Revisiting the tree edit distance and its backtracing: A tutorial

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Abstract

Almost 30 years ago, Zhang and Shasha (1989) published a seminal paper describing an efficient dynamic programming algorithm computing the tree edit distance, that is, the minimum number of node deletions, insertions, and replacements that are necessary to transform one tree into another. Since then, the tree edit distance has been widely applied, for example in biology and intelligent tutoring systems. However, the original paper of Zhang and Shasha can be challenging to read for newcomers and it does not describe how to efficiently infer the optimal edit script. In this contribution, we provide a comprehensive tutorial to the tree edit distance algorithm of Zhang and Shasha. We further prove metric properties of the tree edit distance, and describe efficient algorithms to infer the cheapest edit script, as well as a summary of all cheapest edit scripts between two trees.

A reference implementation of the algorithms presented in this work can be found at https://pypi.org/project/edist/.

Change Note: On September 6, 2022, Daniel Germann and me identified a problem in the prior version of Algorithm 6. In particular, we noticed that a purely iterative backtracing scheme failed to appropriately take subtree boundaries into account. Therefore, I now switched to a recursive writeup, which is consistent with the reference implementation. Theorem 16 and the following example have been updated, accordingly. Thanks go to Daniel Germann for pointing me to this mistake.

1 Introduction

The tree edit distance (TED, Zhang and Shasha 1989) between two trees \( \bar{x} \) and \( \bar{y} \) is defined as the minimum number of nodes that need to be replaced, deleted, or inserted in \( \bar{x} \) to obtain \( \bar{y} \). This makes the TED an intuitive notion of distance, which has been applied in a host of different application areas (Pawlik and Augsten 2011), for example to compare RNA secondary structures and phylogenetic trees in biology (Akutsu 2010; S. Henikoff and J. G. Henikoff 1992; McKenna et al. 2010; Smith and Waterman 1981), or to recommend edits to students in intelligent tutoring systems (Choudhury, Yin, and Fox 2016; Freeman, Watson, and Denny 2016; Nguyen et al. 2014; Paaßen et al. 2018a; Rivers and Koedinger 2015). As such, the TED has certainly stood the test of time and is still of great interest to a broad community. Unfortunately, though, a detailed tutorial on the TED seems to lack, such that users tend to treat it as a black box. This is unfortunate as the TED lends itself for straightforward adjustments to the application domain at hand, and this potential remains under-utilized.

This contribution is an attempt to provide a comprehensive tutorial to the TED, enabling users to implement it themselves, adjust it to their needs, and compute not only the distance as such but also the optimal edits which transform \( \bar{x} \) into \( \bar{y} \). Note that we focus here on the original version of the TED with a time complexity of \( O(m^2 \cdot n^2) \) and a space complexity of \( O(m \cdot n) \), where \( m \) and \( n \) are the number of nodes in \( \bar{x} \) and \( \bar{y} \), respectively (Zhang and Shasha 1989). Recent innovations have improved the worst-case time complexity to cubic time (Pawlik and Augsten 2011; Pawlik and Augsten 2016), but require deeper knowledge regarding tree decompositions. Furthermore, the practical runtime complexity of the original TED algorithm is still competitive for balanced trees, such that we regard it as a good choice in many practical scenarios (Pawlik and Augsten 2011).
Our tutorial roughly follows the structure of the original paper of Zhang and Shasha\textsuperscript{[1989]}, that is, we start by first defining trees (section 2.1) and edit scripts on trees (section 2.2), which are the basis for the TED. To make the TED more flexible, we introduce generalized cost functions on edits (section 2.3), which are a good interface to adjust the TED for custom applications. We conclude the theory section by introducing mappings between subtrees (section 2.4), which constitute the interface for an efficient treatment of the TED.

These concepts form the basis for our key theorems, namely that the cheapest mapping between two trees can be decomposed via recurrence equations, which in turn form the basis for Zhang and Shasha’s dynamic programming algorithm for the TED (section 3). Finally, we conclude this tutorial with a section on the backtracing for the TED, meaning that we describe how to efficiently compute the cheapest edit script transforming one tree into another (section 4).

A reference implementation of the algorithms presented in this work can be found at \url{https://pypi.org/project/edist/}

## 2 Theory and Definitions

We begin our description of the tree edit distance (TED) by defining trees, forests, and tree edits, which provides the basis for our first definition of the TED. We will then revise this definition by permitting customized costs for each edit, which yields a generalized version of the TED. Finally, we will introduce the concept of a tree mapping, which will form the basis for the dynamic programming algorithm.

### 2.1 Trees

**Definition 1** (Alphabet, Tree, Label, Children, Leaf, Subtree, Parent, Ancestor, Forest). We define an alphabet as an arbitrary set $X$.

We define a tree $\bar{x}$ over the alphabet $X$ as an expression of the form $x(\bar{x}_1, \ldots, \bar{x}_R)$, where $x \in X$, and $\bar{x}_1, \ldots, \bar{x}_R$ is a (possibly empty) list of trees over $X$. We denote the set of all trees over $X$ as $\mathcal{T}(X)$.

We call $x$ the label of $\bar{x}$, and we call $\bar{x}_1, \ldots, \bar{x}_R$ the children of $\bar{x}$. If a tree has no children (i.e. $R = 0$), we call it a leaf. In terms of notation, we will generally omit the brackets for leaves, i.e. $x$ is a notational shorthand for the tree $x()$.

We define a subtree of $\bar{x}$ as either $\bar{x}$ itself, or as a subtree of a child of $\bar{x}$. Conversely, we call $\bar{x}$ the parent of $\bar{y}$ if $\bar{y}$ is a child of $\bar{x}$, and we call $\bar{x}$ an ancestor of $\bar{y}$ if $\bar{x}$ is either the parent of $\bar{y}$ or an ancestor of the parent of $\bar{y}$. We call the multi-set of labels for all subtrees of a tree the nodes of the tree.

We call a list of trees $\bar{x}_1, \ldots, \bar{x}_R$ from $\mathcal{T}(X)$ a forest over $X$, and we denote the set of all possible forests over $X$ as $\mathcal{T}(X)^*$. We denote the empty forest as $\epsilon$.

As an example, consider the alphabet $X = \{a, b\}$. Some example trees over $X$ are $a$, $b$, $a(a)$, $a(b)$, $b(a, b)$, and $a(b(a, b), b)$.

An example forest over this alphabet is $a, b, b(a, b)$. Note that each tree is also a forest. This is important as many of our proofs in this paper will be concerned with forests, and these proofs apply to trees as well.

Now, consider the example tree $\bar{x} = a(b(c, d), e)$ from Figure 1 (left). $a$ is the label of $\bar{x}$, and $b(c, d)$ as well as $e$ are the children of $\bar{x}$. Conversely, $\bar{x}$ is the parent of $b(c, d)$ and $e$. The leaves of $\bar{x}$ are $c, d,$ and $e$. The subtrees of $\bar{x}$ are $\bar{x}, b(c, d), c, d,$ and $e$. The nodes of $\bar{x}$ are $a, b, c, d,$ and $e$.

