On the Repeat-Annotated Phylogenetic Tree Reconstruction Problem

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Abstract. A new problem in *phylogenetic inference* is presented, based on recent biological findings indicating a strong association between *reversals* (aka *inversions*) and *repeats*. These biological findings are formalized here in a new mathematical model, called *repeat-annotated phylogenetic trees* (RAPT). We show that, under RAPT, the evolutionary process — including both the tree-topology as well as internal node genome orders — is *uniquely* determined, a property that is of major significance both in theory and in practice. Furthermore, the repeats are employed to provide linear-time algorithms for reconstructing both the genomic orders and the phylogeny, which are NP-hard problems under the classical model of *sorting by reversals* (SBR).

1 Introduction

Phylogenetic inference and ancestral genome order reconstruction are important problems in evolutionary, genetic, and bioinformatic studies [Sankoff, 2003,Bourque et al., 2005] . In these problems one seeks to reconstruct the phylogeny of a given set of organisms as well as the genomic order (*i.e.*, the order of the genomic segments) of their ancestors; see for example Figures 1a and 1c. Here, a one-to-one mapping of the orthologous segments of the two strains *Xanthomonas campestris* pathovar *campestris* ATCC 33913 (*X. campestris*) [da Silva et al., 2002] and 8004 (*X. campestris* 8004) [Qian et al., 2005] is presented schematically. These bacteria cause black rot disease in crucifers such as *Brassica* (cabbage) and *Arabidopsis* (mustard), which results in severe losses in agricultural yield world-wide [da Silva et al., 2002] . This figure suggests that 3 reversals have affected the two bacteria since their divergence. However, during the speciation of which of the two bacteria have these reversals occurred and what is the ancestral genomic order? Figure 1

Using current methods, reconstructing ancestral genomic order involves solving a multiple *sorting by reversals* (SBR) problem. In SBR, which has been thoroughly examined over the last two decades [Watterson et al., 1982, Kececioglu and Sankoff, 1993, Kececioglu and Sankoff, 1994, Bafna and Pevzner, 1996, Berman and Hannenhali, 1996, Chen and Skiena, 1996,Kaplan et al., 1997,Bafna and Pevzner, 1998,Hannenhalli and Pevzner, 1999,Gu et al., 1999, Bader et al., 2001, Christie and Irving, 2001, Bergeron et al., 2002, Hartman, 2003, Hartman and Sharan, 2004, Bergeron et al., 2004, Tannier and Sagot, 2004, Bender et al., 2004,Swidan et al., 2004,Bergeron et al., 2005,Bergeron, 2005], one represents the one-to-one orthologous mappings as permutations and the inversion mutations as reversal operations. The goal of the SBR optimization problem is to find a phylogeny and corresponding reversal scenarios along its branches with the minimum number of reversals. In SBR, however, the ancestral genomic order cannot be implied based solely on the comparison of a pair of genomes, as is needed for the bacteria pair in Figure 1a. Moreover, adding one more organism to enable the deduction of the ancestral order (in which case the problem is known as the *median problem* [Sankoff and Blanchette, 1998])makes this task NP-hard [Caprara, 1999]. Nonetheless, this problem was addressed by both exhaustive search and heuristic techniques [Moret et al., 2001, Bourque and Pevzner, 2002].

The ancestral genome order reconstruction problem described above extends to reconstructing large phylogenetic trees over multiple input leaves (including or excluding the recovery of genomic order in internal nodes). Current phylogenetic inference methods, based on different biological evidence ranging from phenotypic morphologies to various genotypic mutations — including point mutations (distance-based, maximum-likelihood, and parsimony approaches), gene insertions and deletions (the Dollo parsimony approach), and genome rearrangements (distance-based and parsimony approaches) — are computationally hard. Moreover, current approaches often yield many alternative solutions; choosing the most sound phylogeny among them has very important biological consequences, but is yet a very challenging task [Martin et al., 2002, Wolf et al., 2001, Brocchieri, 2001] .

In this paper we investigate a new approach to phylogenetic inference and ancestral genome order reconstruction. The new approach is inspired by a recent biological discovery regarding the role of *repeats*, *i.e.*, short genomic sequences that are highly similar to each other, in inducing reversals (or recombinations in general). Several studies indicate a strong association between repeats and recombination events [Rocha, 2004, Rocha, 2003b, Achaz et al., 2003, Rocha, 2003a, Rocha et al., 1999]. As reviewed in [Bzymek and Lovett, 2001, Kowalczykowski et al., 1994] , repeats cause rearrangements, either by a mechanism of *illegitimate recombination* [Smith, 1989], or by a mechanism of *homologous recombination* [Rothstein et al., 2000, Lusetti and Cox, 2002] (see Figure 2 for an illustration of this phenomenon). Moreover, these findings demonstrate that most of the repeats engaged in reversals correspond to *mobile* DNA elements, *i.e.*, regions of DNA that selfishly duplicate and move into new sites [Mahillon and Chandler, 1998]. Hence, these repeats are usually found only in the organism affected by the reversals; see, *e.g.*, [Parkhill et al., 2003] . This new and important information regarding the repeats became accessible recently with the availability of many sequenced genomes and its automatic generation is made possible by the development of accurate comparative genome mapping methods, see, *e.g.*, [Swidan et al., 2006, Qian et al., 2005]. The new data motivates the enhancement of previous phylogenetic models with additional information in the form of repeat "footprints", in order to make their predictions more realistic and increase their potential for producing biologically relevant insights. Figure 2

Qian *et al.* (2005) demonstrate an initial utilization of repeats in the task of ancestral genome order reconstruction of the *Xanthomonas campestris* bacteria. They have identified two identical IS1478-related insertion sequences (corresponding to the repeat pair $-b, b$ in Figure 1b) spanning a putative recombination site. Moreover, they predicted a rearrangement scenario for transforming one genome to the other — see `http://www.genome.org/content/vol0/issue2005/images/data/gr.3378705/DC1/SI_Fig_2.gif` for a detailed (and vivid) animation of their prediction. We continue their analysis by applying our approach to the very same data: in Figures 1b and 1d we incorporate the information regarding the repeats into the mapping. In addition to the repeat pair reported by Qian *et al.*, we identify two more pairs spanning two putative recombination sites. According to the repeats, one inversion occurred during the speciation of *X. campestris*, while two inversions occurred during the speciation of *X. campestris* 8004. Given this information, deducing the ancestral genomic order is straightforward, as shown in Figure 1d.

The above example demonstrates how repeats can be utilized to uniquely determine the order of the ancestral genomic segments — based solely on pairwise genomic comparisons. Furthermore, it shows that the "repeat footprints" aid in the efficient computation of ancestral genomic orders. To generalize these observations, in Section 2 we formalize the biological assumptions introduced above into a theoretical evolutionary model. In Section 3 we study the pairwise case and present two important results: uniqueness of the solutions and simplification of the computation. In Section 4 we show that these two results scale up to the more general case of multiple genomes. For a formal overview of the combinatorial results of this paper we refer the reader to Section 2.1.

2 A Formal Model Based on Repeats

The model described in this paper is based on the following biological assumptions:

1. Reversals are usually induced by *inverted* repeat pairs, *i.e.*, repeats having opposite orientations [Kowalczykowski et al., 1994, Bzymek and Lovett, 2001] .
2. Repeats engaged in reversals — corresponding mostly to mobile DNA elements — are easily identified on the borders of reversed genomic segments, and are present only in the affected organism [Kowalczykowski et al., 1994, Parkhill et al., 2003, Qian et al., 2005].
3. The information mapping each repeat to its pair-mate is part of the input[1].
4. Each repeat has a very low probability for causing a reversal that remains fixed in the population [Hughes, 2000, Swidan et al., 2006] . Therefore, in our model we assume that each repeat causes up to one reversal.

Note that though the above assumptions may not capture the great variety found in real biological problems, it is easy to check if a given set of input genomes follows these assumptions. Furthermore, as demonstrated by the theoretical results listed in Section 2.1, the assumptions above offer a solid basis for potential future extensions and enhancements.

Based on Assumption 3, the input to our problem comprises sequences, referred to as *repmaps*, of both permutation elements, belonging to a set N, and paired repeats, belonging to a set R. Each permutation element appears exactly once in the repmap, while each repeat appears exactly twice. In addition to the permutation elements (represented by numbers) and based on Assumption 1, the repeats (represented by lowercase characters) are also signed.

[1]This information can be obtained using techniques similar to those standardly used for preparing permutations.

Given a repmap s, two repeat elements $s_i, s_j \in R$ are considered a pair if $|s_i| = |s_j|$ (*i.e.*, their absolute values are equal). If they have opposite signs ($s_i = -s_j$) we refer to them as an *inverted repeat pair*; otherwise they are called a *direct repeat pair.* The set of repeats appearing in s is denoted by $R(s) = \{|s_i|, s_i \in R\}$ and referred to as the *repeat set.* We denote the restriction of s to the permutation elements in N by $s|_N$ and refer to it as the *induced permutation.* The restriction of s to the repeat elements is denoted by $s|_R$ and is referred to as the *repeat subsequence.*

Example. Consider the repmap $s = \ 1 \ \ a \ \ -4 \ \ -a \ \ -b \ \ 3 \ \ 2 \ \ -b \ \ 5$. Here, $+a, -a$ is an inverted repeat pair, while $-b, -b$ is a direct repeat pair. Moreover, we have $R(s) = \{a, b\}$. The induced permutation is $s|_N = \ 1 \ \ -4 \ \ 3 \ \ 2 \ \ 5$, and the repeat subsequence is given by $s|_R = \ a \ \ -a \ \ -b \ \ -b$. Figure 3

The next three definitions are intended to formalize the biological assumptions (1-4) into a mathematical model of an evolutionary process. The first definition is based on Assumption 1, as follows.

