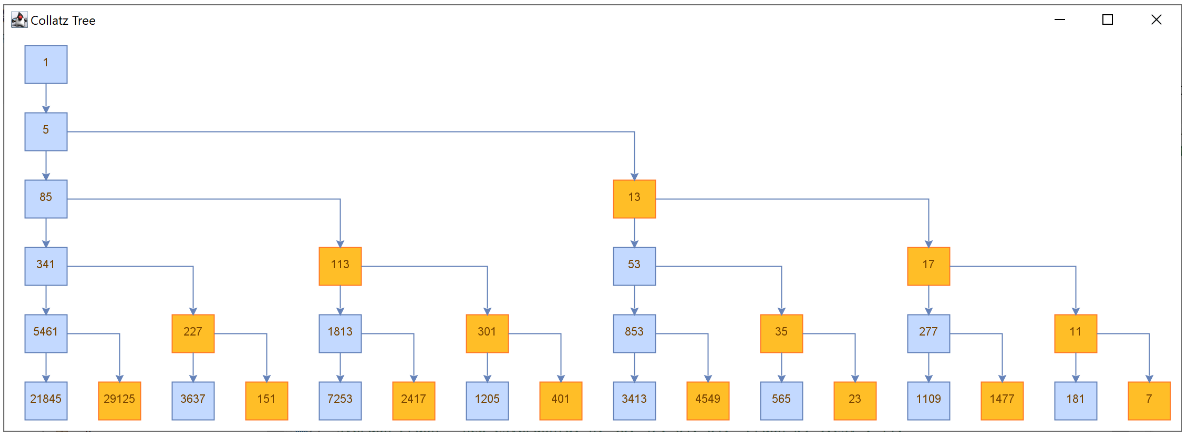

Figure 3.1: The Collatz Tree transformed to the binary tree $T_{\geq 0}$

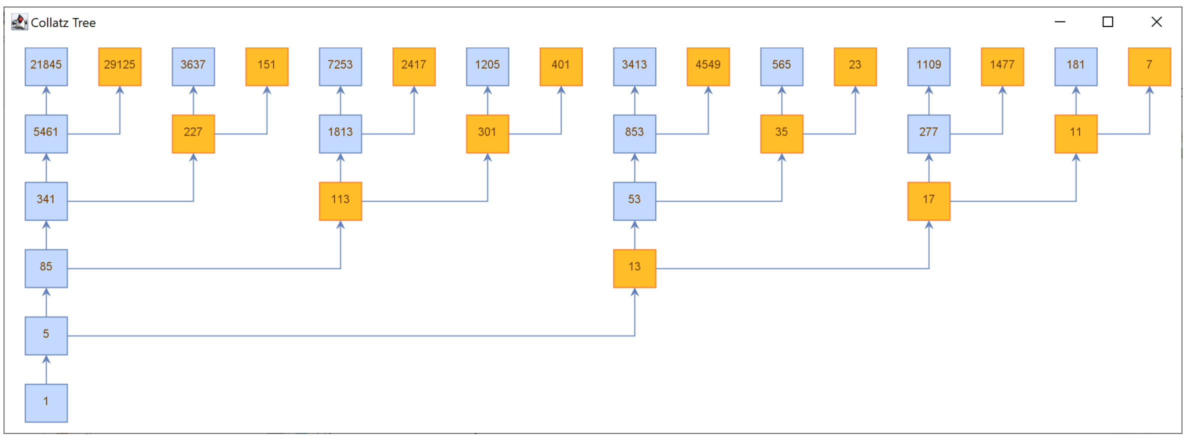

Figure 3.2: The binary tree $T_{\geq 0}$ with *bottom-to-top* layout orientation

To clarify the terminology, it should be mentioned that Jan and Alissa M. Kleinnijenhuis in their manuscripts [53], [59] denote the original Collatz tree T_C while we call it H_U. They denote the Syracuse Tree T_T which in our nomenclature is referred to as $H_{C,3}$.

Nodes that are highlighted orange in figures 3.1, 3.2 are called *prunable* and they are exactly those nodes resulting as output of the *Rightward* function. For navigating within this binary tree, Jan Kleinnijenhuis and Alissa M. Kleinnijenhuis [53] defined an *Upward* function $U(n)$ and a *Rightward* function $R(n)$ as follows:

$$U(n) = \begin{cases} 4n+1 & n \equiv 1 \pmod 6 \\ 16n+5 & n \equiv 5 \pmod 6 \end{cases} \qquad R(n) = \begin{cases} (2^2n-1)/3 & n \in [1]_{18} \cup [13]_{18} \\ (2^3n-1)/3 & n \in [5]_{18} \\ (2^4n-1)/3 & n \in [7]_{18} \\ (2^1n-1)/3 & n \in [11]_{18} \cup [17]_{18} \end{cases} \tag{3.1}$$

The domain and codomain of both functions consist of the two residue classes $[1]_6, [5]_6$, which form the multiplicative (cyclic) group $\mathbb{Z}_6^* = \{1,5\} = \langle 5 \rangle$. Consequently, the domain and codomain exclude all integers divisible by 2 and 3, which is due to the fact that this binary tree (just like our tree $H_{C,3}$) does not contain even numbers and additionally all leaves – namely those nodes labeled with an integer divisible by three – were deleted. The function $U(n)$ is very similar to the function 2.3 and to the more general function 2.20 (when setting $n = 1, k = 3$) which both calculate the right-sibling of a given vertex. This is clear, since siblings (parallel) in $H_{C,3}$ are successors (serial) in the binary tree $T_{\geq 0}$. In the end, for a node v_0 having a leaf as right-sibling in $H_{C,3}$, the function $U(v_0)$ is defined as $v_1 = 4v_0 + 1$ executed twice $v_1 = 4(4v_0 + 1) + 1 = 16v_0 + 5$, because we must skip this leaf. Recall that all leafs in $H_{C,3}$ are excluded from the binary tree without exception. For any $n \in [5]_6$ it applies that $U(n) \equiv 16n + 5 \equiv \mathbf{1} \bmod (6)$ since $6 \mid 16n + 5 - \mathbf{1}$ resulting in $6 \mid 16(5 + k \cdot 6) + 5 - \mathbf{1}$, see 2.6, and analogously for any $n \in [1]_6$ it applies that $U(n) \equiv 4n + 1 \equiv \mathbf{5} \bmod (6)$ since $6 \mid 4n + 1 - \mathbf{5}$ resulting in $6 \mid 4(1 + k \cdot 6) + 1 - \mathbf{5}$. Therefore executing the Upward function twice in a row leads unconditionally to $U^2(n) = 16(4n + 1) + 5 = 4(16n + 5) + 1 = 64n + 21$.

While we displayed trees from top to down, it is sometimes usual to draw trees in a bottom-to-top fashion as Kleinnijenhuis [59] do. The Rightward function corresponds to what we call left-child and the Upward function relates to the right-child which is commonly used in the context of binary trees [82, p. 246].

Jan and Alissa M. Kleinnijenhuis [53] defined the set $N(T_C) = N(H_U)$ that contains the labels of all nodes, to which a path from the root in H_U exists, in other words, this set contains all integers n for which the orbit of n under the (uncompressed) Collatz function 1.1 converges to 1. Furthermore they introduced $S_{\geq 0}$ as the node set containing integers that are neither divisible by 2 nor by 3. The set S_{-1} comprises on the contrary all numbers, which are divisible by 2 or 3. In order to comprehend the structure of these sets S, let us take a look at the following list showing which tree includes which node set, see also the ancillary files of [53], [59]:

Original Collatz tree	$N(T_C) = N(H_U)$	$=$	$\mathbb{N}^+$ if the Collatz conjecture holds	
Syracuse tree	$N(T_T) = N(H_{C,3})$	$=$	$N(T_C) \setminus 2\mathbb{N}$	
Binary tree $T_{\geq 0}$	$N(T_{\geq 0}) = S_{\geq 0}$	$=$	$N(T_C) \setminus S_{-1}$	$= S_0 \cup S_1 \cup S_2 \ldots$
Binary tree $T_{\geq 1}$	$N(T_{\geq 1}) = S_{\geq 1}$	$=$	$N(T_C) \setminus \bigcup_{i=-1}^{0} S_i$	$= S_1 \cup S_2 \cup S_3 \ldots$
Binary tree $T_{\geq j}$	$N(T_{\geq j}) = S_{\geq j}$	$=$	$N(T_C) \setminus \bigcup_{i=-1}^{j-1} S_i$	$= \bigcup_{i=j}^{\infty} S_i$

Let us describe these sets using multiplicative groups. The set $S_{\geq 0} = \mathbb{Z}_6^*$ can be understood as the multiplicative group modulo 6 and the set $S_{-1} = \mathbb{Z}/6\mathbb{Z} \setminus \mathbb{Z}_6^* = \{0, 2, 3, 4\}$ as the set of all non-invertible elements (non-units) of $\mathbb{Z}/6\mathbb{Z}$.