### 2.2 Tree Edits

Next, we shall consider edits on trees, that is, functions which change trees (or forests). In particular, we define:

**Definition 2** (Tree Edit, Edit Script). A tree edit over the alphabet $X$ is a function $\delta$ which maps a forest over $X$ to another forest over $X$, that is, a tree edit $\delta$ over $X$ is any kind of function $\delta : \mathcal{T}(X)^* \rightarrow \mathcal{T}(X)^*$.
In particular, we define a deletion as the following function del.

\[ \text{del}(\epsilon) := \epsilon \]

\[ \text{del}(x(y_1, \ldots, y_n), x_2, \ldots, x_R) := y_1, \ldots, y_n, x_2, \ldots, x_R \]

We define a replacement with node \( y \in \mathcal{X} \) as the following function \( \text{rep}_y \).

\[ \text{rep}_y(\epsilon) := \epsilon \]

\[ \text{rep}_y(x(y_1, \ldots, y_n), x_2, \ldots, x_R) := y(y_1, \ldots, y_n), x_2, \ldots, x_R \]

And we define an insertion of node \( y \in \mathcal{X} \) as parent of the trees \( l \) to \( r - 1 \) as the following function \( \text{ins}_{y,l,r} \).

\[ \text{ins}_{y,l,r}(x_1, \ldots, x_R) := \begin{cases} x_1, \ldots, x_R & \text{if } r > R + 1, l > r, \text{ or } l < 1 \\ x_1, \ldots, x_{l-1}, y, x_{l+1}, \ldots, x_R & \text{if } 1 \leq l = r \leq R + 1 \\ x_1, \ldots, x_{l-1}, y(x_1, \ldots, x_{r-1}), x_{r+1}, \ldots, x_R & \text{if } 1 \leq l < r \leq R + 1 \end{cases} \]

We define an edit script \( \delta \) as a list of tree edits \( \delta_1, \ldots, \delta_T \). We define the application of an edit script \( \delta = \delta_1, \ldots, \delta_T \) to a tree \( \bar{x} \) as the composition of all edits, that is: \( \delta(\bar{x}) := \delta_1 \circ \cdots \circ \delta_T(\bar{x}) \), where \( \circ \) denotes the contravariant composition operator, i.e. \( f \circ g(x) := g(f(x)) \).

Let \( \Delta \) be a set of tree edits. We denote the set of all possible edit scripts using edits from \( \Delta \) as \( \Delta^* \). We denote the empty script as \( \epsilon \).

As an example, consider the alphabet \( \mathcal{X} = \{a, b\} \) and the edit rep\(_a\), which replaces the first node in a forest with a \( b \). If we apply this edit to the example tree \( a(b, a) \), we obtain \( \text{rep}_a(a(b, a)) = b(a, a) \).

Now, consider the edit script \( \delta := \text{del}, \text{rep}_a, \text{ins}_{a,1,3} \), which yields the following result for the example tree \( a(b, a) \).

\[ \delta(a(b, a)) = \text{del} \circ \text{rep}_a \circ \text{ins}_{a,1,3}(a(b, a)) = \text{rep}_a \circ \text{ins}_{a,1,3}(b, a) = \text{ins}_{a,1,3}(a, a) = a(a, a) \]

Note that tree edits are defined over forests, not only over trees. This is necessary because, as in our example above, deletions may change trees into forests and need to be followed up with insertions to obtain a tree again.

Based on edit scripts, we can define the TED.

**Definition 3** (Edit Distance). Let \( \mathcal{X} \) be an alphabet and \( \Delta \) be a set of tree edits over \( \mathcal{X} \). Then, the TED according to \( \Delta \) is defined as the function

\[ d_\Delta : T(\mathcal{X}) \times T(\mathcal{X}) \rightarrow \mathbb{N} \quad (1) \]

\[ d_\Delta(\bar{x}, \bar{y}) = \min_{\delta \in \Delta^*} \left\{ ||\delta|| : \delta(\bar{x}) = \bar{y} \right\} \quad (2) \]

In other words, we define the TED between two trees \( \bar{x} \) and \( \bar{y} \) as the minimum number of edits we need to transform \( \bar{x} \) to \( \bar{y} \).

Our definition of tree edit is very broad and includes many edits which are not meaningful in most tasks. Therefore, the standard TED of Zhang and Shasha (1989) is restricted to the three kinds of special edits listed above, namely deletions, which remove a single node from a forest, insertions, which insert a single node into a forest, and replacements, which replace a single node in a forest with another node. Up to now, we have only defined versions of these edits which apply to the first node in a forest. We now go on to define variants which can be applied to any node in a given forest. To this end, we need a way to uniquely identify single nodes in a forest. We address this problem via the concept of a pre-order (sometimes called depth-first-search order). The pre-order just lists all subtrees of a forest recursively, starting with the first tree in its forest, followed by the pre-order of its children and the pre-order of the remaining trees. More precisely, we define the pre-order as follows.
Definition 4 (Pre-Order). Let \( X = x(y_1, \ldots, y_n), \bar{x}_2, \ldots, \bar{x}_R \) be a (non-empty) forest over some alphabet \( \mathcal{X} \). Then, we define the pre-order of \( X \) as the list
\[
\pi(X) := x(y_1, \ldots, y_n), \bar{x}_2, \ldots, \bar{x}_R,
\]
where \( \oplus \) denotes list concatenation.

We define the pre-order of the empty forest as \( \pi(\epsilon) = \epsilon \).

As a shorthand, we denote the label of \( \bar{x}_i \) as \( x_i \).

We define the size of the forest \( X \) as the length of the pre-order, that is, \( |X| := |\pi(X)| \).

Further, we define \( p_x(i) \) as the pre-order index of the parent of \( \bar{x}_i \), that is, \( \bar{x}_{p_x(i)} \) is the parent of \( \bar{x}_i \). If there is no parent, we define \( p_x(i) := 0 \).

Finally, we define \( r_x(i) \) as the child index of \( \bar{x}_i \), that is, \( \bar{x}_{r_x(i)} \) is the \( r_x(i) \)th child of \( \bar{x}_{p_x(i)} \). If \( p_x(i) = 0 \), we define \( r_x(i) \) as the index of \( \bar{x}_i \) in the forest, that is, \( \bar{x}_i \) is the \( r_x(i) \)th tree in \( X \).

Consider the example of the tree \( \bar{x} = a(b(c, d), e) \) from Figure 1 (left). Here, the pre-order is \( \pi(\bar{x}) = a(b(c, d), e), b(c, d), c, d, e \). Figure 1 (right) lists for all \( i \) the subtrees \( \bar{x}_i \), the nodes \( x_i \), the parents \( p_x(i) \), and the child indices \( r_x(i) \).

Based on the pre-order, we can specify replacements, deletions, and insertions as follows:

Definition 5 (Replacements, Deletions, Insertions). Let \( \mathcal{X} \) be some alphabet, let \( \bar{x}_1 = x(y_1, \ldots, y_n) \) be a tree over \( \mathcal{X} \), and let \( X = \bar{x}_1, \ldots, \bar{x}_R \) be a (non-empty) forest over \( \mathcal{X} \).

We define a deletion of the \( i \)th node as the following function \( \text{del}_i \).

\[
\text{del}_i(X) := \begin{cases} 
X & \text{if } i < 1 \\
\text{del}(X) & \text{if } i = 1 \\
x(\text{del}_{i-1}(y_1, \ldots, y_n), \bar{x}_2, \ldots, \bar{x}_R) & \text{if } 1 < i \leq |\bar{x}| \\
\bar{x}_1, \text{del}_{i-|\bar{x}_1|}(\bar{x}_2, \ldots, \bar{x}_R) & \text{if } i > |\bar{x}_1| 
\end{cases}
\]

We define \( \text{del}_i(\epsilon) = \epsilon \).

We define a replacement of the \( i \)th node with \( y \in \mathcal{X} \) as the following function \( \text{rep}_{i,y} \).

\[
\text{rep}_{i,y}(X) := \begin{cases} 
X & \text{if } i < 1 \\
\text{rep}_y(X) & \text{if } i = 1 \\
x(\text{rep}_{i-1,y}(y_1, \ldots, y_n), \bar{x}_2, \ldots, \bar{x}_R) & \text{if } 1 < i \leq |\bar{x}_1| \\
\bar{x}_1, \text{rep}_{i-|\bar{x}_1|,y}(\bar{x}_2, \ldots, \bar{x}_R) & \text{if } i > |\bar{x}_1| 
\end{cases}
\]

We define \( \text{rep}_{i,y}(\epsilon) = \epsilon \).