Definition 1 (Legal Reversal)**.** Let $s = s_1, \ldots, s_n$ be a repmap and let $\rho = \rho(i, j)$ for $1 < i < j < n$ be a reversal affecting the subsequence $s_i, \ldots, s_j$ in s. The reversal ρ is called *legal* if it is bordered by an inverted repeat pair, *i.e.*, if $s_{i-1} = -s_{j+1}$ (see Figure 3c). We say then that ρ *fulfills* the repeat pair s_{i-1}, s_{j+1}.

The next two definitions are both based on Assumptions 2 and 4.

Definition 2 (Legal Scenario)**.** Given a reversal sequence $\varrho = \rho_1, \ldots, \rho_m$ affecting s, we say that ϱ is a *legal scenario relative to a subset of repeat pairs* $\mathscr{R} \subseteq R(s)$ if $\forall i \in \{1, \ldots, m\}, \rho_i$ is a legal reversal when acting on $s \cdot \rho_1 \cdots \rho_{i-1}$ and if ϱ fulfills each repeat in $\mathscr{R}$ exactly once (see Figure 3c). If $\mathscr{R} = R(s)$, we refer to ϱ simply as a *legal scenario.* If $\mathscr{R} \neq R(s)$ is obvious from the context, we refer to ϱ as a *partially legal scenario.*

Definition 3 (RAPT)**.** Given a repmap S (ancestor), a *Repeat-Annotated Phylogenetic Tree* originating in S (see Figure 4) is a triplet (T, f, g), where $T = (V, E)$ is a directed tree with root $v_r \in V$ such that all the inner nodes (except perhaps the root) are of degree ≥ 3, $f : V \rightarrow (R \cup N)^*$ maps *assignments* (*i.e.*, repmaps) to the nodes, and $g : E \rightarrow 2^{R(S)}$ maps *labels* to the edges, such that:

1. The edge labels are a partition of $R(S)$, *i.e.*, for every two edges $e, e' \in E : g(e) \cap g(e') = \emptyset$ and $\bigcup_{e \in E} g(e) = R(S)$.
2. The assignments to the nodes fulfill the following two requirements:
    (a) The assignment to the root v_r equals S, that is $f(v_r) = S$.
    (b) Assuming $u \in V$ is the immediate parent of $v \in V$ and that $e \in E$ is the edge connecting them, we require that $g(e) \subset R(f(u))$ and that there exists a legal scenario $\rho_1, \ldots, \rho_m$ with respect to $g(e)$ such that $(f(u) \cdot \rho_1 \cdots \rho_m)|_N = f(v)|_N$ (Definition 2).
3. The repeat set $R(s)$ of a leaf repmap s contains only repeats that engaged in reversals at some point during the history of s, *i.e.*, $R(s) = g(\text{path}(v_r, s))$.

Figure 4

2.1 The Main Results of This Paper

In this paper we study the following problems: Can one reconstruct an unknown RAPT (T, f, g) given, as input, a set L of the corresponding leaf repmaps? More specifically, does L uniquely determine the RAPT? Are the legal scenarios linking the assignments in the RAPT nodes unique? Furthermore, can one efficiently reconstruct the unknown RAPT and the corresponding scenarios? Herein we summarize the answers to these questions.

First, in Section 3, we consider the basic case in which the tree T of the RAPT contains a single leaf and a single ancestor. Since in this case both the tree T and the labels g are trivially determined, our results pertain to both the scenario and the ancestral assignment reconstructions, as follows:

Uniqueness: We show that the ancestral assignment is uniquely determined (Section 3.1). This result is surprising given the ambiguity of the scenarios. (Section 3.2).

Complexity: We give a linear-time algorithm for reconstructing the ancestor (Section 3.3.1). Contrary to the classical SBR problem, our algorithm utilizes the constraints introduced by the repeats to calculate the unique ancestor. This algorithm is then employed to solve the problem of reconstructing a plausible legal scenario, by a reduction to SBR (Section 3.3.2).

Next, in Section 4, the multiple leaf RAPT is studied. Based on the results obtained for the single leaf case, it is straightforward to show that, in the multiple leaf case, the tree topology T, the edge labels g, and the leaf repmaps L both uniquely determine the induced permutations in the inner node assignments and also enable their reconstruction in linear-time. Hence, the complexity and uniqueness issues are reduced to the pair (T, g). To investigate the latter, we introduce a new data structure, which is an abstraction of such (T, g) pairs, called *set-tries* (see Figure 4), which are trie-like structures over sets instead of words (Section 4.1). In terms of this abstraction, our results can be formulated as follows:

Uniqueness: We show that the leaf set collection uniquely determines the underlying set-trie(Section 4.2).

Complexity: We give a linear-time algorithm to efficiently reconstruct set-tries from an input leaf set collection(Section 4.3).

3 The Single Leaf RAPT

Throughout this section, we assume without loss of generality that the repmaps are given in an easy to handle format, as follows. Consider a repmap (ancestor) S to which a legal scenario ϱ was applied and denote the result by $s = S \cdot \varrho$ (the notation of S denoting the ancestor and s denoting the descendant is used consistently throughout this section). We assume that S (and hence s) starts and ends with a permutation element (otherwise it can be padded). In addition, we assume that S (and hence s) does not contain successive permutation elements (or otherwise they can be united to form a single new permutation element). Figure 5

Whereas uniting successive permutation elements into a single element is straightforward, dealing with successive repeat elements in the input sequence is more challenging. For instance, having successive repeats implies that the corresponding breakpoints may have been reused (the issue of breakpoint reuse has been repeatedly debated in the literature and is currently controversial [Sankoff and Trinh, 2005, Trinh et al., 2004, Pevzner and Tesler, 2003,Bourque and Pevzner, 2002,Peng et al., 2006]). From a modeling point of view, however, successive repeats distinguish the RAPT problem from the SBR problem: when they are present in a repmap, its set of legal scenarios (see Definition 2) and the set of SBR scenarios [Kececioglu and Sankoff, 1993] of its induced permutation are not necessarily the same, as demonstrated in Figure 3. This is due to the fact that SBR aims to minimize the number of reversals, whereas RAPT is driven by the objective of fulfilling the constraints imposed by the repeats. Still, for a subset of the repmaps, both sets of legal and SBR scenarios are equal. We refer to these special repmaps as "normalized" and define them below. Normalized repmaps serve as stepping stones for our study; see Figures 3 and 5.

Definition 4 (Normalized Repmap)**.** A repmap S is a *normalized repmap* if between every two repeats in it there is a permutation element from N.

3.1 Asserting Uniqueness of Ancestor

In this section we prove that all legal scenarios lead to the same ancestral repmap. This result is surprising, given the richness of the set of all legal scenarios (see Section 3.2 and Figure 6) . We first consider the special subclass of normalized repmaps(Claim 1–Lemma 7). In this subclass, the proof of uniqueness involves a breakpoint counting argument, showing that all legal scenarios are optimal sorting scenarios (namely SBR scenarios). Next, we extend the uniqueness claim from the subset of normalized repmaps to the general repmap case(Claim 8–Theorem 10). The proof here is achieved by transforming any given repmap to a corresponding normalized one and by asserting that this transformation indeed preserves the uniqueness property.

Without loss of generality, we assume that $S|_N$ is sorted (the elements can be always renamed to accommodate this order). In the following we show that legal scenarios affecting normalized repmaps are SBR scenarios.

Claim 1. *Let S be a repmap, ϱ a legal scenario, and $s = S \cdot \varrho$. Then S is normalized iff s is normalized.*

Proof. Assume S is normalized. We show that s is normalized as well. The other direction is obtained by changing the roles of S and s.

The proof is by induction on m, the number of reversals in the scenario ϱ.

Base case: for $m = 1$, assume the first reversal ρ_1 fulfills the inverted repeat S_i and its pair-mate S_j, where $i < j$. Since S is normalized, we have $S_{i+1}, S_{j-1} \in N$ (notice that $i + 1 \leq j - 1$). Denote $t = S \cdot \rho_1$. Then we get $t_{i-1}, t_i, t_{i+1} = S_{i-1}, S_i, -S_{j-1}$ and $t_{j-1}, t_j, t_{j+1} = -S_{i+1}, S_j, S_{j+1}$, and hence each of the repeats t_i and t_j is still surrounded by permutation elements. The rest of the repmap stays trivially normalized.

The induction step is established similarly. □

Definition 5 (Surrounding)**.** Given a repmap t, the *surrounding* of an element t_i is the subsequence of elements t_{i-1}, t_i, t_{i+1}.

Claim 2. *Let S be a normalized repmap and $\varrho = \rho_1, \ldots, \rho_m$ a partially legal scenario (see Definition 2). Denote $t = S \cdot \rho_1$, where ρ_1 fulfills the inverted repeat pair S_i and S_j. Then the surroundings of the fulfilled repeats $S_i = t_i$ and its pair-mate $S_j = t_j$ remain contiguous throughout the rest of the reversals in ϱ.*

Proof. By Claim 1, t is normalized. Thus, the surrounding of t_i, namely t_{i-1}, t_i, t_{i+1}, and the surrounding of t_j, namely t_{j-1}, t_j, t_{j+1}, contain no repeats. Since the inverted repeat pair t_i and t_j is already fulfilled, and since it is assumed that each repeat pair is fulfilled exactly once, no reversal can cut through their surroundings. □

By induction on Claim 2 we get the following corollary.