The set S_0 consists of all nodes resulting as output of $R(n)$ within the binary tree $T_{\geq 0}$. These are the orange highlighted nodes displayed by figures 3.1, 3.2. In other words, S_0 is the codomain of the function $R(n)$ operating on nodes within $T_{\geq 0}$. The binary tree $T_{\geq 0}$ can be transformed to a (pruned) binary tree $T_{\geq 1}$. For this, the prunable nodes will be deleted and their neighbors reconnected. The upward neighbor of a pruned node will then be identified as pruning candidate for a later transformation of the resulting tree $T_{\geq 1}$ to a more pruned tree $T_{\geq 2}$.

The set S_1 contains all nodes that are (as per the description above) identified as pruning candidates for the next transformation of $T_{\geq 1}$ to $T_{\geq 2}$. After having transformed $T_{\geq 1}$ to

$T_{\geq 2}$, the more pruned binary tree $T_{\geq 2}$ contains nodes that are identified as pruning candidates for another upcoming transformation of $T_{\geq 2}$ to $T_{\geq 3}$ – these nodes are elements of the set S_2. This pruning algorithm is repeatedly applied in the same pattern. And in this way we obtain the sets $S_1, S_2, S_3, \ldots$ and so forth. Generally, we can write these sets in the form $S_j = \{n \in N(T_{j-1}) \mid U^{-j}(n) \in S_0\}$. Kleinnijenhuis found out that the codomain $\mathbb{N}^U$ of the Upward function contains 5 residue classes modulo 96, namely $\{5, 29, 53, 77, 85\} = \mathbb{N}^U$ and the codomain $\mathbb{N}^R$ of the Rightward function comprises 27 residue classes modulo 96, namely $\{1, 7, 11, 13, 17, 19, 23, 25, 31, 35, 37, 41, 43, 47, 49, 55, 59, 61, 65, 67, 71, 73, 79, 83, 89, 91, 95\} = \mathbb{N}^R$. The union of both sets $\mathbb{N}^U \cup \mathbb{N}^R$ forms the non-cyclic multiplicative group $\mathbb{Z}^*_{96}$, whose generating set is $\{5, 17, 31\}$ (see [84], [85]). All elements of the Upward function's codomain have the same remainder 5 when divided by 8.

For each subset X of a group G, the intersection over all subgroups (of G) that contain this subset X is [86, p. 34]:

$$\langle X \rangle = \bigcap_{X \subseteq U \leq G} U$$

Firstly it applies $\langle X \rangle \leq G$ meaning that this intersection is again a subgroup of G. It is generated by the *generating set* X and it is the smallest subgroup of G containing every element of X [86, p. 35]. Secondly, $\langle X \rangle \subseteq U$ for each subgroup U (of G) containing X. Thirdly, when there is only a single element x in X, then $\langle X \rangle$ is usually written as $\langle x \rangle$ and in this case, $\langle x \rangle$ is the cyclic subgroup of G – such situations we have already seen in section 2.6. Let us refer back to $\mathbb{Z}^*_{96}$. In this example, $\langle \{5, 17, 31\} \rangle$ is the subgroup generated by $\{5, 17, 31\}$ and therefore every element of $\mathbb{Z}^*_{96}$ is of the form $5^l 17^m 31^n$ where $l \in \{0, 1, \ldots, 7\}$ because the element 5 has order 8, and similarly $m, n \in \{0, 1\}$ since both elements 17 and 31 have order 2. Non-cyclic groups can be cyclic decomposed, which is detailed by Gallian and Rusin [87] and Cheng [88] using the concept of the external direct product [86, p. 79], [78, p. 156] and the internal direct product [86, p. 80], [78, p. 183]. A comprehensive table of cyclic decompositions of multiplicative non-cyclic groups of integers modulo n up to $n = 130$ is provided by Wolfdieter Lang [84].

Let us take a closer look at the (cyclic) multiplicative group $\mathbb{Z}^*_{18} = \{1, 5, 7, 11, 13, 17\} = \langle 5 \rangle$ which has an order $ord(\mathbb{Z}^*_{18}) = 6$. Having the generator 5 coprime to the modulus 18, we obtain the congruence $5^{\phi(18)} \equiv 1 \pmod{18}$ in accordance with Euler's theorem 2.11. This allows us to infer from $5^6 \equiv 5^{6(n+1)} \equiv 5^j 5^{6n+6-j} \equiv 1 \pmod{18}$ the congruences given by 3.4 (on the left).

If a natural number divides another, $m \mid n$, as in our case $3 \mid 18$, then for two integers a, b the following implication holds, see [68, p. 21]:

$$a \equiv b \pmod{n} \rightarrow a \equiv b \pmod{m} \tag{3.2}$$

This means in our case $w \cdot 5^{6n+6} \equiv 1 \pmod{18} \rightarrow w \cdot 5^{6n+6} \equiv 1 \pmod{3}$. In fact, Euler's theorem (2.11) gives us two congruences $5^{\phi(18)} \equiv 1 \pmod{18}$ and $2^{\phi(3)} \equiv 1 \pmod{3}$. The latter is obvious, because $\mathbb{Z}^*_3 = \langle 2 \rangle$. Since $\phi(18) = 6$ and $\phi(3) = 2$, every power of five with an exponent divisible by 6 and every power of two with an exponent divisible by 2 belong to the residue classes $[1]_{18}$ and $[1]_3$.

Because of $[1]_{18} = [5^0]_{18}, \ldots, [13]_{18} = [5^4]_{18}$ and finally $[11]_{18} = [5^5]_{18}$ we obtain the congruences on the left side in 3.4. The exponents are indicated by the j. For example, it follows from $w \in [13]_{18}$ that $[w \cdot 5^{6n+2}]_{18} = [w]_{18} \cdot [5^{6n+2}]_{18} = [13]_{18} \cdot [5^{6n+2}]_{18} = [5^4]_{18} \cdot [5^{6n+2}]_{18} = [5^{6n+6}]_{18} = [1]_{18}$, because $6n + 6$ is divisible by 6 (Euler's theorem).

From the equality of the residue classes modulo 18 and modulo 3 (according to equation 3.2) it follows for $w \in [13]_{18}$ from $[w]_{18} \cdot [5^{6n+2}]_{18} = [13]_{18} \cdot [5^{6n+2}]_{18} = [1]_{18}$ the following equation:

$$[1]_3 = [w]_3 \cdot [5^{6n+2}]_3 = [13]_3 \cdot [5^{6n+2}]_3 \tag{3.3}$$

Just replacing 18 with 3, that is the homomorphism given by the map $f : \mathbb{Z}_n^* \to \mathbb{Z}_m^*$ with $f(r \bmod n) = r \bmod m$ as long as $\gcd(r \bmod n, n) = 1$ leads to $\gcd(r \bmod m, m) = 1$. By Euclid, we know that in the case r is coprime to n then it is also coprime to every factor m of n. That is why a homomorphism exist to the congruences shown in 3.4 (on the right).

Using the fact that $[5^{6n}]_{18} = [5^0]_{18} = [1]_{18}$ and thus $[5^{6n+k}]_{18} = [5^k]_{18} = [5]_{18}^k = [5]_3^k$, we obtain from equation 3.3:

$$[1]_3 = [13]_3 \cdot [5]_3^2 = [13]_3 \cdot [2]_3^2$$

Therefore $[13]_{18} \cdot 4 = [13]_3 \cdot 4 \equiv 1 \pmod 3$. The third and the last row in 3.4 are obtained in the same way. The powers of two that appear in the other rows result from the fact that we can always add or remove even powers of two because $[2^2]_3 = [1]_3$.