Finally, we define an insertion of node \( y \in \mathcal{X} \) as parent of the children \( l \) to \( r-1 \) of the \( i \)th node as the following function \( \text{ins}_{i,y,l,r} \).

\[
\text{ins}_{i,y,l,r}(X) := \begin{cases} 
X & \text{if } i < 0 \\
\text{ins}_{y,l,r}(X) & \text{if } i = 0 \\
x(\text{ins}_{i-1,y,l,r}(y_1, \ldots, y_n), \bar{x}_2, \ldots, \bar{x}_R) & \text{if } 1 \leq i \leq |\bar{x}_1| \\
\bar{x}_1, \text{ins}_{i-|\bar{x}_1|,y,l,r}(\bar{x}_2, \ldots, \bar{x}_R) & \text{if } i > |\bar{x}_1| 
\end{cases}
\]
Definition 6 (Cost function). A cost function $c$ over some alphabet $\mathcal{X}$ with $- \notin \mathcal{X}$ is defined as a function $c : (\mathcal{X} \cup \{ - \}) \times (\mathcal{X} \cup \{ - \}) \to \mathbb{R}$, where $-$ is called the special gap symbol.

Now, let $c$ be a cost function over $\mathcal{X}$. Then, we define the cost $C(\delta, X)$ of an edit $\delta \in \Delta_{\mathcal{X}}$ as zero if $\delta(X) = X$, i.e. if the edit does not change the input forest.

Otherwise, we define the cost of a replacement $\text{rep}_{i,y}$ with respect to some input forest $X$ as $C(\text{rep}_{i,y}, X) := c(x_i, y)$; we define the cost of a deletion $\text{del}_i$ with respect to some input forest $X$ as $C(\text{del}_i, X) := c(x_i, -)$; and we define the cost of an insertion $\text{ins}_{i,y,l,r}$ with respect to some input forest $X$ as $C(\text{ins}_{i,y,l,r}, X) := c(-, y)$.

Finally, we define the cost $C(\delta, X)$ of an edit script $\delta = \delta_1, \ldots, \delta_T$ with respect to some input forest $X$ recursively as $C(\delta, X) := C(\delta_1, X) + C((\delta_2, \ldots, \delta_T), \delta_1(X))$, with the base case $C(\epsilon, X) = 0$ for the empty script.

Intuitively, the cost of an edit script is just the sum over the costs of any single edit in the script.
As an example, consider our example script in Figure 2. For this script we obtain the cost:

\[
C\left(\text{rep}_{1, x}, \text{del}_{2, x}, \text{del}_{2, \text{rep}_{2, g}}, \text{del}_{3, a(b(c, d), e)}\right) \\
= c(a, f) + C\left(\text{del}_{2, x}, \text{del}_{2, \text{rep}_{2, g}}, \text{del}_{3, f(b(c, d), e)}\right) \\
= c(a, f) + c(b, -) + C\left(\text{del}_{2, \text{rep}_{2, g}}, \text{del}_{3, f(c, d, e)}\right) \\
= c(a, f) + c(b, -) + c(c, -) + C\left(\text{rep}_{2, g}, \text{del}_{3, f(c, d, e)}\right) \\
= c(a, f) + c(b, -) + c(c, -) + c(d, g) + C\left(\text{del}_{3, f(g, e)}\right) \\
= c(a, f) + c(b, -) + c(c, -) + c(d, g) + c(e, -) + 0
\]

Based on the notion of cost, we can generalize the TED as follows.

**Definition 7** (Generalized Tree Edit Distance). Let \( \mathcal{X} \) be an alphabet, let \( \Delta_{\mathcal{X}} \) be the standard TED edit set over \( \mathcal{X} \), and let \( c \) be a cost function over \( \mathcal{X} \). Then, the generalized TED over \( \mathcal{X} \) is defined as the function

\[
d_c : \mathcal{T}(\mathcal{X}) \times \mathcal{T}(\mathcal{X}) \to \mathbb{R} \\
d_c(\bar{x}, \bar{y}) = \min_{\delta \in \Delta_{\mathcal{X}}} \left\{ C(\delta, \bar{x}) | \delta(\bar{x}) = \bar{y} \right\}
\]

As an example, consider the cost function \( c(x, y) = 1 \) if \( x \neq y \) and \( 0 \) if \( x = y \). In that case, every edit (except for self-replacements) costs 1, such that the generalized edit distance corresponds to the length of the shortest edit script. If we change this cost function to be 0 for a replacement of \( a \) with \( f \), our edit distance between the two example trees in Figure 2 decreases from 5 to 4. If we set the cost \( c(a, a) = -1 \), the edit distance becomes ill-defined, because we can always make an edit script cheaper by appending another self-replacement of \( a \) with \( a \).

This begs the question: Which properties does the cost function \( c \) need to fulfill in order to ensure a “reasonable” edit distance? To answer this question, we first define what it means for a distance to be “reasonable”. Here, we turn to the mathematical notion of a metric.

**Definition 8** (Metric). Let \( \mathcal{X} \) be some set. A function \( d : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) is called a metric if for all \( x, y, z \in \mathcal{X} \) it holds:

\[
d(x, y) \geq 0 \quad \text{(non-negativity)} \\
d(x, x) = 0 \quad \text{(self-equality)} \\
d(x, y) > 0 \text{ if } x \neq y \quad \text{(discernibility)} \\
d(x, y) = d(y, x) \quad \text{(symmetry)} \\
d(x, z) + d(z, y) \geq d(x, y) \quad \text{(triangular inequality)}
\]

All five of these properties make intuitive sense: We require a reasonable distance to not return negative values, we require that every object should have a distance of 0 to itself, we require that no two different objects can occupy the same space, we require that any object \( x \) is as far from \( y \) as \( y \) is from \( x \), and we require that the fastest route from \( x \) to \( y \) is a straight line, that is, there is no point \( z \) through which we could travel such that we reach \( y \) faster from \( x \) compared to taking the direct distance.

Interestingly, it is relatively easy to show that the generalized TED is a metric if the cost function is a metric.

**Theorem 1.** If \( c \) is a metric over \( \mathcal{X} \), then the generalized TED \( d_c \) is a metric over \( \mathcal{T}(\mathcal{X}) \). More specifically:
1. If $c$ is non-negative, then $d_c$ is non-negative.

2. If $c$ is non-negative and self-equal, then $d_c$ is self-equal.

3. If $c$ is non-negative and discernible, then $d_c$ is discernible.

4. If $c$ is non-negative and symmetric, then $d_c$ is symmetric.

5. If $c$ is non-negative, $d_c$ conforms to the triangular inequality.

Proof. Note that we require non-negativity as a pre-requisite for any of the metric conditions, because negative cost function values may lead to an ill-defined distance, as in the example above.

We now prove any of the four statements in turn:

Non-negativity: The TED is a sum of outputs of $c$. Because $c$ is non-negative, $d_c$ is as well.

Self-Equality: The empty edit script $\epsilon$ transforms $x$ to $\bar{x}$ and has a cost of 0. Because $d_c$ is non-negative, this is the cheapest edit sequence, therefore $d_c(x, \bar{x}) = 0$ for all $x$.

Discernibility: Let $\bar{x} \neq \bar{y}$ be two different trees and let $\bar{\delta} = \delta_1, \ldots, \delta_T$ be an edit script such that $\delta(x) = y$. We now define $x_0 = x$ and $x_t$ recursively as $\delta_1(x_{t-1})$ for all $t \in \{1, \ldots, T\}$. Accordingly, there must exist an $t \in \{1, \ldots, T\}$ such that $x_t \neq x_{t-1}$, otherwise $\bar{x} = \bar{y}$. However, in that case, the costs of $\delta_t$ must be $c(x, y)$ for some $x \neq y$. Because $c$ is discernible, $c(x, y) > 0$.

Further, because $c$ is non-negative, $C(\delta, \bar{x})$ is a sum of non-negative contributions with at least one strictly positive contribution, which means that $C(\bar{\delta}, \bar{x}) > 0$. Because this reasoning applies for any script $\delta$ with $\delta(x) = y$, it holds: $d_c(x, \bar{y}) > 0$.