Corollary 3. *Let S be a normalized repmap and $\varrho = \rho_1, \ldots, \rho_m$ a partially legal scenario. Denote $t = S \cdot \rho_1 \cdots \rho_k$ for $k < m$. The surrounding of any fulfilled repeat pair in $\rho_1, \ldots, \rho_k$ remains contiguous throughout the rest of the reversals in ϱ.*

Corollary 3 implies that the surrounding of each repeat in s is the same as its surrounding after the reversal fulfilling it was applied during the scenario ϱ. This observation as well as the following definition and theorem, commonly used in SBR, are helpful for the reconstruction step, which we consider next.

Definition 6 (Breakpoint)**.** Given a repmap s, a *breakpoint* in $t = s|_N$ is a pair of successive elements t_i, t_{i+1}, such that $t_{i+1} - t_i \neq 1$ [Kececioglu and Sankoff, 1993]. A *breakpoint* in s is a pair of permutation elements that is a breakpoint in $s|_N$. If $s|_N$ contains no breakpoints, we call it *sorted*. We call s *sorted* if $s|_N$ is sorted.

Theorem 4 ([Kececioglu and Sankoff, 1993])**.** *Each reversal can create at most two breakpoints.*

Lemma 5. *Let S be a (sorted) normalized repmap and $\varrho = \rho_1, \ldots, \rho_m$ be a legal scenario. Denote $s = S \cdot \varrho$. Then, a legal reversal affecting s eliminates two breakpoints.*

Proof. Suppose the reversal fulfills the inverted repeat pair s_p and s_q in s. Let ρ_k for $k < m$ be the reversal in the scenario ϱ fulfilling this repeat pair. Denote $t = S \cdot \rho_1 \cdots \rho_{k-1}$ and let t_i and t_j be the corresponding elements to s_p and s_q in t, respectively. Without loss of generality, we assume that $i < j$ (otherwise rename p and q). By Corollary 3 the surroundings of s_p must be either $t_{i-1}, t_i, -t_{j-1}$ or $t_{j-1}, -t_i, -t_{i-1}$. Similarly, the surrounding of s_q must be either $-t_{i+1}, t_j, t_{j+1}$ or $-t_{j+1}, -t_j, t_{i+1}$. However, since t_i and t_j are an inverted pair in $t \cdot \rho_k$, and s_p and s_q are an inverted pair in s, t_i and t_j (as well as their surroundings by Corollary 3) must have been affected either both by an odd or both by an even number of reversals throughout $\rho_{k+1}, \ldots, \rho_m$. Therefore, if the surrounding of s_p equals $t_{i-1}, t_i, -t_{j-1}$, then the surrounding of s_q must equals $-t_{i+1}, t_j, t_{j+1}$. If, on the other hand, the surrounding of s_p equals $t_{j-1}, -t_i, -t_{i-1}$ then the surrounding of s_q must equals $-t_{j+1}, -t_j, t_{i+1}$.

In the first configuration, if $q < p$ we get that after performing the legal reversal the surroundings become $-t_{i+1}, t_j, -t_{i-1}$ and $-t_{j+1}, t_i, -t_{j-1}$. Note that t_{i-1} and t_{i+1} are successive in t, and have not been affected by any reversal throughout $\rho_1, \ldots, \rho_{k-1}$. Therefore, they are successive in S as well. A similar claim holds for t_{j-1} and t_{j+1}. Thus, the legal reversal combines two pairs of successive elements and hence reduces the number of breakpoints by 2. The case $p < q$ and the other configuration is dealt with similarly. ☐

By induction on Lemma 5 we get the following corollary.

Corollary 6. *Let S be a normalized repmap and $\varrho = \rho_1, \ldots, \rho_m$ a legal scenario. Denote $s = S \cdot \varrho$. Then, each reversal in a partially legal scenario ϱ' affecting s eliminates two breakpoints.*

Let $k = |R(S)|$ be the number of different repeats in S. Since each repeat is fulfilled exactly once, the number of reversals in a legal scenario affecting S is k as well. By Theorem

4, the number of breakpoints in s is bounded by $2k$. Corollary 6 implies that a legal scenario eliminates $2k$ breakpoints and does not create new ones. Thus, all legal scenarios must be SBR scenarios and hence lead to the same unique ancestral permutation $S|_N$. Because the induced permutation of the reconstructed ancestor is unique, and by a similar argument to the one used in the proof of Lemma 5, the repeats' order and signs in the reconstructed ancestor must be identical to those in S. Therefore, in summary, all legal scenarios lead to the same ancestor, namely S:

Lemma 7. *Let S be a normalized repmap, ϱ a legal scenario, and $s = S \cdot \varrho$. Then, all legal scenarios affecting the (normalized) repmap s result in the same correct ancestor S.*

Now assume that S is a repmap (not necessarily normalized). We need to show that all legal scenarios affecting s result in S. In order to achieve this, we first transform S to a normalized repmap and then apply Lemma 7. The transformation is done by adding rational numbers between successive repeats. Thus, the resulting repmap is no longer a permutation of integers. To distinguish it, we refer to it as an *extended repmap*.

Claim 8. *Let S be a sorted repmap, ϱ a legal scenario, and $s = S \cdot \varrho$. There exists an extended normalized repmap S' such that S is a subsequence of S', $S|_R = S'|_R$, and S' is sorted.*

Proof. Let $S_j \cdots S_k \in R^*$, for $j < k$, be a block of successive repeats in S surrounded by permutation elements $S_{j-1}, S_{k+1} \in N$. Adding the rational number $S_{j-1}+(i-j+1)/(k-j+1)$ after the repeat S_i for $i \in \{j, \ldots, k-1\}$ and repeating the process for all blocks of successive repeats result in a sorted (extended) normalized repmap S' having S as a subsequence, which fulfills $S|_R = S'|_R$ as well. $\square$

Note that since the repeat sequences in S and S' are the same, the legal scenarios affecting S and S' are also the same. Thus we apply ϱ to S' and denote the result by $s' = S' \cdot \varrho$. Since the elements of S in S' undergo the same scenario when applying ϱ to either of S or S', the relative order between these elements in s and s' is the same. This observation establishes the following claim:

Claim 9. *Let S be a repmap, ϱ a legal scenario, and $s = S \cdot \varrho$. Let S' be the normalization of S as in Claim 8 and let $s' = S' \cdot \varrho$. Then s is a subsequence of s'.*

Claim 9 implies that s and s' have the same set of legal scenarios. However, s' is normalized. Let ϱ' be a legal scenario affecting s and s' (see Figure 5). By Lemma 7, we know that $S' = s' \cdot \varrho'$. By applying Claim 9 to s, s' and ϱ' (where $S \leftarrow s, S' \leftarrow s', \varrho \leftarrow \varrho'$), we get that $P = s \cdot \varrho'$ is a subsequence of $S' = s' \cdot \varrho'$, and is hence sorted. Since, by definition, S is a subsequence of S' as well, and P and S have exactly the same elements, we get that $P = S$. Thus, we conclude that all legal scenarios on s must result in the same correct ancestor S.

Theorem 10 (Uniqueness)**.** *Let S be a repmap, ϱ a legal scenario, and $s = S \cdot \varrho$. Then, all legal scenarios affecting s result in the same correct ancestor S.*

3.2 Are the Reconstructed Scenarios Unique?

Theorem 10 would have been trivial to prove had there been a single legal scenario affecting s, or alternatively, if all the legal scenarios affecting s were "very similar" (as defined below). In this section we show that such is not the case, and that these scenarios might be significantly different.

Given two disjoint reversals, one can always reorder them to get different scenarios. However, these scenarios, despite being different, are "very similar", and trivially yield the same ancestral repmap. Formally, we define "very similar" as an equivalence relation over the space of scenarios as follows: Given a reversal ρ affecting a repmap s, we define the image $\mathrm{Im}(\rho)$ of the reversal ρ to be the set of permutation elements in s that the reversal affects.

Example. Suppose $s = \; 1 \;\; a \;\; -4 \;\; -a \;\; [-b \;\; 3 \;\; 2 \;\; b] \;\; 5$, and $\rho = \rho(5,8)$ (designated by the brackets [ ]), then $\mathrm{Im}(\rho) = \{3, 2\}$.

Thus, given a scenario $\varrho = \rho_1, \ldots, \rho_m$, we define the image of the scenario to equal the set of images collected from all its reversals: $\mathrm{Im}(\varrho) = \{\mathrm{Im}(\rho_i) : i \in \{1, \ldots, m\}\}$. Given two legal scenarios ϱ_1 and ϱ_2 affecting the same repmap s, we say that they are equivalent, and denote $\varrho_1 \equiv \varrho_2$, if they affect the same sets of elements in s, *i.e.*, $\mathrm{Im}(\varrho_1) = \mathrm{Im}(\varrho_2)$. One can easily verify that the above relation is an equivalence relation over the space of scenarios.