Based on equation 2.7 we can state that $a \equiv b \pmod m$ implies $(a + m) \equiv b \pmod m$. Let us set $a = w \cdot 2^{2n+2}$ and $b = 1$ and $m = 3$, then we obtain $(w \cdot 2^{2n+2} + 3) \equiv 1 \pmod 3$ and using a factor $i \in \mathbb{N}$ we obtain the more general congruence $(w \cdot 2^{2n+2} + 3i) \equiv 1 \pmod 3$. As a consequence the congruences in 3.4 are true, while $w \cdot 5^{6n+6} = w \cdot 2^{2n+2} + 3 \cdot i$ or rather while $3 \mid (5^{6n+6} - 2^{2n+2})$. These conditions continue $3 \mid (5^{6n+5} - 2^{2n+3})$ and $3 \mid (5^{6n+4} - 2^{2n+4})$ and so forth.

$$\begin{array}{llllll}
j = 0, & w \in [1]_{18} & w \cdot 5^{6n+6} \equiv 1 \pmod{18} & & w \cdot 2^{2n+2} \equiv 1 \pmod 3 \\
j = 1, & w \in [5]_{18} & w \cdot 5^{6n+5} \equiv 1 \pmod{18} & & w \cdot 2^{2n+3} \equiv 1 \pmod 3 \\
j = 2, & w \in [7]_{18} & w \cdot 5^{6n+4} \equiv 1 \pmod{18} & & w \cdot 2^{2n+4} \equiv 1 \pmod 3 \\
j = 3, & w \in [17]_{18} & w \cdot 5^{6n+3} \equiv 1 \pmod{18} & & w \cdot 2^{2n+1} \equiv 1 \pmod 3 \\
j = 4, & w \in [13]_{18} & w \cdot 5^{6n+2} \equiv 1 \pmod{18} & & w \cdot 2^{2n+2} \equiv 1 \pmod 3 \\
j = 5, & w \in [11]_{18} & w \cdot 5^{6n+1} \equiv 1 \pmod{18} & & w \cdot 2^{2n+1} \equiv 1 \pmod 3
\end{array} \tag{3.4}$$

The inverse upward function, which can be understood as a downward function $U^{-1}(n) = D(n)$ is defined as follows:

$$D(n) = U^{-1}(n) = \begin{cases} \frac{n-1}{4} & n \equiv 5 \pmod{24} \\ \frac{n-5}{16} & n \equiv 85 \pmod{96} \end{cases}$$

The modular conditions are deduced as follows: We have $D(n) = \frac{n-1}{4}$ if $\frac{n-1}{4} \equiv 1 \pmod 6$ and $D(n) = \frac{n-5}{16}$ if $\frac{n-5}{16} \equiv 5 \pmod 6$. For $a, b \in \mathbb{Z}$ and $n, m \in \mathbb{N}$ we can apply the following modular arithmetic rule [68, p. 21]:

$$a \equiv b \pmod n \leftrightarrow m \cdot a \equiv m \cdot b \pmod{m \cdot n} \tag{3.5}$$

This leads to $D(n) = n - 1$ if $n - 1 \equiv 4 \pmod{24}$ and $D(n) = n - 5$ if $n - 5 \equiv 80 \pmod{96}$.

Now we make the use of another modular arithmetic rule, which for two given congruences $a \equiv b \pmod n$ and $c \equiv d \pmod n$ states that [68, p. 19]:

$$a + c \equiv b + d \pmod n \qquad \text{and} \qquad a \cdot c \equiv b \cdot d \pmod n \tag{3.6}$$

This finally leads to $D(n) = n-1$ if $n \equiv 5 \pmod{24}$ and $D(n) = n-5$ if $n \equiv 85 \pmod{96}$.

The rightward function that operates on the tree of pruning level 1, thus the tree $T_{\geq 1}$, is can be expressed as the right-to-left composition $R_{\geq 1}(n) = U \circ R \circ U^{-1}(n) = U \circ R \circ D(n)$ and it is defined as follows:

$$R_{\geq 1}(n) = \begin{cases} (8D(n)-1)/3 & 2D(n) \equiv 4 \bmod 18 \wedge D(n) \in [11]_{18} \cup [17]_{18} \\ (16D(n)-1)/3 & 4D(n) \equiv 4 \bmod 18 \wedge D(n) \in [11]_{18} \cup [13]_{18} \\ (32D(n)-1)/3 & 2D(n) \equiv 16 \bmod 18 \wedge D(n) \in [11]_{18} \cup [17]_{18} \vee D(n) \in [5]_{18} \\ (64D(n)-1)/3 & 4D(n) \equiv 16 \bmod 18 \wedge D(n) \in [1]_{18} \cup [13]_{18} \vee D(n) \in [7]_{18} \end{cases}$$

$$R_{\geq 2}(n) = \begin{cases} (32D^2(n)-1)/3 & 2D^2(n) \in [4]_{18} \wedge D^2(n) \in [11]_{18} \vee 8D^2(n) \in [4]_{18} \wedge D^2(n) \in [17]_{18} \\ (64D^2(n)-1)/3 & D^2(n) \in [1]_{18} \cup [13]_{18} \wedge 4D^2(n), 16D^2(n) \in [4]_{18} \\ (128D^2(n)-1)/3 & D^2(n) \in [11]_{18} \cup [17]_{18} \wedge (2D^2(n) \in [4]_{18} \wedge 8D^2(n) \in [16]_{18} \vee \\ & 2D^2(n) \in [16]_{18} \wedge 32D^2(n) \in [4]_{18}) \\ (256D^2(n)-1)/3 & D^2(n) \in [1]_{18} \vee D^2(n) \in [7]_{18} \cup [13]_{18} \wedge 64D^2(n) \in [4]_{18} \\ (512D^2(n)-1)/3 & 32D^2(n) \in [16]_{18} \wedge (2D^2(n) \in [16]_{18} \wedge D^2(n) \in [11]_{18} \cup [17]_{18} \vee D^2(n) \in [5]_{18}) \\ (1024D^2(n)-1)/3 & 64D^2(n) \in [16]_{18} \wedge (D^2(n) \in [7]_{18} \vee 4D^2(n) \in [16]_{18} \wedge D^2(n) \in [1]_{18} \cup [13]_{18}) \end{cases}$$

Figure 3.3 shows the complete chain of tree transformations, beginning from the original Collatz tree, over the Syracuse tree to the binary tree and pruned ones.

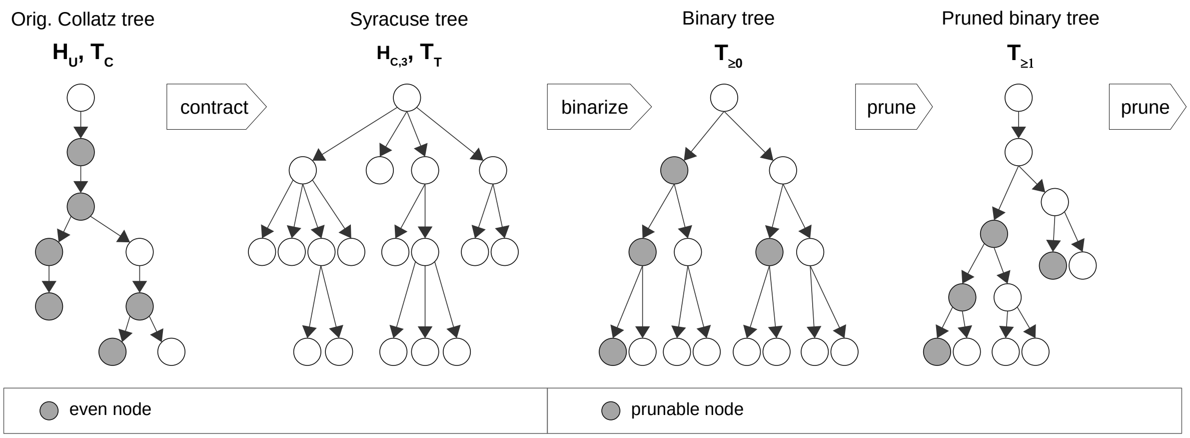

Figure 3.3: Transformation chain, beginning from the original Collatz tree up to pruned binary trees

4. Cycles in the Collatz Graph

4.1 A remark about cycles

In graph theory, a path of length $n \geq 1$ that starts and ends at the same vertex is called a circuit. A circuit, in which no vertex is repeated with the sole exception that the initial vertex is the terminal vertex, is called a cycle. A cycle of length n is referred to as an n-cycle. For these definitions, we rely on [45, p. 599], [89, p. 35] and [90, p. 445]. Furthermore, we call a cycle originating from the root a trivial cycle.