Symmetry: Let $\bar{\delta} = \delta_1, \ldots, \delta_T$ be the cheapest edit script which transforms $\bar{x}$ to $\bar{y}$. Now, we can inductively construct an inverse edit script as follows: If $\bar{\delta}$ is the empty script, then the empty script also transforms $\bar{y}$ to $\bar{x}$. If $\bar{\delta}$ is not empty, consider the first edit $\delta_1$:

- If $\delta_1 = \text{rep}_{i,y}$, we construct the edit $\delta_1^{-1} = \text{rep}_{i,x}$. For this edit it holds: $\delta_1 \circ \delta_1^{-1}(\bar{x}) = \bar{x}$. Furthermore, for the cost it holds: $C(\delta_1, \bar{x}) = c(x, y) = c(y, x) = C(\delta_1^{-1}, \delta_1(\bar{x}))$.
- If $\delta_1 = \text{ins}_{i,y,t,r}$, we construct the edit $\delta_1^{-1} = \text{del}_{i'}$ where $i'$ is the index of the newly inserted node in the forest $\delta_1(\bar{x})$. Therefore, we obtain $\delta_1 \circ \delta_1^{-1}(\bar{x}) = \bar{x}$. Further, for the cost it holds: $C(\delta_1, \bar{x}) = c(\bar{x}, y) = c(y, \bar{x}) = C(\delta_1^{-1}, \delta_1(\bar{x}))$.
- If $\delta_1 = \text{del}_i$, we construct the edit $\delta_1^{-1} = \text{ins}_{i,x_i,r_i}$. That is, we construct an insertion which re-inserts the node that has been deleted by $\delta_1$, and uses all its prior children. Therefore, we obtain $\delta_1 \circ \delta_1^{-1}(\bar{x}) = \bar{x}$. Further, for the cost it holds: $C(\delta_1, \bar{x}) = c(x_i, \bar{x}_i) = c(\bar{x}_i, x_i) = C(\delta_1^{-1}, \delta_1(\bar{x}))$.

It follows by induction that we can construct an entire script $\bar{\delta}^{-1}$, which transforms $\bar{y}$ to $\bar{x}$, because $\bar{x} = \bar{\delta} \circ \bar{\delta}^{-1}(\bar{x}) = \bar{\delta}^{-1}(\bar{y})$. Further, this script costs the same as $\bar{\delta}$, because $C(\bar{\delta}^{-1}, \bar{\delta}(\bar{x})) = C(\bar{\delta}^{-1}, \bar{x})$.

Because $\bar{\delta}$ was by definition a cheapest edit script which transforms $\bar{x}$ to $\bar{y}$ we obtain: $d_c(\bar{y}, \bar{x}) \leq C(\bar{\delta}^{-1}, \bar{x}) = C(\bar{\delta}, \bar{x}) = d_c(\bar{x}, \bar{y})$. It remains to show that $d_c(\bar{y}, \bar{x}) \geq d_c(\bar{x}, \bar{y})$.

Assume that $d_c(\bar{y}, \bar{x}) < d_c(\bar{x}, \bar{y})$. Then, there is an edit script $\tilde{\delta} = \delta_1, \ldots, \delta_T'$ which transforms $\bar{y}$ to $\bar{x}$ and is cheaper than $d_c(\bar{x}, \bar{y})$. However, using the same argument as before, we can generate an inverse edit script $\tilde{\delta}^{-1}$ with the same cost as $\tilde{\delta}$ that transforms $\bar{x}$ to $\bar{y}$, such that $d_c(\bar{x}, \bar{y}) \leq d_c(\bar{y}, \bar{x}) < d_c(\bar{x}, \bar{y})$, which is a contradiction. Therefore $d_c(\bar{y}, \bar{x}) = d_c(\bar{x}, \bar{y})$.

Triangular Inequality: Assume that there are three trees $\bar{x}$, $\bar{y}$, and $\bar{z}$, such that $d_c(\bar{x}, \bar{z}) + d_c(\bar{z}, \bar{y}) < d_c(\bar{x}, \bar{y})$. Now, let $\delta$ and $\delta'$ be cheapest edit scripts which transform $\bar{x}$ to $\bar{z}$ and $\bar{z}$ to $\bar{y}$ respectively, that is, $\delta(\bar{x}) = \bar{z}$, $\delta'(\bar{z}) = \bar{y}$, $C(\delta, \bar{x}) = d_c(\bar{x}, \bar{z})$, and $C(\delta', \bar{z}) = d_c(\bar{z}, \bar{y})$. The concatenation of both scripts $\delta'' = \delta \circ \delta'$ is per construction a script such that $\delta''(\bar{x}) = \delta \circ \delta'(\bar{x}) = \bar{y}$ and $C(\delta'', \bar{x}) = C(\delta, \bar{x}) + C(\delta', \bar{z}) = d_c(\bar{x}, \bar{z}) + d_c(\bar{z}, \bar{y})$. It follows that $d_c(\bar{x}, \bar{z}) + d_c(\bar{z}, \bar{y}) < d_c(\bar{x}, \bar{y}) \leq d_c(\bar{x}, \bar{z}) + d_c(\bar{z}, \bar{y})$ which is a contradiction. Therefore, the triangular inequality holds.

$\square$
As an example of the symmetry part of the proof, consider again Figure 2. Here, the inverse script for $\delta = \text{rep}_{1,f}, \text{del}_2, \text{del}_2, \text{rep}_{2,g}, \text{del}_3$ is $\delta^{-1} = \text{ins}_{1, e, 2, 2}, \text{rep}_{2,d}, \text{ins}_{1,c,1,1}, \text{ins}_{1,b,1,3}, \text{rep}_{1,a}$. For the cost we obtain:

$$C \left( \text{ins}_{1,e,2,2}, \text{rep}_{2,d}, \text{ins}_{1,c,1,1}, \text{ins}_{1,b,1,3}, \text{rep}_{1,a}, f(g) \right)$$

$$= c(-, e) + C \left( \text{rep}_{2,d}, \text{ins}_{1,c,1,1}, \text{ins}_{1,b,1,3}, \text{rep}_{1,a}, f(g, e) \right)$$

$$= c(-, e) + c(g, d) + C \left( \text{ins}_{1,c,1,1}, \text{ins}_{1,b,1,3}, \text{rep}_{1,a}, f(d, e) \right)$$

$$= c(-, e) + c(-, d) + c(-, c) + C \left( \text{ins}_{1,b,1,3}, \text{rep}_{1,a}, f(c, d, e) \right)$$

$$= c(-, e) + c(-, d) + c(-, c) + c(-, b) + C \left( \text{rep}_{1,a}, f(b(c, d), e) \right)$$

$$= c(-, e) + c(-, d) + c(-, c) + c(g, b) + c(f, a) + C \left( e, a(b(c, d), e) \right)$$

$$= c(-, e) + c(-, d) + c(-, c) + c(g, b) + c(f, a) + 0,$$

which is exactly the same cost as for the script $\bar{\delta}$, if $c$ is symmetric.

### 2.4 Mappings

While edit scripts capture the intuitive notion of editing a tree, they are not a viable representation to develop an efficient algorithm. In particular, edit scripts are highly redundant, in the sense that there may be many different edit scripts which transform a tree $\bar{x}$ into a tree $\bar{y}$ and have the same cost. For example, to transform the tree $\bar{x} = a(b(c,d), e)$ to the tree $\bar{y} = f(g)$, we can not only use the edit script in Figure 2 but we could also use the script $\text{del}_5, \text{del}_3, \text{del}_2, \text{rep}_{2,g}, \text{rep}_{1,t}$, which has the same cost, irrespective of the cost function. To avoid these redundancies, we need a representation which is invariant against changes in order of the edits, and instead just counts which nodes are deleted, which nodes are inserted. Such a representation is offered by tree mappings.

**Definition 9 (Tree Mapping).** Let $X$ and $Y$ be forests over some alphabet $\mathcal{X}$, and let $m = |X|$ and $n = |Y|$.