We can now check the "complexity" of the set of legal scenarios affecting a repmap s relative to the above defined equivalence relation. More specifically, the question is whether the set of legal scenarios affecting a repmap s is contained in a single equivalence class? Figure 6 demonstrates that such is not the case. Figure 6

3.3 Algorithms for Ancestor and Scenarios Reconstruction

Given a repmap $s = S \cdot \varrho$, where S and ϱ are unknown, we present a linear-time algorithm for reconstructing S and a sub-quadratic algorithm for reconstructing a possible legal scenario ϱ', where, by Theorem 10, $S = s \cdot \varrho'$. The reconstruction of the ancestor in linear-time is made possible by utilizing the constraints introduced by the repeats and the strong connection established between the repeats and their surroundings in normalized repmaps(Corollaries 3 and 6). In fact, we first show how to transform s to a normalized repmap s' for which the ancestor S' is sorted[2] based only on the repeat subsequence $s|_R$ (see Figure 5). Then we simply rename the matching elements from S' to obtain S (see Figure 3b). Unlike Claim 8, where we transformed a *sorted* repmap to an extended normalized one, here the transformation to a normalized format is done based on the repeats in s and without knowing the ancestor repmap S.

[2]Note that, unlike the previous section, here we can no longer assume without loss of generality that S is sorted.

After computing the ancestor S, we solve the problem of finding a legal scenario transforming s to S in sub-quadratic time by a reduction to SBR. In the general case, as exemplified in Figures 3c and 3d, applying SBR to $s|_N$ may yield illegal scenarios. This is due to the fact that SBR aims to minimize the number of reversals, while RAPT is driven by the objective of fulfilling the constraints imposed by the repeats. However, this barrier is overcome here by transforming a repmap to its normalized format, which intuitively uses $O(|s|)$ additional "virtual" permutation elements to simulate the constraints imposed by the repeats (see Figures 3a and 3b). Thus, to reconstruct a legal scenario, we apply SBR algorithms to the permutation elements of s' and S' and show that the resulting scenario is legal on s. Note that whereas reconstructing the ancestor in linear-time is made possible thanks to the constraints introduced separately by each repeat pair, calculating a legal scenario is complicated by the interaction between the constraints introduced by the different repeat pairs.

3.3.1 Reconstructing the Unique Ancestral Repmap S

Reconstructing the ancestral repmap S can be naïvely achieved by applying some of the techniques demonstrated in [Kaplan et al., 1997, Bergeron, 2005] to the *overlap graph* constructed over the repeat pairs. This approach, however, yields a quadratic-time algorithm for both reconstructing the ancestor and finding a legal scenario.

Here, we present a different approach (with lower complexity) for tackling the problem. Let S be an ancestral repmap, ϱ a legal scenario affecting S, and $s = S \cdot \varrho$. Consider a transformation of S yielding a normalized sorted repmap S', and let $s' = S' \cdot \varrho$. According to the above and since all the transformations are reversible, calculating s' from s can be done by the following series of transformations:

$$s \longrightarrow S \longrightarrow S' \longrightarrow s'.$$

However, since S is unknown, this path is intractable. Yet, surprisingly, calculating s' from s can alternatively be done based on the repeat sequence $s|_R$ and without knowing S. Intuitively, this can be explained as follows. Since s' is normalized, the locations of the permutation elements are constrained by the locations of the repeats. Moreover, as Corollaries 3 and 6 show, each permutation element is constrained by the repeat next to it. Thus, the position of a permutation element can be determined from local information (the position of a single repeat) in constant time, and the whole repmap can be reconstructed in linear-time. Note that the above transformation implies that the diagram having S, S', s, and s' as its vertices is commutative (Figure 5).

Before describing the reconstruction algorithm formally, we give an example illustrating its strategy.

Example. Consider the sequence s and the corresponding sequence s' in Figure 3a and suppose that we wish to recover s' based on $s|_R$. The first and second elements in s' are easily fixed, since s' must always start with 1 and the second element in s' always equals to the repeat appearing in the second position of s. Fixing the third element in s' is more challenging. For that, we consider the second element in both s and s', *i.e.*, the repeat $-a$, and its corresponding pair-mate — the repeat a. By Corollary 3 we know that, since S' is sorted and normalized, once the repeat pair $\{-a, a\}$ got fulfilled while transforming S' to s', the surroundings of both repeats remain contiguous. In particular, the permutation element 2, which appears directly after the repeat $-a$ in S' (see Figure 3b) must appear in the surrounding of the repeat a in s'; its exact position (*i.e.*, before or after the repeat) is determined based on two factors: whether the repeat pair is inverted or direct, and whether the preceding permutation element 1 appears before the repeat $-a$ or after it. In this example, since the repeat pair is inverted and since the preceding permutation element 1 appears before the repeat $-a$, the permutation element 2 must precede the repeat a in s'(this results from a similar argument to the one presented in the proof of Lemma 5). The sign of the permutation element 2 is determined via a similar consideration.

The idea demonstrated in the above example is generalized via the following lemma:

Lemma 11. *Let P be a sorted normalized repmap, ϱ a legal scenario affecting it, and $p = P \cdot \varrho$. Consider a permutation element of p, $1 \neq p_i \in N$. Given the index of the preceding permutation element $p_i - 1$, the index j of the successive permutation element $p_i + 1$ is determined by i, p_i, and the repeat subsequence $p|_R$.*

Proof. Consider the repeats p_{i-1} and p_{i+1} surrounding p_i, and let $p_{i'}$ and $p_{i''}$ be their counterpart repeats, respectively. By Corollary 3, the neighboring permutation elements $p_i - 1$ and $p_i + 1$ are neighbors to the repeats $p_{i'}$ and $p_{i''}$. Since the index of $p_i - 1$ is given, we know near which repeat it is found. Suppose first that $p_i - 1$ is found near the repeat $p_{i'}$ (the other case is handled similarly). This implies that $p_i + 1$ is found near the repeat $p_{i''}$. Moreover, by Corollary 6, the sign and the relative order between $p_i + 1$ and the repeat $p_{i''}$ is determined by the sign of p_i and whether the repeat pair $p_{i''}$ and p_{i+1} is a direct or an inverted pair. □

As exemplified above, since the permutation element 1 always appears with a positive sign in the first index, then — similarly to the proof of Lemma 11 — we can determine both the index and the sign of the permutation element 2. Note that for determining the index of element 2 we need to know the index of the preceding element, its value (in this case 1), and the repeat sequence $s'|_R = s|_R$. By induction, one can determine the index of the permutation element k in s' based on the indices of the preceding permutation elements $k-1, k-2$ and the repeat sequence $s|_R$. Thus, Lemma 11 implies that the repmap s' can be deduced from the repeat sequence of s. Moreover, calculating the index of the successive permutation element as demonstrated in Lemma 11 can be done in constant time. Therefore, s' can be reconstructed in linear-time.

Lemma 12. *Given a repmap $s = S \cdot \varrho$, where both the ancestor S and the legal scenario ϱ are unknown, let S' be the sorted normalization of S and $s' = S' \cdot \varrho$. The normalized repmap s' can be calculated in linear-time and linear-space based on the repeat sequence $s|_R$.*

After calculating the repmap s', determining S is a matter of renaming the repmap S' according to the correspondency established between the permutation elements of s and s'. Thus, the calculation follows the path $s \rightarrow s' \rightarrow S' \rightarrow S$. Figures 3a and 3b give an example illustrating this process and Algorithm `getAncestor` implements this idea. Figure 7

Theorem 13 (Time Complexity)**.** *Given a repmap $s = S \cdot \varrho$, Algorithm* `getAncestor(`s`)` *reconstructs the ancestor S in linear time ($O(|s|)$).*

3.3.2 Reconstructing a Legal Scenario

Unlike the ancestor repmap reconstruction, the scenario reconstruction involves look-ahead to avoid conflicts between repeat pairs. This problem is best demonstrated by an example.

Example. Consider the following repmap:

$$1 \quad a \quad -b \quad -2 \quad -a \quad -c \quad -4 \quad b \quad 3 \quad c \ .$$

Suppose we were first to fulfill the inverted repeat pair b and $-b$. Such a choice would turn the other two repeat pairs (a and c) into direct-repeat pairs. Thus, we reach a deadlock without getting a legal scenario.

As demonstrated in the above example, choosing a legal reversal sequence that avoids deadlocks is a delicate matter. We address this problem by utilizing the fact that we can calculate the normalized repmaps s' and S' in linear-time (Section 3.3.1). When both repmaps are known, we show that an SBR reversal sequence sorting $s'|_N$ (to $S'|_N$) corresponds to a legal scenario transforming s to S. Currently, the best algorithm for solving SBR works in sub-quadratic time [Tannier and Sagot, 2004]. Hence, we get a sub-quadratic algorithm for reconstructing a legal scenario.

Consider a normalized repmap p resulting from a legal scenario affecting a sorted and normalized repmap P. Lemma 5 states that a legal reversal affecting p reduces the breakpoint count by 2. The following lemma claims the opposite direction, and is proved similarly.

Lemma 14. *Given a sorted normalized repmap P, let ϱ be a legal scenario, and let $p = P \cdot \varrho$. Any reversal ρ that eliminates two breakpoints, such that ρ affects a subsequence of p that begins and ends with permutation elements, is a legal reversal.*

Proof. Since p is normalized and ρ affects a subsequence of it having permutation elements on both its edges, ρ must be bordered by repeats. By the proof of Lemma 5, these repeats must correspond to an inverted repeat pair. $\square$

By induction on Lemma 14 we get the following corollary.