In order for the cycles to become graphically visible, we now require that in a graph H two vertices v_1 and v_2 are one and the same if the label of both nodes are identical: $l_{V(H)}(v_1) = l_{V(H)}(v_2) \rightarrow v_1 = v_2$. As a consequence, there is no guarantee that the graph precisely refers to the algebraic structure of a free monoid anymore. A free monoid requires that each of its elements can be written in one and only one way.

When different nodes collapse on one, the graph is no longer necessarily a tree. Let us point to the monoid S^*, which we introduced in section 2.1. Take for example four of its elements, the empty string e, the strings qqr, $qqrqqr$, and $qqrqqrqqr$. These elements lie as well within the subset $U \subset T \subset S^*$, and they are represented by nodes of the tree H_U that all have the same label $1 = ev_{S^*}(qqr, 1) = ev_{S^*}(qqrqqr, 1) = ev_{S^*}(qqrqqrqqr, 1)$. These nodes are one and the same, the root of H_U. Visually, then in H_U a directed edge goes from the vertex labeled with 4 back to the root node. Analogically, in $H_{C,3}$ a loop connects the root to itself, since due to the path contraction even labeled nodes do not exist in $H_{C,3}$. The aforementioned example reflects the trivial cycle of the Collatz sequence.

Figure 4.1 depicts a section of $H_{C,5}$, which includes the 3-cycle $43, 17, 27$. Because of the two non-trivial cycles $(43, 17, 27)$ and $(83, 33, 13)$, in $H_{C,5}$ there does not exist a path between the root and the vertex 43 and between the root and the vertex 83. Hence, $H_{C,5}$ is said to be a disconnected graph. Generally, a graph is called a disconnected graph if it is impossible to walk (along its edges) from any vertex to any other [89, pp. 46-47].

The following considerations focus on non-trivial cycles, and therefore on cycles that do not originate from the root, but cause the graph to be a disconnected graph. Utilizing the example of the graph $H_{C,5}$ we are able to deduct from the cycle $(43, 17, 27)$ the simple and self-evident equality $\textit{left-child}^3(43) = 43$:

$$\textit{left-child}(43) = \tfrac{1}{5} * \left(43 * 2^1 - 1\right) = 17$$
$$\textit{left-child}(17) = \tfrac{1}{5} * \left(17 * 2^3 - 1\right) = 27$$
$$\textit{left-child}(27) = \tfrac{1}{5} * \left(27 * 2^3 - 1\right) = 43$$

Obviously, the authors note, it would be interesting to find out what circumstances en-

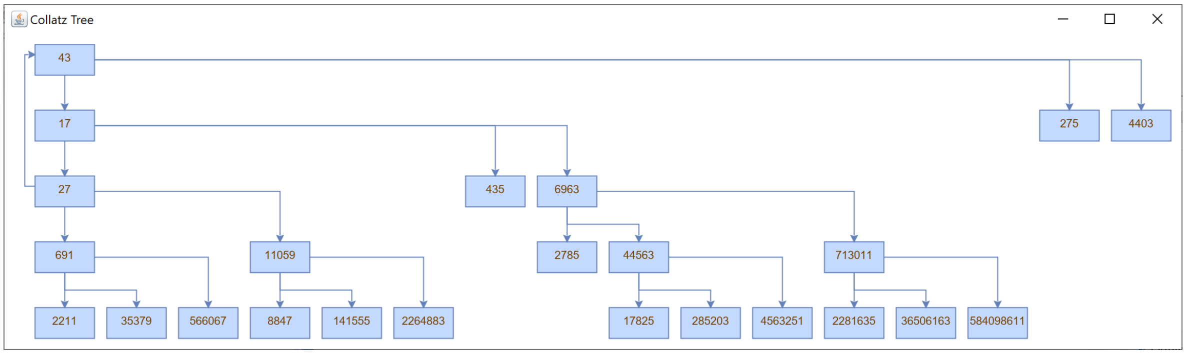

Figure 4.1: Section of $H_{C,5}$ including the 3-cycle $43, 17, 27$

able a graph to have non-trivial cycles, whether it be the $5x+1$ variant, the $7x+1$ variant of H_C or any variant $H_{C,k}$ with $k \geq 1$.

4.2 Which variants of H_C have non-trivial cycles?

The generalization of the relationship between successive nodes, given by equation 2.18 leads to the condition for an existence of an n-cycle in any $kx+1$ variant of H_C, which looks analogous to the condition given by equation 2.2 that specifies $H_{C,3}$ has a cycle:

$$2^{\alpha} = \prod_{i=1}^{n} \left(k + \frac{1}{v_i} \right) \tag{4.1}$$

The natural number α is the sum of edges that have been contracted between the vertices v_i forming the cycle, in other words α is the number of divisions by 2 within the sequence. The natural number n is the cycle length and k obviously specifies the variant of H_C. Since between each vertex at least one edge has been contracted (at least one division by 2 took place), we know that our exponent alpha is greater than or equal to the sequence length:

$$\alpha \geq n \tag{4.2}$$

In their 2020 publication Koch et al. [19] provide a list of cycles for different values of k, identified with a linear search performed by a Python script [1]. Table 4.1 lists all these discovered cycles (refer to [19] for details on the discovery procedure and search intervals). Note that the cycles in table 4.1 are written in reverse order, i.e. in the order which corresponds to the Collatz sequence. To obtain the cycles in terms of graph theory referring to the graph H_C, read them from right to left.

k	cycle	α	non-trivial
1	1	1	
3	1	2	
5	1,3	5	
5	13,33,83	7	✓
5	27,17,43	7	✓
7	1	3	
15	1	4	
31	1	5	
63	1	6	
127	1	7	
181	27,611	15	✓
181	35,99	15	✓
255	1	8	
511	1	9	

Table 4.1: Known n-cycles in $kx+1$ variants of H_C for $k \leq 1000$, $n \leq 100$

Based on the results shown in table 4.1 we state the following theorem 4.1 that renders more precisely the prerequisite for cycles that may occur in any variants of H_C.

Theorem 4.1 An n-cycle can only exist in a graph $H_{C,k}$, if the following equation holds:

$$2^{\bar{\alpha}} = 2^{\lfloor n \log_2 k \rfloor + 1} = \prod_{i=1}^{n} \left(k + \frac{1}{v_i} \right)$$

The statement behind theorem 4.1 consists in the claim that, in order for an n-cycle to occur, the exponent α has to be $\bar{\alpha} = \lfloor n \log_2 k \rfloor + 1$. This statement is true if the following general condition for the validity of the cycle-alpha's upper limit always holds (see [19]):

$$n \log_2 k - \lfloor n \log_2 k \rfloor < 2 - \log_2 \left(\prod_{i=1}^{n} \left(1 + \frac{1}{k v_i} \right) \right) \tag{4.3}$$

A product $\prod(1+a_n)$ with positive terms a_n is convergent if the series $\sum a_n$ converges, see Knopp [91, p. 220]. A similar statement provides Murphy [92], who write the factors in the form $c_n = 1 + a_n$ and explains that if $\prod c_n$ is convergent then $c_n \to 1$ and therefore if $\prod(1+a_n)$ is convergent then $a_n \to 0$. Thus, to verify whether the product in condition 4.3 is converging towards a limiting value, it is sufficient to examine the following sum:

$$\sum_{i=1}^{n} \frac{1}{k v_i}$$

The sum of reciprocal vertices depending only from v_1 is given in appendix A.3.