A tree mapping between $X$ and $Y$ is defined as a set of tuples $M \subseteq \{1, \ldots, m\} \times \{1, \ldots, n\}$, such that for all $(i, j), (i', j') \in M$ it holds:

1. Each node of $X$ is assigned to at most one node in $Y$, i.e. $i = i' \Rightarrow j = j'$.
2. Each node of $Y$ is assigned to at most one node in $X$, i.e. $j = j' \Rightarrow i = i'$.
3. The mapping preserves the pre-order of both trees, i.e. $i \geq i' \iff j \geq j'$.
4. The mapping preserves the ancestral ordering in both trees, that is: if the subtree rooted at $i$ is an ancestor of the subtree rooted at $i'$, then the subtree rooted at $j$ is also an ancestor of the subtree rooted at $j'$, and vice versa.

Intuitively, a tuple $(i, j)$ in a tree mapping $M$ expresses that node $i$ is replaced with node $j$. If an index does not occur in $M$, it is deleted/inserted. The four constraints in the definition of a tree mapping have the purpose to ensure that we can find a corresponding edit script for each mapping. As an example, consider again our two trees $\bar{x} = a(b(c,d), e)$ and $\bar{y} = f(g)$ from Figure 2. The mapping corresponding to the edit script in this figure would be $M = \{(1,1), (4,2)\}$ because node $x_1 = a$ is replaced with node $y_1 = f$ and node $x_4 = d$ is replaced with node $y_2 = g$. All remaining nodes are deleted and inserted, respectively. The empty mapping $M = \{\}$ would correspond to deleting all nodes in $\bar{x}$ and then inserting all nodes in $\bar{y}$, which is also a valid mapping but would likely be more costly.

The set $M = \{(1,1), (1,2)\}$ would not be a valid mapping because the node $x_1 = a$ is assigned to multiple nodes in $\bar{y}$ and thus we can not construct an edit script corresponding to this mapping. For such an edit script we would need a “copy” edit. For the same reason, the set $M = \{(1,1), (2,1)\}$ is not a valid mapping. Here, the node $y_1 = f$ is assigned to multiple nodes in $\bar{x}$. 

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Figure 3: One example mapping between the trees $\bar{x} = a(b(c,d),e)$ and $\bar{y} = f(g)$ (top left) and four sets which are not valid mappings due to violations of one of the four mapping constraints.

$M = \{(1,2),(2,1)\}$ is an example of a set that is not a valid tree mapping because of the third criterion. To construct an edit script corresponding to this mapping we would need a "swap" edit, i.e. an edit which can exchange nodes $x_1 = a$ and $x_2 = b$ in $\bar{x}$. Finally, the set $M = \{(3,1),(5,2)\}$ is not a valid mapping due to the fourth criterion. In particular, the subtree $\bar{y}_2 = g$ in $\bar{y}$, but the subtree $\bar{x}_5 = c$ is not an ancestor of the subtree $\bar{y}_5 = e$. This last criterion is more subtle, but you will find that each edit we can apply - be it replacement, deletion, or insertion - preserves the ancestral order in the tree. Conversely, this means that we can not make a node an ancestor of another node if it was not before. This also makes intuitive sense because it means that nodes can not be mapped to nodes in completely distinct subtrees.

Now that we have considered some examples, it remains to show that we can construct a corresponding edit script for each mapping in general.

**Theorem 2.** Let $X$ and $Y$ be forests over some alphabet $\mathcal{X}$ and let $M$ be a tree mapping between $X$ and $Y$. Then, the output of Algorithm 1 for $X, Y$ and $M$ is an edit script $\delta_M$ over $\Delta_X$, such that $\delta_M(X) = Y$ and

1. If $(i,j) \in M$, then the edit $\text{rep}_{i,y_i}$ is part of the script.
2. For all $i$ which are not part of the mapping - i.e. $\not\exists j: (i,j) \in M$ - the edit $\text{del}_i$ is part of the script.
3. For all $j$ which are not part of the mapping - i.e. $\not\exists i: (i,j) \in M$ - an edit $\text{ins}_{p_r(i,j),y_i,r_i,r_j+R_j}$ for some $R_j$ is part of the script.

Further, no other edits are part of $\delta_M$ than the edits mentioned above. Algorithm 1 runs in $O(m + n)$ worst-case time.

**Proof.** The three constraints are fulfilled because we iterate over all entries $(i,j)$ and create one replacement per such entry, we iterate over all $i \in I$ and create one deletion per such $i$, and we iterate over all $j \in J$ and we create one insertion per such entry. It is also clear that $O(m + n)$ because we iterate over all $i \in \{1, \ldots, m\}$ and over all $j \in \{1, \ldots, n\}$. Assuming that $I$ and $J$ permit insertion as well as containment tests in constant time, and that the list concatenations in ram-descendants are possible in constant time, this leaves us with $O(m + n)$.

It is less obvious that $\delta_M(X) = Y$. We show this by an induction over the cardinality of $M$. First, consider $M = \emptyset$. In that case, we obtain $I = \{1, \ldots, m\}$, $J = \{1, \ldots, n\}$, and $R_0 = \ldots = R_n = 0$. Theorem 2 proves that the conditions of the theorem are satisfied.
Therefore, the resulting script is \( \delta_M = \text{del}_m, \ldots, \text{del}_1, \text{ins}_{p_Y(v_j)}, x_j, r_j, \ldots, \text{ins}_{p_Y(v_n)}, y_n, r_n \). This script obviously first deletes all nodes in \( X \) and then inserts all nodes from \( Y \) in the correct configuration.

Now assume that the theorem holds for all mappings \( M \) between \( X \) and \( Y \) with \( |M| \leq k \), and consider a mapping \( M \) between \( X \) and \( Y \) with \( |M| = k + 1 \).

Let \((i, j)\) be the entry of \( M \) with smallest \( j \), let \( M' = M \setminus \{(i, j)\} \), and let \( \delta_{M'} \) be the corresponding edit script for \( M' \) according to Algorithm 1. Per induction, \( \delta_{M'}(X) = Y' \).

Now, let \( I = \{i||j : (i, j) \in M\}, I' = \{i||j : (i, j) \in M'\}, J = \{j||i : (i, j) \in M\}, \) and \( J' = \{j||i : (i, j) \in M'\}. \) We observe that \( I' = I \cup \{i\} \) and \( J = J \cup \{j\} \), so our resulting script \( \delta_M \) will not delete node \( i \) and not insert node \( j \), but otherwise contain all deletions and insertions of script \( \delta_{M'} \). We also know that node \( x_i \) will be replaced with node \( y_j \), such that all nodes of \( Y \) are contained after applying \( \delta_M \). It remains to show that node \( y_j \) is positioned correctly in \( \delta_M(X) \), such that \( \delta_M(X) = Y \).

Let \( P_M(j) \) be a set that is recursively defined as \( P_M(j') = \emptyset \) if \( j' \notin J \), and \( P_M(j') = \{j'\} \cup P_M(p_Y(j')) \) if \( j' \in J \). In other words, \( P_M(j) \) contains all ancestors of \( j \), until we find an ancestor that is not inserted. Now, consider all inserted ancestors of \( j \), that is, \( P_M(p_Y(j)) \). Further, let \( (n, R_0, \ldots, R_n) = \text{num-descendants}(Y, 0, J) \) and \((n, R'_0, \ldots, R'_n) = \text{num-descendants}(Y, 0, J') \). For all elements \( j' \in P_M(p_Y(j)) \) we obtain \( R_{j'} = R'_{j'} + 1 \), and for all other nodes we obtain \( R_{j'} = R'_{j'} \). In other words, all ancestors of \( j \) which are inserted use one more child compared to before, but no other node will. This additional child is \( j \), such that the ancestral structure is preserved and we obtain \( \delta_M(X) = Y \).