Corollary 15. *Let P be a given sorted normalized repmap, let $\varrho = \rho_1, \ldots, \rho_m$ be a legal scenario, and denote $p = P \cdot \varrho$. Let ϱ' be a scenario (not necessarily legal) in which each reversal eliminates* 2 *breakpoints and affects a subsequence that begins and ends with permutation elements. Then, ϱ' is a partially legal scenario.*

If the scenario eliminates all the breakpoints in p (*i.e.*, it sorts p) then, obviously, it must fulfill all the repeat pairs and is hence legal.

Corollary 16. *Let P be a given sorted normalized repmap, let $\varrho = \rho_1, \ldots, \rho_m$ be a legal scenario, and denote $p = P \cdot \varrho$. Let ϱ' be a scenario (not necessarily legal) in which each reversal eliminates* 2 *breakpoints and affects a subsequence that begins and ends with permutation elements such that $P = p \cdot \varrho'$. Then, ϱ' is a legal scenario.*

Since $p = P \cdot \varrho$, Corollary 6 implies that $p|_N$ has an SBR scenario in which each reversal eliminates 2 breakpoints, and hence all SBR scenarios fulfill this property. Thus, by Corollary 16, all SBR scenarios are legal.

Theorem 17. *Let P be a sorted and normalized repmap, ϱ a legal scenario, and denote $p = P \cdot \varrho$. A solution of SBR on $p|_N$ corresponds to a legal scenario on p.*

Theorems 17 and 13 enable us to find a legal scenario transforming s to S as follows: calculate s' from s (byproduct of Algorithm `getAncestor`) and use SBR to find an optimal scenario sorting $s'|_N$. By Theorem 17 this scenario is legal on s'. Since s and s' have the same repeat sequence, the scenario is legal on s as well. Since computing s' from s can be done in linear-time, the complexity of finding a legal scenario for s is determined by the SBR bottleneck. Currently, the most efficient algorithm for solving SBR has a time complexity of $O(n\sqrt{n \log n})$, where $n = |s|$ [Tannier and Sagot, 2004].

Theorem 18 (Time Complexity)**.** *Given a repmap $s = S \cdot \varrho$, where both the repmap S and the legal scenario ϱ are unknown, one can reconstruct a legal scenario transforming s to S in $O(n\sqrt{n \log n})$ time, where $n = |s|$.*

4 The Multiple Leaf RAPT and Set-tries

In this section we show that the leaf assignments $L = \{s^1, \ldots, s^q\}$ uniquely determine the underlying RAPT (T, f, g) up to (and not including) repeats in the inner nodes, *i.e.*, they dictate the tree topology, the induced permutations in inner node assignments, and the edge labels. We then describe a linear-time algorithm for reconstructing this information from the given input.

The proof of uniqueness is developed in two stages: first, the RAPT is reduced to a new auxiliary data structure called a *set-trie* (see Section 4.1 and Figure 4), which encodes partial information (tree topology and edge labels). Using this reduction, we show that both the tree topology and the edge labels are uniquely determined (Section 4.2) and can be reconstructed in linear-time based on the repeat sets $\{R(s) : s \in L\}$ of the leaf assignments(Section 4.3). Finally, the application of Theorems 10 and 13 to the above findings leads to the conclusion that the induced permutations in the inner node assignments are uniquely determined and can be reconstructed in linear-time based on the tree topology, the edge labels, and the leaf assignments (Section 4.4).

4.1 Set-tries and Monotonic Collections

Word-tries are well-known data structures, commonly used in text compression and database search [Gonnet, 1983]. They are used to store the information about the contents of each node in the path from the root to the node rather than in the node itself, thus grouping words with a common prefix along similar paths. Here we introduce a new data structure which, similarly to word-tries, is also based on a tree topology and path-encoding, however, the leaves of the new data structure correspond to sets instead of words (or sequences), as defined below.

Definition 7 (Set-tries)**.** Let $\mathscr{A} = \{A_1, \ldots, A_k\}$ be a collection of finite subsets of $\mathbb{N}$. A *set-trie st* over $\mathscr{A}$ is a pair $st = (T, g)$, where $T = (V, E)$ is a directed tree with a root v_r such that all the inner nodes (except perhaps the root) are of degree ≥ 3 and $g : E \to 2^{\mathbb{N}}$ are *labels* to the edges. In the following discussion we assume that *assignments* to the nodes $f : V \to 2^{\mathbb{N}}$ are also given. The labels g and the "virtual" assignments f need to fulfill the following requirements:

1. $f(v_r) = \emptyset$ and f is $1:1$ from the leafs of T to $\mathscr{A}$. Given that $u \in V$ is an ancestor of $v \in V$, we require that $f(v) = f(u) \cup g(\text{path}(u, v))$. In particular, this requirement implies $\forall v \in V - \{v_r\} : f(v) = g(\text{path}(v_r, v))$.

2. $\forall e, e' \in E, e \neq e' : g(e) \cap g(e') = \emptyset$. Thus, the node assignments are determined by the edge labels and vice versa.

Figure 4 gives an example of a set-trie and its derivation from a RAPT. We observe the following *monotonicity* property of set collections corresponding to leafs of set-tries(see Section 4.2).

Definition 8 (Monotonic Set Collection)**.** A set collection $\mathscr{A}$ is *monotonic* if, for any three sets $A, B, C \in \mathscr{A}$, either $A \cap B \subseteq A \cap C$ or $A \cap C \subseteq A \cap B$.

4.2 Uniqueness of Set-tries Based on Monotonic Collections

Figure 8

In this section we show that a set-trie is uniquely determined by the monotonic collection assigned to its leafs. However, before addressing the uniqueness issue, we first prove that the leaf assignments in a set-trie indeed correspond to a monotonic collection. Furthermore, we assert that, for any given monotonic collection $\mathscr{A}$, there exists a corresponding set-trie over $\mathscr{A}$. The existence proof is constructive, and serves as the basis for the set-trie reconstruction algorithm presented in Section 4.3.

Lemma 19. *Let $\mathscr{A}$ be a finite collection of finite subsets of $\mathbb{N}$. There exists a set-trie over $\mathscr{A}$ iff $\mathscr{A}$ is monotonic.*

Proof. Assume first that $\mathscr{A}$ has a set-trie st. Consider three sets $A, B, C \in \mathscr{A}$ and let v_A, v_B, v_C be leafs in T such that $f(v_A) = A, f(v_B) = B, f(v_C) = C$. Assume without loss of generality that the inner node $lca(v_A, v_C)$ (namely the least common ancestor) is lower (*i.e.*, further away from the root) than the inner node $lca(v_A, v_B)$. By Definition 7 it is easy to see that $A \cap C = f(lca(v_A, v_C))$ and $A \cap B = f(lca(v_A, v_B))$. Moreover, since $lca(v_A, v_C)$ is lower, we have $f(lca(v_A, v_B)) \subseteq f(lca(v_A, v_C))$, and thus $A \cap B \subseteq A \cap C$ and $\mathscr{A}$ is monotonic.

Next, assume that $\mathscr{A}$ is monotonic. We need to prove that there exists a set-trie over $\mathscr{A}$. We show this by induction on k, the number of sets in $\mathscr{A}$. Base case: for $k = 1$ the claim is trivial. Induction step: assume the claim holds for $k - 1 \geq 1$, we need to prove it for k. Consider the first $k - 1$ sets in $\mathscr{A}$ and denote them by $\mathscr{A}' = \{A_1, \ldots, A_{k-1}\}$. By the induction assumption, there exists a set-trie st' over $\mathscr{A}'$. Note that since $\mathscr{A}$ is monotonic, one can order the sets $A_k \cap A_1, \ldots, A_k \cap A_{k-1}$ in an increasing order (with respect to the containment relation). Let $A_k \cap A_i$ be the maximum set in this collection and let $v \in V$ be the lowest (*i.e.*, furthest away from the root) vertex on the path from v_r to $f^{-1}(A_i)$ such that $f(v) \subseteq A_k$. There exists such a vertex, since v_r fulfills the requirement ($f(v_r) = \emptyset \subseteq A_k$). Note that, by definition, $f(v) \subseteq A_i$, and thus $f(v) \subseteq A_k \cap A_i$. Next, we define the vertex v', which is the son of v in the emerging set-trie (see Figure 8).

To do that, we distinguish between the following two cases: v' exists already in st', in which case it can be either a leaf or an inner node, or v' does not exist in st', and therefore needs to be constructed.

1. If $f(v) = A_k \cap A_i$, let $v' = v$ (v' exists in st'). If v' is a leaf, define a new vertex u and connect it as a son to v', label the connecting edge with the empty set, and define $f(u) = A_i$.

2. If $f(v) \neq A_k \cap A_i$ (v' does not exist in st'), let $e_{tail} \in E'$ be the edge going out of v to the vertex u such that $(A_k \cap A_i - f(v)) \cap f(u) \neq \emptyset$. By the monotonicity assumption,

there is only one such node u. Define a new vertex v', connect it with an edge e' from v and with an edge e'' to u, and define $f(v') = A_k \cap A_i$, $g(e') = f(v') - f(v)$, and $g(e'') = f(u) - f(v')$.

In both cases, create a new vertex w and connect it from v' with an edge e''' such that $f(w) = A_k$, and $g(e''') = f(w) - f(v')$. It is easy to see that the above modification is a set-trie over $\mathscr{A}$. $\square$

We are now ready to prove the *uniqueness* of set tries over monotonic collections.