4.3 Cycles and the product in the condition for cycle-alpha's upper limit

Let us start with the following product equality, which will give us insights into the relationship between cycles and the product in the condition for alpha's upper limit. The variables $V_1, \ldots, V_m$ and $W_1, \ldots, W_n$ are all odd positive integers:

$$(V_1+1)\cdots(V_m+1)\cdot W_1\cdots W_n = V_1\cdots V_m\cdot(W_1+1)\cdots(W_n+1) \tag{4.4}$$

Every natural odd number V can be expressed in the form of $V = v\cdot 2^{\alpha} - 1$ whereby v is an positive odd integer and $\alpha > 0$ is any natural number. This allows us to perform the following substitution (we use α_V for denoting the divisions by two between successive nodes v_i and α_W for divisions by two between successive nodes w_i):

$$\begin{array}{llllll}
V_1 & = v_2 2^{\alpha_{V,1}} - 1 & = kv_1 & W_1 & = w_2 2^{\alpha_{W,1}} - 1 & = kw_1 \\
V_2 & = v_3 2^{\alpha_{V,2}} - 1 & = kv_2 & W_2 & = w_3 2^{\alpha_{W,2}} - 1 & = kw_2 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
V_{m-1} & = v_m 2^{\alpha_{V,m-1}} - 1 & = kv_{m-1} & W_{n-1} & = w_n 2^{\alpha_{W,n-1}} - 1 & = kw_{n-1} \\
V_m & = v_1 2^{\alpha_{V,m}} - 1 & = kv_m & W_n & = w_1 2^{\alpha_{W,n}} - 1 & = kw_n
\end{array} \tag{4.5}$$

The substitution rotating from $v_2 = (kv_1+1)\cdot 2^{-\alpha_{V,1}}$ to $v_m = (kv_{m-1}+1)\cdot 2^{-\alpha_{V,m-1}}$ and finally back to $v_1 = (kv_m+1)\cdot 2^{-\alpha_{V,m}}$ describes a cycle. The result of these substitutions into equation 4.4 is the following equality:

$$\begin{gathered}
v_2 2^{\alpha_{V,1}}\cdots v_m 2^{\alpha_{V,m-1}} v_1 2^{\alpha_{V,m}}\cdot W_1\cdots W_n = V_1\cdots V_m\cdot w_2 2^{\alpha_{W,1}}\cdots w_n 2^{\alpha_{W,n-1}} w_1 2^{\alpha_{W,n}} \\
v_2 2^{\alpha_{V,1}}\cdots v_m 2^{\alpha_{V,m-1}} v_1 2^{\alpha_{V,m}}\cdot kw_1\cdots kw_n = kv_1\cdots kv_m\cdot w_2 2^{\alpha_{W,1}}\cdots w_n 2^{\alpha_{W,n-1}} w_1 2^{\alpha_{W,n}}
\end{gathered}$$

The trivial case where $n = m$ and the sum of exponents are equal $\sum_{i=1}^{m}\alpha_{V,i} = \sum_{i=1}^{n}\alpha_{W,i}$ simplifies the product equality as follows:

$$\begin{gathered}
(V_1+1)\cdots(V_n+1)\cdot W_1\cdots W_n = V_1\cdots V_n\cdot(W_1+1)\cdots(W_n+1) \\
v_1\cdots v_n\cdot \cancel{2^{\alpha_{V,1}+\ldots+\alpha_{V,n}}}\cdot W_1\cdots W_n = V_1\cdots V_m\cdot w_1\cdots w_n\cdot \cancel{2^{\alpha_{W,1}+\ldots+\alpha_{W,n}}}
\end{gathered}$$

This equality becomes immediatly true if $V_1\cdots V_n = W_1\cdots W_n$ which is the less spectacular case. The more interesting case arises from setting $V_i = kv_i$ and $W_i = kw_i$ as given by substitution 4.5 wich turns the product equality into an always true statement as well:

$$\begin{gathered}
v_1\cdots v_n\cdot W_1\cdots W_n = V_1\cdots V_m\cdot w_1\cdots w_n \\
v_1\cdots v_n\cdot k^n\cdot w_1\cdots w_n = k^n\cdot v_1\cdots v_n\cdot w_1\cdots w_n
\end{gathered}$$

Example 4.1 The following exemplarly product equality fullfills equation 4.4, whereby $V_1 = 65$, $V_2 = 165$, $V_3 = 415$ and $W_1 = 135$, $W_2 = 85$, $W_3 = 215$:

$$(65+1)(165+1)(415+1)\cdot 135\cdot 85\cdot 215 = 65\cdot 165\cdot 415\cdot (135+1)(85+1)(215+1)$$

We perform the following substitutions:

$$\begin{aligned}
V_1 &= 65 &&= v_2 2^{\alpha_{V,1}} - 1 = 33\cdot 2^1 - 1 = 5v_1 & W_1 &= 135 &&= w_2 2^{\alpha_{W,1}} - 1 = 17\cdot 2^3 - 1 = 5w_1\\
V_2 &= 165 &&= v_3 2^{\alpha_{V,2}} - 1 = 83\cdot 2^1 - 1 = 5v_2 & W_2 &= 85 &&= w_3 2^{\alpha_{W,2}} - 1 = 43\cdot 2^1 - 1 = 5w_2\\
V_3 &= 415 &&= v_1 2^{\alpha_{V,3}} - 1 = 13\cdot 2^5 - 1 = 5v_3 & W_3 &= 215 &&= w_1 2^{\alpha_{W,3}} - 1 = 27\cdot 2^3 - 1 = 5w_3
\end{aligned}$$

The result of these substitutions is:

$$33\cdot \cancel{2^1}\cdot 83\cdot \cancel{2^1}\cdot 13\cdot \cancel{2^5}\cdot 135\cdot 85\cdot 215 = 65\cdot 165\cdot 415\cdot 17\cdot \cancel{2^3}\cdot 43\cdot \cancel{2^1}\cdot 27\cdot \cancel{2^3}$$

Since the sum of exponents $\alpha_{V,i}$ and $\alpha_{W,i}$ are equal, we can cancel out all powers of two and obtain:

$$v_2 v_3 v_1 W_1 W_2 W_3 = 33\cdot 83\cdot 13\cdot 135\cdot 85\cdot 215 = 65\cdot 165\cdot 415\cdot 17\cdot 43\cdot 27 = V_1 V_2 V_3 w_2 w_3 w_1$$

This product equality becomes true $v_2 v_3 v_1 \cdot k^3 \cdot w_1 w_2 w_3 = k^3 \cdot v_1 v_2 v_3 \cdot w_2 w_3 w_1$ when we set $V_i = kv_i$ and $W_i = kw_i$ (for $i = 1, 2, 3$) which inevitably leads to the two corresponding cycles for $k = 5$ that are already presented by table 4.1.

Let us define the difference $\Delta = (1+1/V_1)(1+1/V_2)\cdots(1+1/V_m) - (1+1/W_1)(1+1/W_2)\cdots(1+1/W_n)$. We know that if this difference is zero, then we have found two cycles, as for example $0 = (1+1/65)(1+1/165)(1+1/415) - (1+1/135)(1+1/85)(1+1/215)$. Can you identify empirically some set pairs $\{V_1, V_2, \ldots, V_m\}$ and $\{W_1, W_2, \ldots, W_n\}$, where the difference is not necessarly zero but a whole number, e.g. $\Delta = 1, 2, 3, \ldots$?

5. Conclusion and Outlook

5.1 Summary

We defined an algebraic graph structure that expresses the Collatz sequences in the form of a tree. Next, the vertex reachability properties were unveiled by examining the relationship between successive nodes in H_C. Moreover, we dealt with graphs that represent other variants of Collatz sequences, for instance $5x+1$ or $181x+1$. The interesting part of both variants is that for these sequences the existence of cycles is known. They serve as the basis for further investigations of the problem.

5.2 Further Research

In subsequent studies, the properties of vertices in H_C might be elaborated upon more closely by taking into account a vertex's label as well as its properties. Moreover we will investigate on the structure of a pruned trees $T_{\geq j}$ including questions on calculating a left-child or right-child within any of these trees.

A. Appendix

A.1 A brief note on the tree $H_{C,1}$

A special case of Collatz trees is the graph $H_{C,1}$ – the $x+1$ variant of H_C. In this case, any sequence of successive nodes along the path from v_n down to v_1 is strictly monotonically increasing. If we run reverse to the edge direction (towards the root), then of course the node sequence is strictly monotonically decreasing. Figure A.1 shows a portion of the graph $H_{C,1}$ starting at its root.