**Algorithm 1** An algorithm to transform a mapping \( M \) into a corresponding edit script \( \delta_M \) according to Theorem 2.

```plaintext
function MAP-TO-SCRIPT(\( X \) and \( Y \), a tree mapping \( M \) between \( X \) and \( Y \).)
    \( I \leftarrow \{i||j : (i, j) \in M\} \).
    \( J \leftarrow \{j||i : (i, j) \in M\} \).
    Initialize \( \delta \) as empty.
    for \((i, j)\) in \( M \) do
        \( \delta \leftarrow \delta \oplus \text{rep}_i, y_j \).  // replacements
    end for
    for \( i \) in \( I \) in descending order do
        \( \delta \leftarrow \delta \oplus \text{del}_i \).  // deletions
    end for
    \((n, R_0, \ldots, R_n) \leftarrow \text{NUM-DESCENDANTS}(Y, 0, J) \).  // number of children for each inserted node
    for \( j \) in \( J \) in ascending order do
        \( \delta \leftarrow \delta \oplus \text{ins}_{p_Y(j)}, y_j, r_j + R_j \).  // insertions
    end for
    return \( \delta \).
end function

function NUM-DESCENDANTS(\( Y \) = \( y(z_1, \ldots, z_k), y_2, \ldots, y_R \), index \( j \), index set \( J \))
    \( \hat{R} \leftarrow \varepsilon \).
    \( \hat{R} \leftarrow 0 \).
    for \( r \leftarrow 1, \ldots, R \) do
        \( j \leftarrow j + 1 \).
        \((\hat{r}_j, \hat{R}_j, \ldots, \hat{R}_j) \leftarrow \text{NUM-DESCENDANTS}(z_1, \ldots, z_k, j, J) \).
        \( \hat{R} \leftarrow \hat{R} \oplus \hat{R}_j \).
        if \( j \notin J \) then
            \( \hat{R} \leftarrow \hat{R} + 1 \).
        else
            \( \hat{R} \leftarrow \hat{R} + \hat{R}_j \).
        end if
    end for
    return \( (j, \hat{R} \oplus \hat{R}) \).
end function
```

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As an example, consider again the mapping $M = \{(1, 1), (4, 2)\}$ between the trees $\bar{x} = a(b(c, d), e)$ and $\bar{y} = f(g)$ from Figure 2. Here we have the non-mapped nodes $I = \{2, 3, 5\}$ and $J = \{\}\$. Therefore, Algorithm 1 returns the script $\text{rep}_{1, \ell}, \text{rep}_{4, g'}, \text{del}_5, \text{del}_3, \text{del}_2$. Note that deletions are done in descending order to ensure that the pre-order indices in the tree do not change for intermediate trees.

For the inverse mapping $M = \{(1, 1), (2, 4)\}$ between $\bar{y}$ and $\bar{x}$ we have $I = \{\}\$ and $J = \{2, 3, 5\}$. Further, the output of $\text{num-descendants}$ is $(n = 5, R_0 = 1, R_1 = 1, R_2 = 1, R_3 = 0, R_4 = 0, R_5 = 0)$. Therefore, we obtain the script $\text{rep}_{1, a}, \text{rep}_{2, d}, \text{ins}_{1, b, 1, 2}, \text{ins}_{2, c, 1, 1}, \text{ins}_{1, e, 2, 2}$. Our next task is to demonstrate that the inverse direction is also possible, that is, we can find a corresponding mapping for each script.

**Theorem 3.** Let $X$ and $Y$ be forests over some alphabet $X$, and let $\delta$ be an edit script such that $\bar{\delta}(X) = Y$. Then, the following, recursively defined set $M_\delta$, is a mapping between $X$ and $Y$:

$$M_\ell := \{(1, 1), \ldots, (m, m)\}$$

$$M_{\delta_1, \ldots, \delta_T} := \begin{cases} M_{\delta_1, \ldots, \delta_{T-1}} & \text{if } \delta_T = \text{rep}_{j, g_j} \\ \{(i, j')|(i, j') \in M_{\delta_1, \ldots, \delta_{T-1}}, j' < j\} \cup \{(i, j')|(i, j') \in M_{\delta_1, \ldots, \delta_{T-1}}, j' > j\} & \text{if } \delta_T = \text{del}_j \\ \{(i, j')|(i, j') \in M_{\delta_1, \ldots, \delta_{T-1}}, j' < j\} \cup \{(i, j')|(i, j') \in M_{\delta_1, \ldots, \delta_{T-1}}, j' > j\} & \text{if } \delta_T = \text{ins}_{p_{\nu}(j), g_j, r_j, R_j} \\ \{(i, j' + 1)|(i, j') \in M_{\delta_1, \ldots, \delta_{T-1}}, j' \geq j\} & \text{if } \delta_T = \text{del}_j \end{cases}$$

where $R_j$ is the number of children of $\bar{x}_j$.

**Proof.** We prove the claim via induction over the length of $\delta$. $M_\ell$ obviously conforms to all mapping constraints.

Now, assume that the claim is true for all scripts $\delta$ with $|\delta| < T$ and consider a script $\delta = \delta_1, \ldots, \delta_T$. Let $\bar{\delta}' = \delta_1, \ldots, \delta_T$. Due to induction, we know that $M_{\bar{\delta}'}$ is a valid mapping between $X$ and $\bar{\delta}'(X)$. Now, consider the last edit $\delta_{T+1}$.

First, we observe that, if $M_{\bar{\delta}'}$ fulfills the first three criteria of a mapping, $M_{\bar{\delta}}$ does as well, because we never introduce many-to-one mappings and respect the pre-order. The only criterion left in question is the fourth, namely whether $M_{\bar{\delta}}$ respects the ancestral ordering of $Y$.

If $\delta_{T+1}$ is a replacement, the tree structure of $\bar{\delta}(X)$ is the same as for $\bar{\delta}'(X)$. Therefore, $M_{\bar{\delta}} = M_{\bar{\delta}'}$ is also a valid mapping between $X$ and $Y$.

If $\delta_{T+1}$ is a deletion del$_j$, then node $g_j$ in $\bar{\delta}'(X)$ is missing from $Y$ and all subtrees with pre-order indices higher than $j$ decrease their index by one, which is reflected by $M_{\bar{\delta}}$. Further, $M_{\bar{\delta}}$ only removes a tuple, but does not add a tuple, such that all ancestral relationships present in $M_{\bar{\delta}'}$ were also present in $M_{\bar{\delta}}$. Finally, a deletion does not break any of the ancestral relationships because any ancestor of $g_j$ remains an ancestor of all children of $g_j$ in $Y$. Therefore, $M_{\bar{\delta}}$ is a valid mapping between $X$ and $Y$.

If $\delta_{T+1}$ is an insertion ins$_{p_{\nu}(j), g_j, r_j, R_j}$, then $g_j$ is a new node in $Y$ and all subtrees with pre-order indices as high or higher than $j$ in $\bar{\delta}'(X)$ increase their index by one, which is reflected by $M_{\bar{\delta}}$. Further, $M_{\bar{\delta}}$ leaves all tuples intact, such that all ancestral relationships of $M_{\bar{\delta}'}$ are preserved. Finally, an insertion does not break any ancestral relationships because $g_{p_{\nu}(j)}$ is still an ancestor of all nodes it was before, except that there is now a new node $g_j$ in between. Therefore, $M_{\bar{\delta}}$ is a valid mapping between $X$ and $Y$.

As an example, consider the edit scripts shown in Figure 2. For the script $\bar{\delta} = \text{rep}_{1, \ell}, \text{del}_2, \text{del}_2, \text{rep}_{2, g'}, \text{del}_3$, which transforms the tree $\bar{x} = a(b(c, d), e)$ into the tree $\bar{y} = f(g)$, we obtain the following map-
all replacements, and is shifted for all deletions and insertions up until now. In particular, the mapping starts as a one-to-one mapping, is left unchanged for edits from Figure 2. For each edit of the script, the mapping is updated to be consistent with all mappings.

Figure 4: An illustration of the recursive construction of the corresponding mapping $M_j$ for three edits from Figure 2. For each edit of the script, the mapping is updated to be consistent with all edits up until now. In particular, the mapping starts as a one-to-one mapping, is left unchanged for all replacements, and is shifted for all deletions and insertions.