Lemma 20 (Uniqueness)**.** *Let $\mathscr{A}$ be a monotonic collection. There exists a unique set-trie over $\mathscr{A}$.*

Proof. By Lemma 19, there exists a set-trie over $\mathscr{A}$. Here we prove that this trie is unique by induction on k, the number of sets in the collection $\mathscr{A}$. Base case: for $k = 1$, the claim is trivial. Induction step: assume the claim holds for $k - 1 \geq 1$, and consider a collection $\mathscr{A}$ over k sets. By contradiction, let st and st' be two different set-tries over $\mathscr{A}$. Consider the collection of the first $k-1$ sets in $\mathscr{A}$ and denote it by $\mathscr{A}'$. Trivially, the restrictions $st|_{\mathscr{A}'}$ and $st'|_{\mathscr{A}'}$ are set-tries over $\mathscr{A}'$. By the induction assumption $st|_{\mathscr{A}'} = st'|_{\mathscr{A}'}$. In particular, if the tree topologies of st and st' differ, then $\text{path}_{st}(v_r, f^{-1}(A_k)) \neq \text{path}_{st'}(v'_r, f'^{-1}(A_k))$ (the paths in st and st' respectively). Let d and d' be the direct parents of $f^{-1}(A_k)$ and $f'^{-1}(A_k)$ in T and T' respectively. By Definition 7 and since the paths are not equal, $g(\text{path}_{st}(v_r, d))$ and $g'(\text{path}_{st'}(v'_r, d'))$ are not equal. Without loss of generality, assume that $\exists a \in g(\text{path}_{st}(v_r, d))$ and $a \notin g'(\text{path}_{st'}(v'_r, d'))$. By Definition 7, $a \in g(\text{path}_{st}(v_r, d)) \subseteq g(\text{path}_{st}(v_r, f^{-1}(A_k)))$ and hence $a \in A_k$. Let $A_i \neq A_k$ be a descendant of d (by Definition 7 all internal nodes are of degree ≥ 3. If d is the root and has only A_k as its child, then the tree is trivial). By similar reasoning, we have that $a \in A_i$. However, since $a \notin g'(\text{path}_{st'}(v'_r, d'))$, we must have that $a \in g'(\text{path}_{st'}(d', f'^{-1}(A_k)))$. Thus a is not in $g'(\text{path}_{st'}(v'_r, f'^{-1}(A_i)))$. A contradiction.

Note that the assignments to the inner nodes are uniquely determined by the tree topology, since we have $f(lca(A_i, A_j)) = A_i \cap A_j$. Furthermore, the edge labels are uniquely determined by the inner node assignments, since for an edge $e \in E$ going from u to v, $u \xrightarrow{e} v$, we have $g(e) = f(u) - f(v)$. $\square$

4.3 A Linear-time Algorithm for Set-trie Construction

Adding an element to a standard word-trie utilizes the fact that the labels on the path from the root to the leaf representing the word preserve the original order of the characters in the word. Such is not the case when dealing with sets. It is easy to see that adapting the current strategies used in constructing word-tries [Gonnet, 1983] to the task of set-trie reconstruction results in algorithms with quadratic-time complexity. In this section we present a more efficient method with linear-time complexity ($\Theta(|\mathscr{A}|)$ where $|\mathscr{A}| = \sum_{j=1}^{k} |A_j|$). We describe an algorithm to construct the set-trie via incremental leaf insertions, based on the induction described in the proof of Lemma 19 and we use the same notation. At step k of the algorithm, the set-trie st' is updated with the leaf node corresponding to A_k. As elaborated in the proof of Lemma 19 and as demonstrated in Figure 8, the leaf insertion requires two consecutive operations: Figure 9

1. `Find`: Identify the node $v \in V'$ which is the lowest vertex such that $f(v) \subseteq A_k$, and the edge $e_{tail} \in E'$ which is the edge connecting v to the vertex u such that $(A_k \cap A_i - f(v)) \cap f(u) \neq \emptyset$. In addition, compute the sets $B = g(e_{tail}) \cap A_k$ (elements common to the label of e_{tail} and the new set A_k) as well as $C = A_k - \cup_{j=1}^{k-1} A_j$ (new elements to be added to the current set-trie).

2. `Split`: Use the result of the `Find` operation to update the set-trie $st' = (T', g')$ with the new leaf.

The above `Find` and `Split` operations need to be distinguished from the classical disjoint set operations surveyed in [Galil and Italiano, 1991]. Here, tricks such as path compression cannot be applied since the set-trie is defined by its topology. Further, note that strategies such as employing numbering on the edges to reflect their level in the tree in order to support efficient `Find` queries are likely to yield inefficient solutions, since the numbering could change dynamically via `Split` operations. Therefore, the crux of our solution is in utilizing monotonicity to efficiently (in $O(|A_k|)$) maintain information regarding the local neighborhood of each edge. This information is then used to enable an efficient implementation of both operations in time-complexity that is linear in the size of each set $O(|A_k|)$. Summing up over all leaves in $\mathscr{A}$ then yields a linear-time complexity, $\Theta(|\mathscr{A}|)$. The pseudo-codes for the linear time `Find` (Algorithm 2) and `Split` (Algorithm 3) are given below. Figure 10

Lemma 21 (`Find`). *Given a monotonic set collection $\mathscr{A} = \{A_1, \ldots, A_\ell\}$ and a set-trie st' over $\mathscr{A}' = \{A_1, \ldots, A_{k-1}\}$, where $2 \leq k \leq \ell$, Algorithm 2 performs* `Find` *(A_k) in time complexity that is linear in the set size $O(|A_k|)$.*

Proof. Explicitly constructing the edge label function $g(\cdot)$ and using it to find v and e_{tail} is likely to yield an inefficient solution because of the need to perform set intersection and subtraction operations. Instead, we construct a quasi-inverse function by mapping each element in $\cup_{A \in \mathscr{A}} A$ to the edge whose label contains it (if any). This way, the node v can be efficiently found via two passes over the elements of A_k, as follows. Similarly to the proof of Lemma 19, consider $e_{tail} \in E'$, the lowest (*i.e.*, furthest away from the root) edge whose label intersects with A_k (if none exists then $e_{tail} = null$ and we consider it as pointing to the root v_r). Clearly, e_{tail} leads into v if $f(v) = A_k \cap A_i$, and otherwise e_{tail} is the edge connecting v with u (see the proof of Lemma 19 for a reminder of the notation). For $a \in A_k$, let $e_a \in E'$ denote the edge with $a \in g'(e_a)$ (*i.e.*, the quasi-inverse function) and let $e'_a \in E'$ denote the edge immediately preceding e_a in T' — see Figure 8 for an example ($e_a = e'_a = null$ if a does not appear in T'). In the first pass, the edges in $\{e'_a : a \in A_k\}$ are marked (*i.e.*, for each $a \in A_k$ first the edge e_a is queried, and the edge e'_a which precedes e_a is marked). Let $b \in g(e_{tail}) \cap A_k$ (by definition $g(e_{tail}) \cap A_k \neq \emptyset$ if $e_{tail} \neq null$). Note that $e_b = e_{tail}$. Because of the extremity of e_{tail}, we know that it is the only edge among $\{e_a : a \in A_k\}$ that was not marked in the first scan. Therefore, finding $B = \{b \in A_k : e_b \neq null \text{ is unmarked}\} = g(e_{tail}) \cap A_k$, and hence e_{tail}, as well as $C = \{c \in A_k : e_c = null\} = A_k - \cup_{j=1}^{k-1} A_j$ can be computed via one additional pass over the elements of A_k (the variables e_{tail}, B, and C are the output of the `Find` operation and are used as input to the `Split` operation to follow). Clearly, both e_a and e'_a can be queried in constant time, *e.g.*, by maintaining the correspondences $a \to e_a$ and $e_a \to e'_a$ in two arrays, namely aToEdge and prevEdge in the pseudo-code, respectively. The two passes are computed in $O(|A_k|)$, and hence the `Find` has a linear-time complexity. $\square$

Lemma 22 (`Split`)**.** *Given a monotonic set collection $\mathscr{A} = \{A_1, \ldots, A_\ell\}$, a set-trie st' over $\mathscr{A}' = \{A_1, \ldots, A_{k-1}\}$, where $2 \leq k \leq \ell$, as well as e_{tail}, B, and C, the result of the* `Find` *(A_k) operation (Algorithm 2), Algorithm 3 performs* `Split` *(A_k) in time complexity that is linear in the set size $O(|A_k|)$.*

Proof. First we analyze the implementation of the `Split` operation for the more challenging case of adding v' as a new node. Then we analyze the implementation in the other case (see the proof of Lemma 19). Let A_k be the set to be inserted in the set-trie $st' = (T', g')$. Apply the `Find` operation to it, and consider its result, namely the edge to be split e_{tail}, the set B of elements appearing in both A_k as well as in the label of e_{tail} (*i.e.*, $B = A_k \cap g(e_{tail})$), and the set C of elements appearing in A_k but not in the set-trie st' (*i.e.*, $C = A_k - \cup_{j=1}^{k-1} A_j$). The `Split` operation needs to cut the edge e_{tail} according to the set B, so that instead of a single edge

$$v \xrightarrow[g(e_{tail})]{e_{tail}} u$$

we get two new edges

$$v \xrightarrow[B]{e'} v' \xrightarrow[g(e_{tail})-B]{e''} u \ .$$

Furthermore, we need to add a leaf w corresponding to the set A_k and an edge connecting it to v' with C as the edge's label: $v' \xrightarrow[C]{e'''} w$ (see Figure 8). Let aToEdge and prevEdge be arrays as introduced in the `Find` implementation, let count denote a global variable keeping count of the total number of edges in the set-trie at any given moment, and let edgeElementsCount denote an additional array mapping each edge to the number of elements in its label $e \longrightarrow |g(e)|$. These arrays and counters are used to implement `Split` in $O(A_k)$ as follows: Create a new vertex v' and a new edge e' pointing from v to v' (using the global counter count). Let all the elements in B point to e', $v \xrightarrow[B]{e'} v'$ (by changing their values in aToEdge). This implies that only elements in $g(e_{tail}) - B$ now point to e_{tail}. Instead of adding a new edge e'' connecting v' to u (which would require $O(g(e_{tail}) - B)$ time), redefine e_{tail} to connect v' to u: $v' \xrightarrow[g(e_{tail})-B]{e_{tail}} u$. Update both the number of elements contained in the labels of each of e' and e_{tail} (in the edgeElementsCount array) as well as their preceding edges (in the prevEdge array). This implicitly establishes the new path

$$v \xrightarrow[B]{e'} v' \xrightarrow[g(e_{tail})-B]{e''} u \ .$$

Next, construct the edge $v' \xrightarrow[C]{e'''} w$ by adding a new vertex w and a new edge e''', update the edge's number of elements, its preceding edge, and let the elements in C point to it.

