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Eldar Sultanow | Christian Koch | Sean Cox

Collatz Sequences in the Light of Graph Theory

Second Version

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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, that one needs to show that this tree covers all (odd) natural numbers. A structured reachability analysis is hitherto not available. This paper does not claim to solve this million dollar problem. Rather, the objective is to investigate the problem from a graph theory perspective. We first define a tree that consists of nodes labeled with Collatz sequence numbers. This tree will then be transformed into a sub-tree that only contains odd labeled nodes. Finally, we provide relationships between successive nodes.

1.1 Motivation

The Collatz conjecture is a number theoretical problem, which has puzzled countless researchers using myriad approaches. Presently, there are scarcely any methodologies to describe and treat the problem from the perspective of the Algebraic Theory of Automata. Such an approach is promising with respect to facilitating the comprehension of the Collatz sequence's "mechanics". The systematic technique of a state machine is both simpler and can fully be described by the use of algebraic means.

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

1.2 Related Research

The Collatz conjecture is one of the unsolved mathematical Millennium problems [1]. 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 it is not reversible.

In his book "The Ultimate Challenge: The 3x+1 Problem" [2], along with his annotated bibliographies [3], [4] and other manuscripts like an earlier paper from 1985 [5], Lagarias has reseached 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 [6] 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 [7] 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 [8], 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 [9] 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 $x = 5 = 1010000\ldots = x_0x_1x_2\ldots$, 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 [5] and it is the inverse of the map Φ introduced by Bernstein [10]. 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 [11]. 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 this problem has been provided by Berg and Meinardus [12], [13] as well as Gerhard Opfer [14], 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 [15] contradicted Opfer's attempted proof.

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 [16], [17]. It is acknowledged that in order to prove the Collatz conjecture, then one needs to demonstrate that this tree covers all (odd) natural numbers.

The Stopping Time theory has been introduced by Terras [18], [19], [20]. He 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.

Many other approaches exist as well. From an algebraic perspective Trümper [21] analyzes The Collatz Problem in light of an Infinite Free Semigroup. Kohl [22] generalized the problem by introducing residue class-wise affine, in short, by utilizing rcwa mappings. A polynomial analogue of the Collatz Conjecture has been provided by Hicks et al. [23] [24] 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 [7].

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 $id_{\mathbb{Q}} = e$. 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 [25, 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 $E(G) = \left\{\{f, f \circ s\} \mid f \in F, s \in \left(S \cup S^{-1}\right) \setminus \{e\}\right\}$ [25, p. 57]. More precisely, the vertices are *labeled* by the elements (strings) of F.

In conformance with graph-theoretical precepts [26], [27], [28] 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 [21] 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" [29, p. 26], [25, 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 [30, p. 127], [31, p. 155], [32, p. 54] and [33, p. 188]. We define the evaluation function $ev_{S^*} : S^* \times \{1\} \to \mathbb{Q}$ that evaluates an element of S^*, id est a composition of q and r, for the given input value 1.