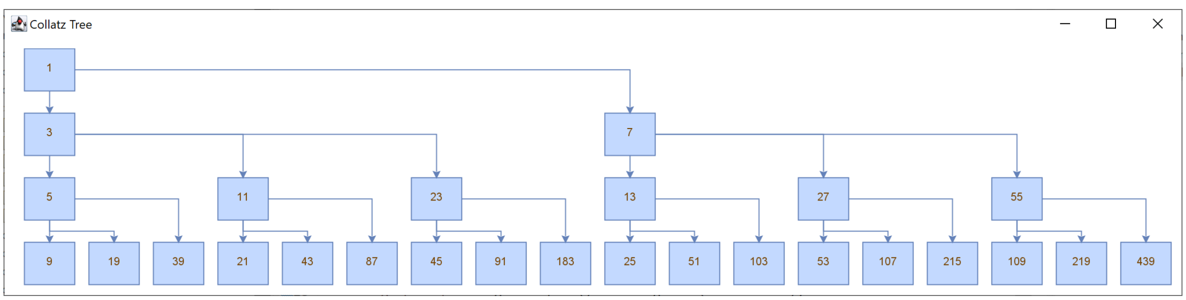

Figure A.1: Section of the graph $H_{C,1}$ starting at its root (without branches that reflect a subsequence containing the trivial cycle)

A.2 Algorithm for pruning binary trees $T_{\geq j}$

Binary trees as introduced in chapter 3 inspired by Kleinnijenhuis [53], [59] can iteratively be pruned (the way Kleinnijenhuis originally invented it). Listing A.1 implements this pruning algorithm.

```python
def shrinkRoot(self):
  self.root = self.root.successors[0]
  self.root.predecessor = None

def prune(self):
  self.shrinkRoot()
  new_prunables = []
  for node in self.prunable_nodes:
    if node.predecessor is not None:
      if len(node.successors) > 1 and len(node.predecessor.successors) > 1:
        node.predecessor.successors[1].successors.append(node.successors[1])
        node.predecessor.successors[1].successors.reverse()
        node.successors[1].predecessor = node.predecessor.successors[1]
        node.successors[1].prunable = True
        new_prunables.append(node.successors[1])
      node.predecessor.successors.remove(node)
      node.predecessor = None
      self.labels.remove(node.label)
  self.prunable_nodes = new_prunables
  return self
```

Listing A.1: Python function for pruning a binary tree $T_{\geq j}$ [93]

Listing A.1 is only intended to illustrate the pruning algorithm in a simplifying manner. To run pruning on trees with arbitary large numbers, we refer to the professional Python API by Koch [1].

A.3 The sum of reciprocated vertices depending only on v_1

One condition deduced from theorem 2.1 is the product condition 4.3, which specifies the validity of the cycle-alpha's upper limit. This condition requires the sum $1/kv_1 + 1/kv_2 + 1/kv_3 + \ldots$ to be limited. In order to formulate this sum independently from the successive vertices $v_2, v_3, \ldots$, we substitute these as follows:

$$\begin{aligned}
v_1 &= v_1 \\
v_2 &= \frac{kv_1 + 1}{2^{\alpha_1}} \\
v_3 &= \frac{k^2 v_1 + k + 2^{\alpha_1}}{2^{\alpha_1+\alpha_2}} \\
v_4 &= \frac{k^3 v_1 + k^2 + k \cdot 2^{\alpha_1} + 2^{\alpha_1+\alpha_2}}{2^{\alpha_1+\alpha_2+\alpha_3}} \\
&\vdots
\end{aligned} \tag{A.1}$$

$$v_{n+1} = \frac{k^n v_1 + \sum_{j=1}^{n} k^{j-1} 2^{\alpha_1+\ldots+\alpha_n - \sum_{l>n-j} \alpha_l}}{2^{\alpha_1+\ldots+\alpha_n}} \tag{A.2}$$

The sum of the reciprocated vertices can be expressed as a term that depends from v_1 and from the number of contracted edges, id est the number of dvisions by two, between two successive vertices $\alpha_1, \alpha_2, \alpha_3, \ldots$:

$$\sum_{i=1}^{n+1} \frac{1}{kv_i} = \frac{1}{k}\left(\frac{1}{v_1} + \sum_{i=1}^{n} \frac{1}{v_{i+1}}\right) = \frac{1}{k}\left(\frac{1}{v_1} + \sum_{i=1}^{n} \frac{2^{\alpha_1+\ldots+\alpha_i}}{k^i v_1 + \sum_{j=1}^{i} k^{j-1} 2^{\alpha_1+\ldots+\alpha_n - \sum_{l>i-j}\alpha_l}}\right)$$

A.4 The product of reciprocated vertices incremented by one

In a similar way to deduce the sum of reciprocated vertices depending only on v_1 as performed in A.3, we evolve the product formula depending only on v_1:

$$\prod_{i=1}^{n+1}\left(1 + \frac{1}{kv_i}\right) = 1 + \frac{2^{\alpha_1+\ldots+\alpha_n} + k \cdot 2^{\alpha_1+\ldots+\alpha_{n-1}} + \ldots + k^{n-1} \cdot 2^{\alpha_1} + k^n}{k^{n+1} v_1} \tag{A.3}$$

$$= 1 + \frac{2^{\alpha_1+\ldots+\alpha_n} + k \cdot \sum_{j=1}^{i} k^{j-1} 2^{\alpha_1+\ldots+\alpha_n - \sum_{l>i-j}\alpha_l}}{k^{n+1} v_1} \tag{A.4}$$

$$= 1 + \frac{2^{\alpha_1+\ldots+\alpha_n} + k \cdot (v_{n+1} \cdot 2^{\alpha_1+\ldots+\alpha_n} - k^n v_1)}{k^{n+1} v_1}$$

$$= \frac{2^{\alpha_1+\ldots+\alpha_n}(1 + kv_{n+1})}{k^{n+1} v_1} \tag{A.5}$$

We inserted the sum used in equation A.2 into the above-given equation A.3 and then obtained equation A.4. Let us divide this product by the last factor and consider the product in the condition for cycle-alpha's upper limit, which iterates to n instead of $n+1$:

$$\prod_{i=1}^{n}\left(1 + \frac{1}{kv_i}\right) = \frac{\prod_{i=1}^{n+1}\left(1 + \frac{1}{kv_i}\right)}{\frac{kv_{n+1}+1}{kv_{n+1}}} = \frac{2^{\alpha_1+\ldots+\alpha_n}\cancel{(1 + kv_{n+1})}kv_{n+1}}{k^{n+1} v_1 \cancel{(kv_{n+1}+1)}} = \frac{2^{\alpha_1+\ldots+\alpha_n} v_{n+1}}{k^n v_1} \tag{A.6}$$

The above-shown equation A.6 becomes simplified, when we replaced the numerator by equation A.5. The question which sequence maximizes its last member v_{n+1} ties into the question: Which sequence maximizes the product? The product formula A.6 does not depend from all vertices $v_1, v_2, \ldots, v_n$, it depends only from $2^\alpha = 2^{\alpha_1+\ldots+\alpha_n}$, from the first vertex v_1 and the final one v_{n+1}.