If v' exists in the set-trie st', then splitting e_{tail} is not required. One needs only to add w (and perhaps one additional vertex if v' is a leaf).

□

By applying the above `Find` and the `Split` operations via incremental additions of sets from $\mathscr{A}$ to the set-trie, it is possible to construct the tree topology T and to implicitly construct the edge labels g in linear-time ($O(|\mathscr{A}|)$). Explicitly constructing g from aToEdge can be done in linear-time by a straightforward single pass over the array aToEdge.

Theorem 23 (Time Complexity)**.** *Given a monotonic collection $\mathscr{A}$, a set-trie over $\mathscr{A}$ can be constructed in linear-time ($\Theta(|\mathscr{A}|)$).*

4.4 From Set-tries Back to RAPT

Based on Definition 3 it is easy to see that the collection of repeat sets $\{R(s) : s \in L\}$ is monotonic. In particular, a RAPT (T, f, g) with leaf assignments $L = \{s^1, \ldots, s^q\}$ can be readily mapped to a set-trie (T', g') with node assignments f' as follows: define $T' = T$, $g' = g$, and $\forall s \in L : f'(s) = R(s)$, *i.e.*, the leaf assignments of the set-trie are the repeat sets of the leaf assignments of the RAPT. Figure 4 gives an example illustrating this mapping. Since, by Lemma 20, a set-trie is uniquely determined by its leaf assignments, we imply that the repeat sets $\{R(s) : s \in L\}$ uniquely determine the tree topology T and the edge labels g of the RAPT. Thus, to prove the uniqueness of the RAPT, it is sufficient to show that the induced permutations in the inner node assignments are uniquely determined by T, g, and L. However, this result is immediately established by Theorem 10.

Theorem 24 (Uniqueness)**.** *The leaf assignments L uniquely determine the underlying RAPT up to (and not including) repeats in the inner nodes.*

Based on the linear-time algorithm for reconstructing set-tries (Theorem 23) and the linear-time algorithm for reconstructing ancestral assignments (Theorem 13), we get a linear-time algorithm for reconstructing a RAPT from its leaf assignments.

Theorem 25 (Time Complexity)**.** *Given the leaf assignments L of an unknown RAPT, reconstructing the RAPT (up to repeats in the inner nodes) can be done in linear-time ($\Theta(|L|)$).*

5 Acknowledgment

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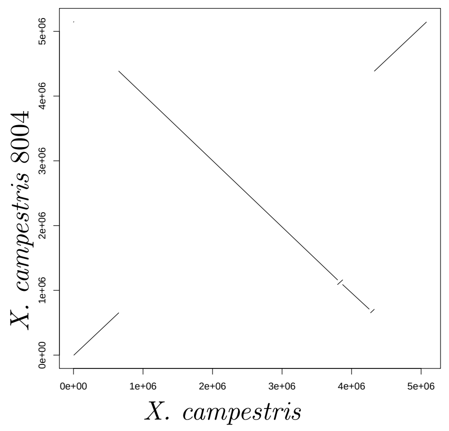
List of Figures



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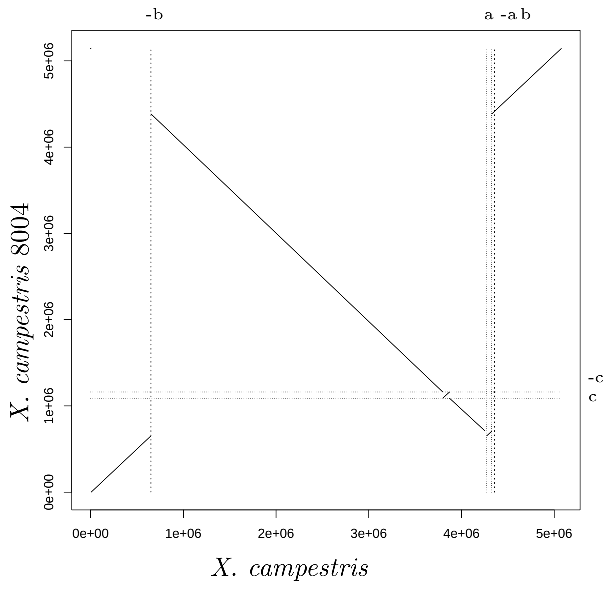

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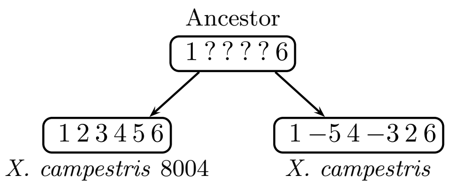

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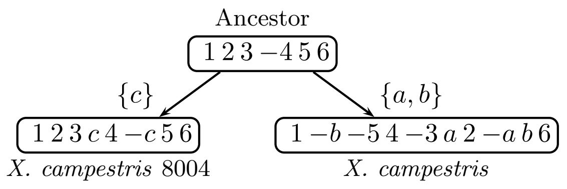

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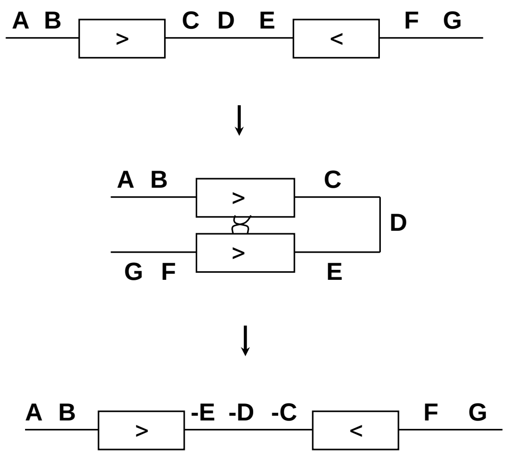
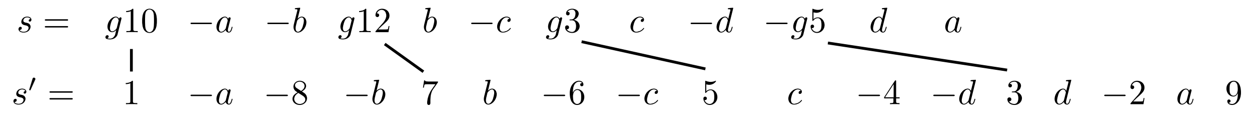
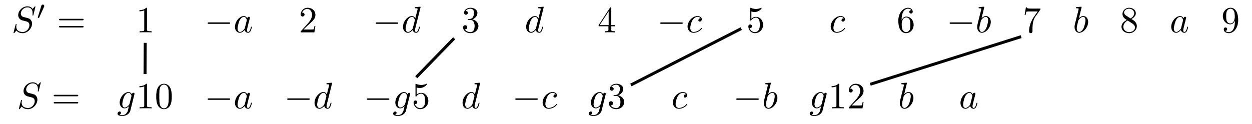


Figure 2


$s =$ $g10$ $-a$ $-b$ $g12$ b $-c$ $g3$ c $-d$ $-g5$ d a
$s' =$ 1 $-a$ -8 $-b$ 7 b -6 $-c$ 5 c -4 $-d$ 3 d -2 a 9

(a)


$S' =$ 1 $-a$ 2 $-d$ 3 d 4 $-c$ 5 c 6 $-b$ 7 b 8 a 9
$S =$ $g10$ $-a$ $-d$ $-g5$ d $-c$ $g3$ c $-b$ $g12$ b a

(b)

$$\begin{array}{rcccccccccccc}
s^* = & 1 & -a & -b & [4] & b & -c & 3 & c & -d & 2 & d & a \\
 & 1 & -a & -b & -4 & b & -c & [3] & c & -d & 2 & d & a \\
 & 1 & -a & -b & -4 & b & -c & -3 & c & -d & [2] & d & a \\
 & 1 & -a & [-b & -4 & b & -c & -3 & c & -d & -2 & d] & a \\
S^* = & 1 & -a & -d & 2 & d & -c & 3 & c & -b & 4 & b & a
\end{array}$$

(c)

$$\begin{array}{rcccc}
s^*|_N = & 1 & [4 & 3] & 2 \\
 & 1 & -3 & [-4 & 2] \\
 & 1 & [-3 & -2] & 4 \\
S^*|_N = & 1 & 2 & 3 & 4
\end{array}$$