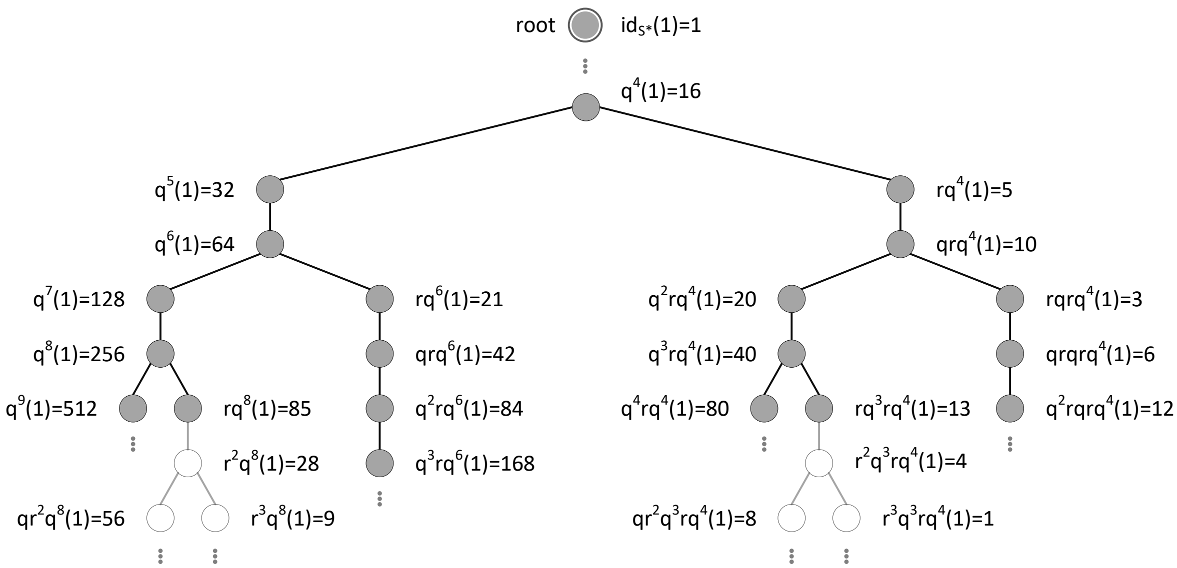

Figure 2.1: Small section of H_T with darkly highlighted subtree H_U

Furthermore we define the corestriction $ev^0_{S^*}$ of ev_{S^*} to $\mathbb{N}$. Since a corestricion of a function resricts the function's codomain [34, p. 3], the function $ev^0_{S^*}$ operates on a subset $T \subset S^*$ that contain only those compositions of q and r, which return a natural number when inputting the value 1.

The set T forms not 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 ***level of a vertex*** *or often called* ***depth of a vertex*** *is the length of the path from the root to this vertex [35, p. 804]. In other words, it is the vertex's distance (the number of edges in the path) from the root. The* ***height of a vertex*** *is its level plus one* $level(v) + 1 = height(v)$*, see [36, p. 169].*

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:

- ***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 arbitary 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 [37, p. 15].

- ***H_U* is a rooted tree:** According to Rosen [35, 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 [38, p. 52], for example, who distinguish between an undirected and directed rooted tree.

- ***H_U* is an out-tree:** There is exactly one path from the root to any other node [38, p. 52], which means that edge directions go from parents to children [39, 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* [39, p. 108].

- ***H_U* is a labeled tree:** For defining a labeled graph, Ehrig et al. [40, 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 $l_{V(H_U)}(v) = ev^0_{S^*}(l_{V(G)}(\iota(v)), 1)$, whereby $\iota : V(H_U) \hookrightarrow V(G)$ is the inclusion map [41, 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 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. Visually, we obtain H_C by contracting all edges in H_U that have an even-labeled target vertex, which (due to contraction) gets "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 [42, p. 27] and Loehr [43].

The tree H_C 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" [42, 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 is shown in figure 2.2. Other definitions of the same tree exist, see for example Conrow [44] or Bauer [45, p. 379].

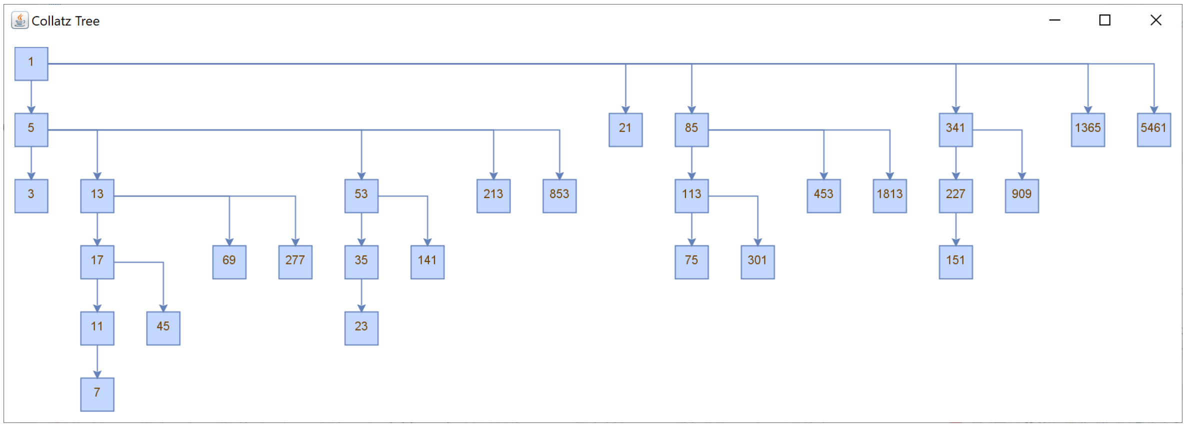

Figure 2.2: Small section of H_C

2.3 Relationship of successive nodes in H_C

Let v_1 and v_{1+n} be two vertices of H_C, where v_1 is reachable from v_{1+n} with $level(v_1) - level(v_{1+n}) = n$. Hence, a path $(v_{1+n}, \dots, v_1)$ exists between these two vertices. Theorem 2.1 specifies the following relationship between v_1 and v_{1+n}.