A.5 Engel expansions maximize the node v_{n+1}

A sequence $v_{n+1}, v_n, \ldots, v_2, v_1$ describing a path in $H_{C,3}$ from v_{n+1} down to v_1 allows at most one division by 2 between two successive nodes. Dividing only once between two successive nodes, maximizes the v_{n+1}, but it is not obvious that this maximizes the product contained in condition 4.3. Such a sequence forms the following ascending continued fraction (for the classical case $b = 2, k = 3$ see [94, p. 11]):

$$v_{n+1} = \frac{k\dfrac{k\dfrac{k\dfrac{kv_1+1}{b}+1}{b}+1}{b}+1}{b} \cdots = \frac{k^n v_1 + \sum_{i=0}^{n-1} k^i b^{n-1-i}}{b^n} = \frac{k^n v_1}{b^n} + \frac{k^n - b^n}{(k-b)b^n} \tag{A.7}$$

The sum of the products of the powers of k and b, contained in equation A.7, can be simplified by converting this sum into the form $(k-b)(b^{n-1}+kb^{n-2}+k^2b^{n-3}+\ldots+k^{n-3}b^2+k^{n-2}b+k^{n-1})=k^n-b^n$ as follows:

$$k^n-b^n=k^n\left(1-\frac{b^n}{k^n}\right)=k^n\left(1-\frac{b}{k}\right)\left(1+\frac{b}{k}+\frac{b^2}{k^2}+\ldots+\frac{b^{n-3}}{k^{n-3}}+\frac{b^{n-2}}{k^{n-2}}+\frac{b^{n-1}}{k^{n-1}}\right)=\left(1-\frac{b}{k}\right)\sum_{i=0}^{n-1}k^n\left(\frac{b}{k}\right)^i$$
$$=k\cdot\left(1-\frac{b}{k}\right)\cdot k^{n-1}\cdot\left(\frac{b^{n-1}}{k^{n-1}}+\frac{b^{n-2}}{k^{n-2}}+\frac{b^{n-3}}{k^{n-3}}+\ldots+\frac{b^2}{k^2}+\frac{b}{k}+1\right)$$
$$=(k-b)(b^{n-1}+kb^{n-2}+k^2b^{n-3}+\ldots+k^{n-3}b^2+k^{n-2}b+k^{n-1})$$

Example A.1 A concrete example (where $b=2$ and $k=3$) for such a sequence is $v_1=31$, $v_2=47$, $v_3=71$, $v_4=107$, $v_5=161$. And, to follow that example, we can calculate the label of the vertex v_5 in a straightforward way:

$$v_5=v_{n+1}=\frac{3^4(31+1)-2^4}{2^4}=161$$

Besides, by choosing a vertex $v_1=2^{n+1}-1$, we are able to infinitely generate sequences each forming an ascending continued fraction. As per equation A.7 the last member in this sequence is the odd labeled vertex $v_{n+1}=3^n\cdot 2-1$.

Ascending variants of a continued fraction, such as used in equation A.7, shall not be confused with continued fractions as treated for example in [95], [96], [97]. These ascending continued fractions correspond to the so-called "Engel Expansions" [98].

As illustrated below, we can formulate the ascending continued fractions in a generalized fashion, whereas the analogy to A.7 is given by $b_1=b_2=b_3=b_4=b$ and $a_1=k^0$, $a_2=k^1$, $a_3=k^2$ and $a_4=k^3+k^4v_1$:

$$\frac{a_1+\frac{a_2+\frac{a_3+\frac{a_4}{b_4}}{b_3}}{b_2}}{b_1}\cdots=\frac{a_1}{b_1}+\frac{a_2}{b_1b_2}+\frac{a_3}{b_1b_2b_3}+\frac{a_4}{b_1b_2b_3b_4}+\cdots$$

The generalized equation A.7 may be used to compute any of the above-named ascending continued fraction that has $a_i=k^{i-1}$, $b_i=b$ for $i\in\mathbb{N}$ and $a_n=k^{n-1}+k^nv_1$.

A.6 Include more divisions by two into an Engel expansion

For calculating the largest possible v_{n+1}, we considered so far Engel expansions which contain only n division by two within a Collatz sequence of $n+1$ memebers. In the following we include m additional divisions by two and thus a total of $m+n$ divisions. We look at two corner cases:

- the one where we do the additional m divisions by 2 at the end and
- the one where we do these additional divisions at the very beginning.

The first case is our starting point to examine how the swapping a division by two affects the node v_{n+1}. For this, let us compare the Engel expansion where we devide by 2^m afterwards with one where we divide by 2 in the penultimate step and by 2^{m-1} in last step. One can immediately recognize the following inequality with a mere look:

$$\frac{1+\frac{3+\frac{3^2+\frac{3^3+3^4v_1}{2}}{2}}{2}}{2\cdot 2^m} < \frac{1+\frac{3+\frac{3^2+\frac{3^3+3^4v_1}{2}}{2}}{2\cdot 2}}{2\cdot 2^{m-1}}$$

To put it simply, in the expansion on the right side of the above-shown inequality we perform one division by two a little bit earlier as we do it in the expansion on the left side of the expansion. Almost all summands of both expansions cancel out each other:

$$\frac{1}{2\cdot 2^m}+\cancel{\frac{3}{2^2\cdot 2^m}+\frac{3^2}{2^3\cdot 2^m}+\frac{3^3+3^4v_1}{2^4\cdot 2^m}} < \frac{1}{2\cdot 2^{m-1}}+\cancel{\frac{3}{2^2\cdot 2\cdot 2^{m-1}}+\frac{3^2}{2^3\cdot 2\cdot 2^{m-1}}\frac{3^3+3^4v_1}{2^4\cdot 2\cdot 2^{m-1}}}$$

The second case deals with Engel expansions where we perform that additional m divisions by two as early as possible. The resulting value decreases, when we make a division by two later:

$$\frac{1+\frac{3+\frac{3^2+\frac{3^3+3^4v_1}{2\cdot 2^{m-1}}}{2\cdot 2}}{2}}{2} < \frac{1+\frac{3+\frac{3^2+\frac{3^3+3^4v_1}{2\cdot 2^m}}{2}}{2}}{2}$$

Also here almost all summands of both Engel expansions, they cancel each other out:

$$\cancel{\frac{1}{2}}+\cancel{\frac{3}{2^2}}+\frac{3^2}{2^3\cdot 2}+\cancel{\frac{3^3+3^4v_1}{2^4\cdot 2\cdot 2^{m-1}}} < \cancel{\frac{1}{2}}+\cancel{\frac{3}{2^2}}+\frac{3^2}{2^3}+\cancel{\frac{3^3+3^4v_1}{2^4\cdot 2^m}}$$

While the first case minimizes the value of the node v_{n+1}, the second case maximizes it. The difference between the maximum and the minimum is given by the following equation:

$$\begin{aligned}
&\frac{3^{n-1}\left(\frac{3v_1+1}{2\cdot 2^m}+1\right)-2^{n-1}}{2^{n-1}}-\frac{3^n\left(v_1+1\right)-2^n}{2^{n+m}}\\
=&\frac{3^{n-1}\cdot\left(3v_1+1+2^{m+1}\right)-2^{n-1}\cdot 2^{m+1}-3^n\left(v_1+1\right)+2^n}{2^{m+1}\cdot 2^{n-1}}\\
=&\frac{3^{n-1}+3^{n-1}\cdot 2^{m+1}-2^{n+m}-3^n+2^n}{2^{n+m}}=\frac{3^{n-1}-3\cdot 3^{n-1}+3^{n-1}\cdot 2^{m+1}-2^{n+m}+2^n}{2^{n+m}}\\
=&\frac{-2\cdot 3^{n-1}+3^{n-1}\cdot 2^{m+1}-2^{n+m}+2^n}{2^{n+m}}=\frac{\left(2\cdot 3^{n-1}-2^n\right)\left(2^m-1\right)}{2^n\cdot 2^m}\\
=&\left(\frac{3^{n-1}}{2^{n-1}}-1\right)\left(1-\frac{1}{2^m}\right)
\end{aligned}$$

This has the consequence that for a given sequence consisting of $n+1$ members, between which a total of $n+m$ divisions have taken place, the permutation of these divisions has a very limited effect on the node v_{n+1} as described by theorem A.1.