(d)

Figure 3:

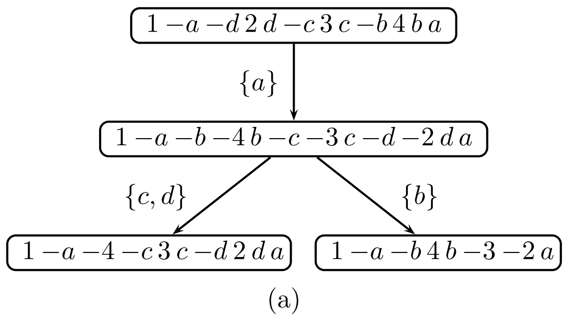
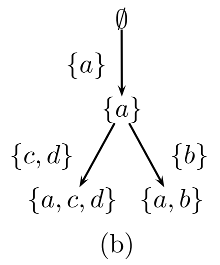

$1\,-a\,-d\,2\,d\,-c\,3\,c\,-b\,4\,b\,a$
$\{a\}$
$1\,-a\,-b\,-4\,b\,-c\,-3\,c\,-d\,-2\,d\,a$
$\{c,d\}$
$\{b\}$
$1\,-a\,-4\,-c\,3\,c\,-d\,2\,d\,a$
$1\,-a\,-b\,4\,b\,-3\,-2\,a$
(a)
$\emptyset$
$\{a\}$
$\{a\}$
$\{c,d\}$
$\{b\}$
$\{a,c,d\}$
$\{a,b\}$
(b)

Figure 4:

$$\begin{tikzcd}
S \arrow[r, "normalize"] \arrow[d, shift right, "\varrho"'] & S' \arrow[d, shift right, "\varrho"'] \\
s \arrow[r, "calculate"] \arrow[u, shift right, "\varrho'"'] & s' \arrow[u, shift right, "\varrho'"']
\end{tikzcd}$$

Figure 5

$$\begin{array}{rccccccccccccccccc}
s = & 1 & a & -7 & b & 3 & c & [6 & -b & -2 & -a & 8 & d & -4] & -c & -5 & d & 9 \\
 & 1 & a & -7 & b & 3 & c & 4 & -d & [-8 & a & 2 & b & -6 & -c & -5] & d & 9 \\
 & 1 & a & -7 & b & [3 & c & 4 & -d & 5 & c & 6] & -b & -2 & -a & 8 & d & 9 \\
 & 1 & a & [-7 & b & -6 & -c & -5 & d & -4 & -c & -3 & -b & -2] & -a & 8 & d & 9 \\
S = & 1 & a & 2 & b & 3 & c & 4 & -d & 5 & c & 6 & -b & 7 & -a & 8 & d & 9
\end{array}$$

(a)

$$\begin{array}{rccccccccccccccccc}
s = & 1 & a & [-7 & b & 3 & c & 6 & -b & -2] & -a & 8 & d & -4 & -c & -5 & d & 9 \\
 & 1 & a & 2 & b & [-6 & -c & -3] & -b & 7 & -a & 8 & d & -4 & -c & -5 & d & 9 \\
 & 1 & a & 2 & b & 3 & c & [6 & -b & 7 & -a & 8 & d & -4] & -c & -5 & d & 9 \\
 & 1 & a & 2 & b & 3 & c & 4 & -d & [-8 & a & -7 & b & -6 & -c & -5] & d & 9 \\
S = & 1 & a & 2 & b & 3 & c & 4 & -d & 5 & c & 6 & -b & 7 & -a & 8 & d & 9
\end{array}$$

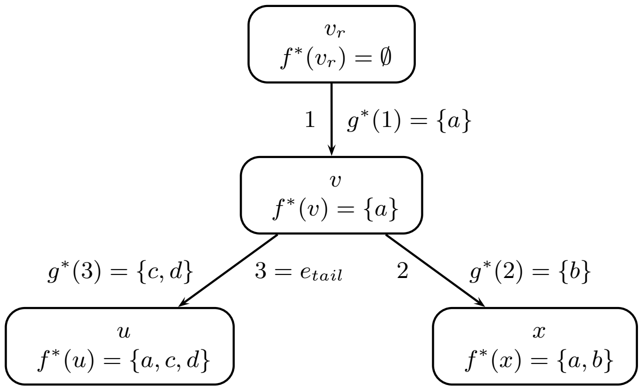
(b)

Figure 6

Algorithm 1: `getAncestor`

```
Data: A repmap $s$.
Result: The ancestor $S$ of $s$.
begin
    $prev \longleftarrow 0$ ; $current \longleftarrow 1$; $k \longleftarrow$ length($s|_R$) ;
    /* Assuming $s'|_R = s|_R$ , $s'[1] = 1$ , $s'[2k+1] = k+1$.                */
    while $current \neq 2k+1$ do
        /* Calculate the index of the successive permutation
           element.                                                             */
        $next \longleftarrow$ getNextIndex($prev$,$current$,$s'$) ;
        /* Calculate the sign of the successive permutation
           element.                                                             */
        $val \longleftarrow$ getNextVal($current$,$next$,$s'$) ;
        $s'[next] \longleftarrow val$ ;
        $prev \longleftarrow current$ ; $current \longleftarrow next$ ;
    /* Rename $S'$ to calculate $S$.                                            */
    return getS($s$,$s'$)
end
```

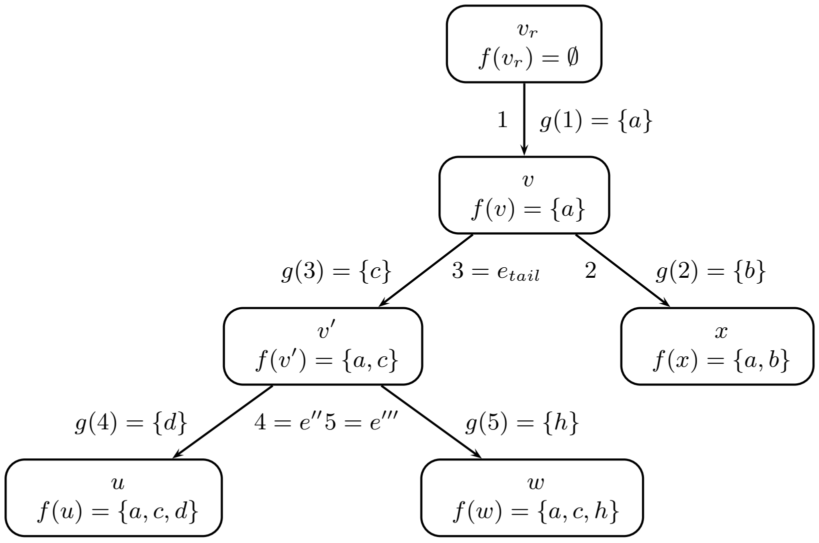
Figure 7



(a)

	a	b	c	d	e	h
e_a	**1**	2	**3**	3	null	null
e'_a	**null**	1	**1**	1	null	null

(b)



(c)

Figure 8

Algorithm 2: `Find`

```
Data: A set $A_k$.
Result: The lowest level edge $e_{tail}$ whose label intersects with $A_k$, the
        non-empty set $B = g(e_{tail}) \cap A_k$, and the set $C = A_k - \cup_{j=1}^{k-1} A_j$.
begin
    $B \longleftarrow \emptyset$ ;
    $C \longleftarrow \emptyset$ ;
    $e_{tail} \longleftarrow 0$;
    for $a \in A_k$ do
        $e \longleftarrow$ aToEdge $[a]$ ;
        mark prevEdge $[e]$ ;
    for $a \in A_k$ do
        if aToEdge $[a] = 0$ then $C \longleftarrow C \cup \{a\}$ ;
        else if aToEdge $[a]$ is unmarked then
            $B \longleftarrow B \cup \{a\}$;
            $e_{tail} \longleftarrow$ aToEdge $[a]$ ;
    return $e_{tail}$,$B$,$C$
end
```

Figure 9

Algorithm 3: `Split`

```
Data: The edge $e_{tail}$, and the two sets $B$ and $C$.
Result: Splitting the edge $e_{tail}$ as follows: adding a new edge $e'$
        according to the set $B$, redefining $e_{tail}$ according to $g(e_{tail}) - B$,
        adding a new edge $e'''$ according to $C$, and updating aToEdge,
        prevEdge, edgeElementsCount, and count.
begin
    if edgeElementsCount $[e_{tail}] \neq |B|$ then
        count $\longleftarrow$ count $+1$;
        $e' \longleftarrow$ count ;
        edgeElementsCount $[e'] \longleftarrow |B|$;
        edgeElementsCount $[e_{tail}] \longleftarrow$ edgeElementsCount $[e_{tail}] - |B|$;
        prevEdge $[e'] \longleftarrow$ prevEdge $[e_{tail}]$ ;
        prevEdge $[e_{tail}] \longleftarrow e'$ ;
        for $b \in B$ do aToEdge $[b] \longleftarrow e'$;
    else $e' \longleftarrow e_{tail}$;
    count $\longleftarrow$ count $+1$ ;
    $e''' \longleftarrow$ count ;
    for $c \in C$ do aToEdge $[c] \longleftarrow e'''$ ;
    prevEdge $[e'''] \longleftarrow e'$ ;
    edgeElementsCount $[e'''] \longleftarrow |C|$;
end
```

Figure 10