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

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:

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

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

$$v_{1+1} = 3v_1 \left(1 + \frac{1}{3v_1}\right) 2^{-a_1} = (3v_1 + 1)\, 2^{-a_1} = v_2$$

The path from v_2 to v_1 can conformly be expressed by a string $rq \cdots q$ of S^*, because of $v_1 =$

$r \circ q^{a_1}(v_2)$. We set $n = n+1$ for the step case, which leads to

$$\begin{aligned} v_{n+2} &= 3^{n+1} v_1 \prod_{k=1}^{n+1} \left(1 + \frac{1}{3v_k}\right) 2^{-a_k} \\ &= 3^{n+1} v_1 \left(1 + \frac{1}{3v_{n+1}}\right) 2^{-a_{n+1}} \prod_{k=1}^{n} \left(1 + \frac{1}{3v_k}\right) 2^{-a_k} \\ &= 3\left(1 + \frac{1}{3v_{n+1}}\right) 2^{-a_{n+1}} 3^n v_1 \prod_{k=1}^{n} \left(1 + \frac{1}{3v_k}\right) 2^{-a_k} \\ &= 3\left(1 + \frac{1}{3v_{n+1}}\right) 2^{-a_{n+1}} v_{1+n} \\ &= (3v_{1+n} + 1)\, 2^{-a_{n+1}} \end{aligned}$$

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

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

$$\begin{aligned} v_1 &= 3^n v_1 \prod_{k=1}^{n} \left(1 + \frac{1}{3v_k}\right) 2^{-a_k} \\ 2^{a_1+\cdots+a_n} &= \prod_{k=1}^{n} \left(3 + \frac{1}{v_k}\right) \end{aligned} \tag{2.2}$$

A similar condition has been formulated by Hercher [46]. 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 only trivial solutions exist since we are multiplying fractional numbers. However, we might change our position on this triviality when we examine the following case of using 5 instead of 3 which indeed forms a cycle in the $5x+1$ variant of Collatz sequences:

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

A detailed elaboration of the divisibility and a deeper understanding of the tree H_C needs to be performed in order to get towards any proof of the Collatz conjecture.

2.4 Relationship of sibling nodes in H_C

In a rooted tree, vertices which have the same parent are called "siblings" [30, p. 702], [35, p. 747]. Sibling vertices thus have 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 $l_{V(H_C)}(v_2) = 4 * l_{V(H_C)}(v_1) + 1$. This fact has been expressed differently by Kak [17] 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):

$$\begin{aligned} v_1 &= \frac{w*2^n-1}{3} \\ v_2 &= \frac{w*2^{n+2}-1}{3} = 4*v_1+1 \end{aligned}$$

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, the vertex v_2 is the right-sibling of v_1 and these two sibling vertices are immediate children of w.