Consider the mapping $M_1$ after the $t$th edit:

- $M_0 = \{(1, 1), (2, 2), (3, 3), (4, 4), (5, 5)\}$
- $M_1 = \{(1, 1), (2, 2), (3, 3), (4, 4), (5, 5)\}$
- $M_2 = \{(1, 1), (3, 2), (4, 3), (5, 4)\}$
- $M_3 = \{(1, 1), (4, 2), (5, 3)\}$
- $M_4 = \{(1, 1), (4, 2), (5, 3)\}$
- $M_5 = \{(1, 1), (4, 2)\}$

Conversely, for the script $\delta^{-1} = \text{ins}_{1,e,2,2, \text{rep}_{1,f, d, \text{ins}_{1,c,1,1, \text{ins}_{1,b,1,3, \text{rep}_{1,a}}}}$, which transforms $\bar{y}$ into $\bar{x}$, we obtain the following mappings.

- $M_0 = \{(1, 1), (2, 2)\}$
- $M_1 = \{(1, 1), (2, 2)\}$
- $M_2 = \{(1, 1), (2, 2)\}$
- $M_3 = \{(1, 1), (2, 3)\}$
- $M_4 = \{(1, 1), (2, 4)\}$
- $M_5 = \{(1, 1), (2, 4)\}$

The influence of the different kinds of edits on the mapping is also illustrated in Figure 4.

Now that we have shown that edit scripts and mappings can be related on a structural level, it remains to show that they are also related in terms of cost. To that end, we need to define the cost of a mapping:

**Definition 10 (Mapping cost).** Let $X$ and $Y$ be forests over some alphabet $\mathcal{X}$, and let $c$ be a cost function over $\mathcal{X}$. Further, let $M$ be a mapping between $X$ and $Y$, let $I = \{i \in \{1, \ldots, |X|\} | \exists j : (i, j) \in M\}$, and let $J = \{j \in \{1, \ldots, |Y|\} | \exists i : (i, j) \in M\}$.

The cost of the mapping $M$ is defined as:

$$C(M, X, Y) = \sum_{(i, j) \in M} c(x_i, y_j) + \sum_{i \in I} c(x_i, -) + \sum_{j \in J} c(\cdot, y_j)$$

For example, consider the mapping $M = \{(1, 1), (4, 2)\}$ between the trees in Figure 2. This mapping has cost

$$C(\{(1, 1), (4, 2)\}, a(b(c, d), e), f(g)) = c(a, f) + c(d, g) + c(b, -) + c(c, -) + c(e, -)$$
Note that this is equivalent to the cost of the edit script \( \delta = \text{rep}_{1,x}, \text{del}_2, \text{del}_2, \text{rep}_{2,y}, \text{del}_3 \). However, the cost of an edit script is not always equal to the cost of its corresponding mapping. For example, consider the two trees \( x = a \) and \( y = b \) and the script \( \delta = \text{rep}_{1,c}, \text{rep}_{1,b} \), which transforms \( x \) to \( y \). Here, the corresponding mapping is \( M = \{ (1,1) \} \) with the cost \( C(M, x, y) = c(a, b) \). However, the cost of the edit script is \( C(\delta, x) = c(a, c) + c(c, b) \), which will be at least as expensive if the cost function conforms to the triangular inequality.

In general, we can show that mappings are at most as expensive as scripts if \( c \) is non-negative, self-equal, and conforms to the triangular inequality.

**Theorem 4.** Let \( X \) and \( Y \) be forests over some alphabet \( X \) and \( c \) be a cost function over \( X \). Further, let \( \delta \) be an edit script over \( \Delta X \) with \( \delta(X) = Y \), and let \( M \) be a mapping between \( X \) and \( Y \). Then it holds:

1. The corresponding script \( \delta_M \) for \( M \) according to Algorithm \( \overline{7} \) has the same cost as \( M \), that is: \( C(M, X, Y) = C(\delta_M, X) \).
2. If \( c \) is non-negative, self-equal, and conforms to the triangular inequality, the corresponding mapping \( M_\delta \) for \( \delta \) according to Theorem \( 6 \) is at most as expensive as \( \delta \), that is: \( C(M_\delta, X, Y) \leq C(\delta, X) \).

**Proof.** Let \( m = |X| \) and \( n = |Y| \), let \( I = \{ i \in \{1, \ldots, m\} | \exists j : (i,j) \in M \} \), and let \( J = \{ j \in \{1, \ldots, n\} | \exists i : (i,j) \in M \} \).

1. Due to Theorem \( 2 \) we know that the script \( \delta_M \) for \( M \) contains exactly one replacement \( \text{rep}_{i,y} \) per entry \( (i,j) \in M \), exactly one deletion \( \text{del}_i \) per unmapped index \( i \in I \) and exactly one insertion \( \text{ins}_{p+1}(j,y), r, r+1 \) per unmapped index \( j \in J \). Therefore, the cost of \( \delta_M \) is:

\[
C(\delta_M, X) = \sum_{(i,j) \in M} c(x_i, y_j) + \sum_{i \in I} c(x_i, -) + \sum_{j \in J} c(-, y_j)
\]  

which is per definition equal to \( C(M, X, Y) \).

2. We show this claim via induction over the length of \( \delta \). First, consider the case \( \delta = \epsilon \). Then, \( X = Y \) and \( M_\delta = \{ (1,1), \ldots, (m,m) \} \). Because \( c \) is self-equal, we obtain for the cost of \( M_\delta \):

\[
C(M_\delta, X, Y) = \sum_{(i,j) \in M_\delta} c(x_i, y_j) = \sum_{i=1}^{m} c(x_i, x_i) = 0 = c(\epsilon, X)
\]

Now, assume that the claim holds for an \( \delta' \) with \( |\delta'| \leq T \), and consider a script \( \delta = \delta_1, \ldots, \delta_T+1 \). Let \( \delta' = \delta_1, \ldots, \delta_T \) and let \( Y' = \delta'(X) \). Then, we consider the last edit \( \delta_T+1 \) and distinguish the following cases:

If \( \delta_T+1 = \text{rep}_{j,y} \), we have \( M_\delta = M_{\delta'} \). Further, if there is an \( i \in \{1, \ldots, m\} \) such that \( (i,j) \in M_{\delta'} \), we obtain for the cost:

\[
C(\delta, X) = C(\delta', X) + c(y_j', y_j) \geq C(M_{\delta'}, X, Y') + c(y_j', y_j) = C(M_\delta, X, Y) - c(x_i, y_j) + c(x_i, y_j') + c(y_j', y_j) \\
\geq C(M_\delta, X, Y) - c(x_i, y_j) + c(x_i, y_j') = C(M_\delta, X, Y)
\]

In case there is no \( i \in \{1, \ldots, m\} \) such that \( (i,j) \in M_{\delta'} \), we obtain for the cost:

\[
C(\delta, X) = C(\delta', X) + c(y_j', y_j) \geq C(M_{\delta'}, X, Y') + c(y_j', y_j) = C(M_\delta, X, Y) - c(-, y_j) + c(-, y_j') + c(y_j', y_j) \\
\geq C(M_\delta, X, Y) - c(-, y_j) + c(-, y_j) = C(M_\delta, X, Y)
\]
If \( \delta_{T+1} = \text{del} \), consider first the case that there exists some \( i \) such that \( (i,j) \in M_{\delta} \). Then, we obtain for the cost:

\[
C(\bar{\delta}, X) = C(\bar{\delta}', X) + c(y_j', -) \quad \text{Induction} \\
\geq C(M_{\delta}, X, Y') + c(y_j', -) \\
= C(M_{\delta}, X, Y) - c(x_i, -) + c(x_i, y_j') + c(y_j', -) \\
\geq C(M_{\delta}, X, Y) - c(x_i, -) + c(x_i, -) = C(M_{\delta}, X, Y)
\]

If there exists no such \( i \), we obtain for the cost:

\[
C(\bar{\delta}, X) = C(\bar{\delta}', X) + c(y_j', -) \quad \text{Induction} \\
\geq C(M_{\delta}, X, Y') + c(y_j', -) \\
= C(M_{\delta}, X, Y) + c(-, y_j') + c(y_j', -) \geq C(M_{\delta}, X, Y)
\]

Finally, if \( \delta_{T+1} = \text{ins}_{p_{y'}(j), y_j, r_j, r_j + R_j} \), we obtain for the cost:

\[
C(\bar{\delta}, X) = C(\bar{\delta}', X) + c(-, y_j) \quad \text{Induction} \\
\geq C(M_{\delta}, X, Y') + c(-, y_j) \\
= C(M_{\delta}, X, Y) - c(-, y_j) + c(-, y_j) = C(M_{\delta}, X, Y)
\]

This concludes our proof by induction.

\[\square\]

It follows directly that we can compute the TED by computing the cheapest mapping instead of the cheapest edit script.