Theorem A.1 Let $v_{n+1}, v_n, \ldots, v_2, v_1$ be a sequence in which a total of $n+m$ divisions took place (a path in which a total of $n+m$ edges has been contracted). No matter how these divisions are permuted, i.e. performed sooner or later, the node v_{n+1} can differ at most by the following product:

$$\left(\frac{3^{n-1}}{2^{n-1}} - 1\right)\left(1 - \frac{1}{2^m}\right)$$

A.7 The product in the condition for alpha's upper limit

Let us take a closer look at the product contained in condition 4.3 for the case $k = 3$ and use the ascending continued fractions for examining this product. The exciting question is, does this product have a limit value even in the case where we only contract a single edge between successive nodes? Setting accordingly the sequence, which maximizes v_{n+1}, into the product expressed by condition 4.3, we obtain a product that is limited, or to be more specific, which in the worst case $v_1 = 1$ converges (for n to infinity) towards 2:

$$\prod_{i=1}^{n}\left(1 + \frac{1}{3v_i}\right) = \prod_{i=1}^{n}\left(1 + \frac{1}{3\frac{3^{i-1}(v_1+1)-2^{i-1}}{2^{i-1}}}\right) = \prod_{i=1}^{n}\frac{3^i(v_1+1)-2^i}{3^i(v_1+1)-3*2^{i-1}} = \frac{1}{v_1} - \frac{1}{v_1}\left(\frac{2}{3}\right)^n + 1 \tag{A.8}$$

The above-illustrated last forming step, simplifies this product significantly into an expression waiving a product formulation. A detailed breakdown including all intermediate steps of this simplification is shown in the appendix **??**. The correctness of this simplification can be proven inductively too, which we detail in appendix **??**. The most important and the most interesting aspect of this result is, that the above simplified term cannot exceed the value 2, whatever you choose to insert into n or into v_1:

$$\frac{1}{v_1} - \frac{1}{v_1}\left(\frac{2}{3}\right)^{n+1} + 1 < 2$$

Since, as shown above, the product cannot exceed the value 2, the logarithmic product expression in the condition 4.3 cannot exceed the value one and this condition becomes a consistently true statement:

$$n\log_2 3 - \lfloor n\log_2 3\rfloor < 2 - 1$$

Thus, for $k = 3$ the condition 4.3 for alphas's upper limit is met for all sequences that maximize v_{n+1}.

A.8 Include additional divisions into the product

How does the product, contained in condition 4.3, look like if we include the additional m divisions into the Engel expansion as per section A.6? To answer this question, we consider the sequence $v_{n+1}, v_n, v_{n-1}, \ldots, v_2, v_1$ and we set $v_2 = \frac{3v_1+1}{2\cdot 2^m}$. Then reusing the continued fraction given by equation A.7, we obtain:

$$v_{n+1} = \frac{3\frac{3\frac{3\frac{3v_1+1}{2\cdot 2^m}+1}{2}+1}{2}+1}{2}\cdots = \frac{3\frac{3\frac{3v_2+1}{2}+1}{2}+1}{2}\cdots = \frac{3^{n-1}(v_2+1)-2^{n-1}}{2^{n-1}} \tag{A.9}$$
$$= \frac{3^{n-1}(\frac{3v_1+1}{2\cdot 2^m}+1)-2^{n-1}}{2^{n-1}} = \frac{3^n v_1 + 3^{n-1} + 3^{n-1}2^{m+1}}{2^{m+n}} - 1$$

The product will be calculated by using equation A.8:

$$\prod_{i=1}^{n}\left(1+\frac{1}{3v_i}\right) = \left(1+\frac{1}{3v_1}\right)\cdot\prod_{i=2}^{n}\left(1+\frac{1}{3v_i}\right) \tag{A.10}$$
$$= \left(1+\frac{1}{3v_1}\right)\cdot\prod_{i=1}^{n-1}\left(1+\frac{1}{3v_{i+1}}\right) = \left(1+\frac{1}{3v_1}\right)\cdot\left(\frac{1}{v_2}-\frac{1}{v_2}\left(\frac{2}{3}\right)^{n-1}+1\right)$$

Finally substituting $v_2 = \frac{3v_1+1}{2\cdot 2^m}$ into equation A.10 leads to the simplified formula of the product:

$$\prod_{i=1}^{n}\left(1+\frac{1}{3v_i}\right) = \left(1+\frac{1}{3v_1}\right)\cdot\frac{1-\left(\frac{2}{3}\right)^{n-1}+v_2}{v_2} = \frac{1+2^{m+1}}{3v_1} - \frac{2^m}{v_1}\left(\frac{2}{3}\right)^n + 1 \tag{A.11}$$

Example A.2 An example provides the sequence $v_1 = 661$, $v_2 = 31$, $v_3 = 47$, $v_4 = 71$, $v_5 = 107$. When we input $v_1 = 661$ with $m = 5$ and $n = 4$ into equation A.9 we retrieve the label of the vertex v_5:

$$v_5 = v_{n+1} = \frac{3^4\cdot 661 + 3^3 + 3^3\cdot 2^6}{2^9} - 1 = 107$$

In this sequence five ($m = 5$) additional divisions by two took place in the first step using v_1:

$$\frac{3\cdot 661 - 1}{2\cdot 2^5} = v_2 = 31$$

Let us now verify the formula for the product by taking this particular example. To this end we input $v_1 = 661$ together with $m = 5$ and $n = 4$ into equation A.11:

$$\left(1+\frac{1}{3\cdot 661}\right)\left(1+\frac{1}{3\cdot 31}\right)\left(1+\frac{1}{3\cdot 47}\right)\left(1+\frac{1}{3\cdot 71}\right) = \frac{1+2^6}{3\cdot 661} - \frac{2^5}{661}\left(\frac{2}{3}\right)^4 + 1 = 1.023215853$$

A.9 Condition for a limited growth of the Engel expansion

Let us look now into the question of what condition must be met to prevent a greater growth than a decline in Collatz sequences. Specifically we consider an Engel expansion comprising $n+1$ sequence members that include m additional divisions by two at the beginning. The last member v_{n+1} in such a sequence can be calulated by formula A.9. In order to restrict the growth of this sequence, we require that the last member has to be smaller than the first one. For this we define the condition $v_{n+1} < v_1$:

$$\frac{3^n v_1 + 3^{n-1} + 3^{n-1} 2^{m+1}}{2^{m+n}} - 1 < v_1$$

By transforming this inequality, which is thoroughly described in the appendix **??** step by step, we obtain the condition:

$$\frac{3^{n-1}\left(2^{m+1} - 2\right)}{2^{m+n} - 3^n} - 1 < v_1 \tag{A.12}$$

A.10 Engel expansions maximize the product

The question which sequence maximizes the target node v_{n+1} ties into the question which sequence maximizes the product in the condition for cycle-alpha's upper limit given by equation 4.3. The product formula that do not depend from all vertices $v_1, v_2, \dots v_n$ has been evolved in appendix A.4. This formla depends only from 2^α, from the starting node v_1 and the target node v_{n+1}:

$$\prod_{i=1}^{n}\left(1 + \frac{1}{kv_i}\right) = \frac{2^{\alpha_1+\ldots+\alpha_n} v_{n+1}}{k^n v_1}$$

In order to maximize this product, one needs to maximize the target node v_{n+1}, which exactly the Engel expansion does. Hence, for a given v_1, the Engel expansion is the worst case sequence maximizing the product in the condition for cycle-alpha's upper limit.

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About our approach

The results published in this paper have been achieved with an interdisciplinary approach. Not surprisingly, we applied classic mathematical theory and reasoning. Since we are convinced that the Collatz problem cannot be solved with classical maths alone, we furthermore used techniques and tools of modern data science. We combined the two fields in different ways. Firstly, we analyzed Collatz sequences and related features empirically, to derive new formulas and theorems. On the other hand, we used data science to challenge our proofs. As suggested by Karl Popper, we tried to falsify them with counterexamples. In the course of our work, we have learned that the combination of the two fields leads to a very efficient working mode.

Our main data science tool was a Python-API, which implements the theorems of this article and is optimized for processing arbitrarily big integers [1]:

https://github.com/c4ristian/collatz

After the generated data has been exported into a comma-separated values (CSV) file, a Java tool reads that file and carries out the visualization of the corresponding Collatz trees [99]:

https://github.com/Sultanow/collatz_java

For quick experiments or retracing the transformation chain as per figure 3.3 some notebooks may provide an efficient playground [93], but it should be noted that these are not designed for large amounts of data and professional use like Christian's API does:

https://github.com/Sultanow/collatz

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Communities

Mathematics is not the easiest discipline. Mistakes happen quickly and symbols, formulas or definitions can sometimes appear contradictory in the literature. The ambiguity/overriding of the notation for powers of an ideal and for the repeated direct product of a ring is only one example. All the more we are grateful for the numerous help from mathematics communities like the Stack Exchange Network, the MatheBoard Community, and Matroids Matheplanet. As an example let us mention Bill Dubuque, for whose instant help in matters of abstract algebra we are very grateful as for the help by many other kind people from the math communities.

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