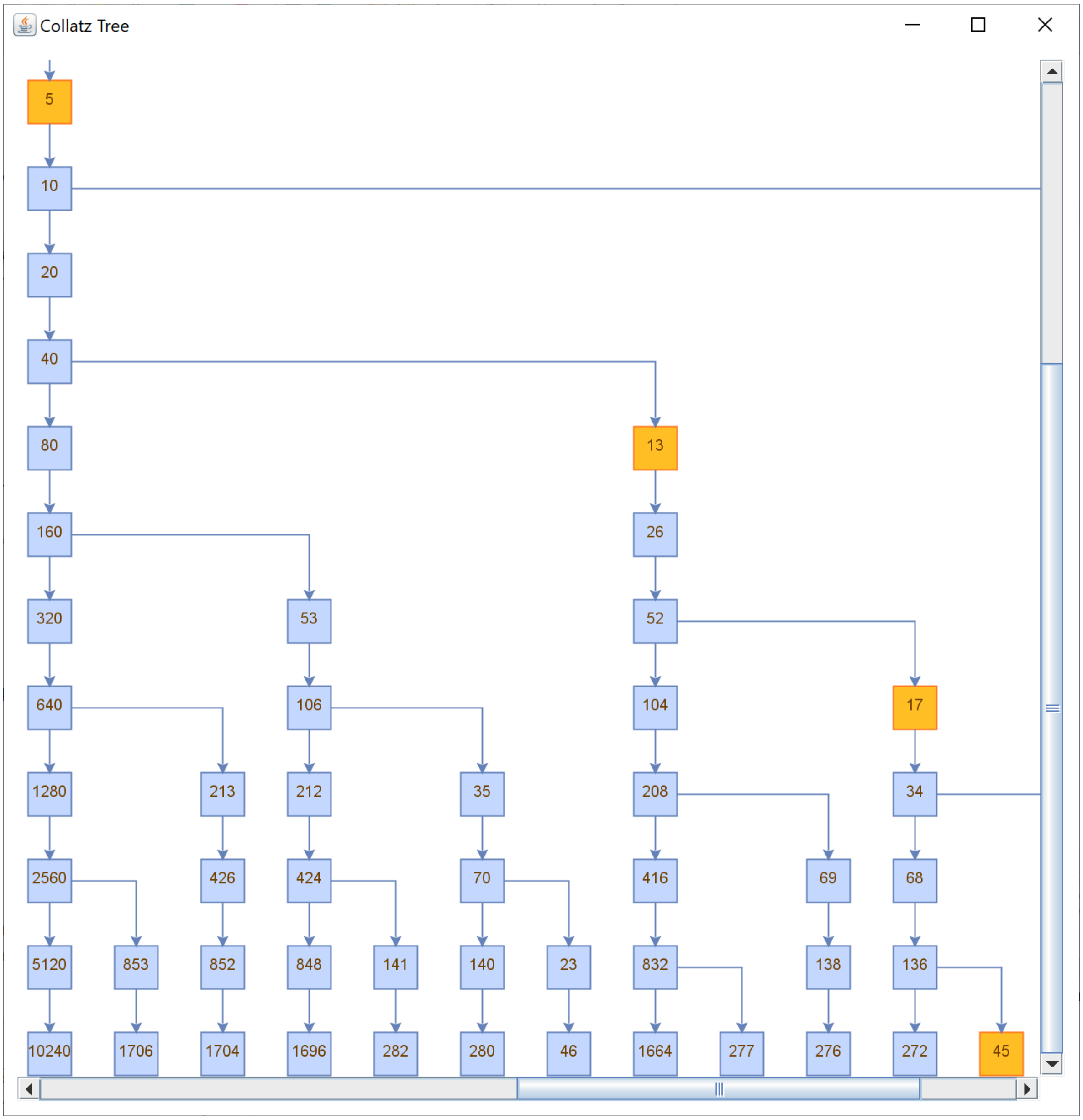

Figure 2.3: Section of H_U containing the path from 5 to 45

2.5 A vertex's n-fold left-child and right-sibling in H_C

Referring to the "left-child, right-sibling representation" of rooted trees [47, 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 shown 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 [47, 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.

Let w be a vertex in H_C and v_0 the left-child of w. The n-fold right-sibling of v_0 can be calculated as follows:

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

When setting $n = 0$, we trivially retrieve the vertex's w left-child:

$$v_0 = \textit{left-child}(w) = \frac{1}{3} * \left(w * 2^{3-w \bmod 3} - 1\right)$$

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 $v_3 = 213$:

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

3. Conclusion and Outlook

3.1 Summary

We defined an algebraic graph structure that expresses the Collatz sequences in the form of a tree. Moreover, we unveiled vertex reachability properties by examining the relationship between successive nodes in H_C. This compact definitory digression serves as a basis for further investigations of the tree H_C.

3.2 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 column, row and label. In addition, future steps may include the dealing with graphs that represent other variants of Collatz sequences, for instance $5x + 1$ or $181x + 1$. The interesting part of both variants just mentioned is that for these the existence of cycles is known.

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About Us

Eldar Sultanow is an Architect at Capgemini. In 2015, he completed his doctoral studies at the Chair of Business Information Systems and Electronic Government at the University of Potsdam. He likes mathematics, computer science and scuba diving.

✉ eldar.sultanow@capgemini.com

Christian Koch is data architect at TeamBank AG and lecturer at the Institute of Technology (Technische Hochschule Georg Simon Ohm) in Nuremberg. He began his career as an IT-Consultant and has since developed analytical systems for various European banks and public institutions. Christian likes programming, data science and swimming.

✉ christian.koch@th-nuernberg.de

Sean Cox is an Analyst at RatPac-Dune Entertainment. He is an expert in mathematics of finance and econometrics. Previously he worked for The Blackstone Group as mathematician and analyst. In his speare time he pursues outdoor activities.

✉ sean.cox@ratpacent.com