**Theorem 5.** Let \( X \) and \( Y \) be forests over some alphabet \( X \) and \( c \) be a cost function over \( X \) that is non-negative, self-equal, and conforms to the triangular inequality. Then it holds:

\[
\min_{\delta \in \Delta_X} \{ C(\delta, X) | \delta(X) = Y}\ = \\
\min \{ C(M, X, Y) | M \text{ is a tree mapping between } X \text{ and } Y \}
\]  

(8)

**Proof.** First, we define two abbreviations for the minima, namely:

\[
d_c^{\text{script}}(X, Y) := \min_{\delta \in \Delta_X} \{ C(\delta, X) | \delta(X) = Y\} \\
d_c^{\text{map}}(X, Y) := \min \{ C(M, X, Y) | M \text{ is a tree mapping between } X \text{ and } Y \}
\]

Let \( \bar{\delta} \) be an edit script such that \( \delta(X) = Y \) and \( C(\delta, X) = d_c^{\text{script}}(X, Y) \). Then, we know due to Theorem 4 that the corresponding mapping \( M_{\bar{\delta}} \) is at most as expensive as \( \bar{\delta} \), i.e. \( C(M_{\bar{\delta}}, X, Y) \leq C(\delta, X) = d_c^{\text{script}}(X, Y) \). This implies: \( d_c^{\text{map}}(X, Y) \leq d_c^{\text{script}}(X, Y) \).

Conversely, let \( M \) be a tree mapping between \( X \) and \( Y \), such that \( C(M, X, Y) = d_c^{\text{map}}(X, Y) \). Then, we know due to Theorem 4 that the corresponding edit script \( \bar{\delta}_M \) has the same cost as \( M \), i.e. \( C(\bar{\delta}_M, X) = C(M, X, Y) \). This implies: \( d_c^{\text{script}}(X, Y) \leq d_c^{\text{map}}(X, Y) \).

This concludes our theory on edit scripts, cost functions, and mappings. We have now laid enough groundwork to efficiently compute the TED.

## 3 The Dynamic Programming Algorithm

To compute the TED between two trees \( \bar{x} \) and \( \bar{y} \) efficiently, we require a way to decompose the TED into parts, such that we can compute the distance between subtrees of \( \bar{x} \) and \( \bar{y} \) and combine those partial TEDs to an overall TED. In order to do that, we need to define what we mean by “partial trees”.

14
Algorithm 2 An algorithm to retrieve the subforest from $i$ to $j$ of a forest $X$.

function SUBFOREST(Forest $X = \bar{x}_1, \ldots, \bar{x}_R$, start index $i$, end index $j$, current index $k$)

\begin{align*}
Y & \leftarrow \epsilon, \\
& \text{for } r = 1, \ldots, R \text{ do} \\
& \quad k \leftarrow k + 1. \\
& \quad \text{Let } x(\bar{y}_1, \ldots, \bar{y}_n) \leftarrow \bar{x}_r. \\
& \quad \text{if } k > j \text{ then} \quad \text{return } (Y, k). \\
& \quad \text{else if } k \geq i \text{ then} \quad (Y', k) \leftarrow \text{SUBFOREST}(\bar{y}_1, \ldots, \bar{y}_n, i, j, k). \\
& \quad \quad Y' \leftarrow Y \oplus x(Y'). \\
& \quad \quad \text{else} \quad (Y', k) \leftarrow \text{SUBFOREST}(\bar{y}_1, \ldots, \bar{y}_n, i, j, k). \\
& \quad \quad Y' \leftarrow Y'. \\
& \quad \text{end if} \quad \text{return } (Y, k). \\
& \text{end for} \quad \text{end function}
\end{align*}

Definition 11 (subforest). Let $X$ be a forest of size $m = |X|$. Further, let $i, j \in \{1, \ldots, m\}$ with $i \leq j$. We define the subforest of $X$ from $i$ to $j$, denoted as $X[i, j]$, as the first output of Algorithm 2 for the input $X$, $i$, $j$, and 0.

As an example, consider the left tree $\bar{x} = a(b(c, d), e)$ from Figure 1 (left). For this example, we find: $X[1, 1] = a$, $X[2, 4] = b(c, d)$, $X[3, 5] = c, d, e$, and $X[2, 1] = \epsilon$.

Note that $X[2, 4] = \bar{x}_2$, that is: The subforest of $\bar{x}$ from 2 to 4 is exactly the subtree rooted at 2. In general, subforests which correspond to subtrees are important special cases, which we can characterize in terms of outermost right leaves.

Definition 12 (outermost right leaf). Let $X$ be a forest of size $m = |X|$. Further, let $i \in \{1, \ldots, m\}$. We define the outermost right leaf of $i$ as

$$rl_X(i) = i + |\bar{x}_i| - 1. \quad (9)$$

Again, consider the tree $\bar{x} = a(b(c, d), e)$ from Figure 2. For this tree, we have $rl_x(1) = 5$, $rl_x(2) = 4$, $rl_x(3) = 3$, $rl_x(4) = 4$, $rl_x(5) = 5$.

More generally, we can show that the subforest from $i$ to its outermost right leaf is always the subtree rooted at $i$.

Theorem 6. Let $X$ be a forest. For any $i \in \{1, \ldots, |X|\}$ it holds:

$$X[i, rl_X(i)] = \bar{x}_i \quad (10)$$

Proof. First, note that the pre-order algorithm (see definition 11) visits parents before children and left children before right children. Therefore, the largest index within a subtree must be the outermost right leaf. The claim follows because the subforest Algorithm 2 visits nodes in the same order as the pre-order algorithm and therefore $X[i, rl_X(i)] = X[i, i + |\bar{x}_i| - 1] = \bar{x}_i$. \hfill \Box

Now, we can define the edit distance between partial trees, which we call the subforest edit distance:

Definition 13 (Subforest edit distance). Let $X$ and $Y$ be forests over some alphabet $\mathcal{X}$, let $c$ be a cost function over $\mathcal{X}$, let $\bar{x}_k$ be an ancestor of $\bar{x}_i$ in $X$, and let $\bar{y}_j$ be an ancestor of $\bar{y}_j$ in $Y$. Then, we define the subforest edit distance between the subforests $X[i, rl_X(k)]$ and $Y[j, rl_Y(l)]$ as

$$D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) := \min_{\delta \in \Delta_X} \left\{ C(\delta, X[i, rl_X(k)]) \middle| \bar{\delta}(X[i, rl_X(k)]) = Y[j, rl_Y(l)] \right\} \quad (11)$$

It directly follows that:
Theorem 7. Let $X$ and $Y$ be trees over some alphabet $\mathcal{X}$ of size $m = |X|$ and $n = |Y|$ respectively. For every $i \in \{1, \ldots, m\}$ and $j \in \{1, \ldots, n\}$ we have:

$$D(X[i, rl_X(i)], Y[j, rl_Y(j)]) = d_c(\bar{x}_i, \bar{y}_j) \tag{12}$$

Proof. From Theorem 6 we know that $X[i, rl_X(i)] = \bar{x}_i$ and $Y[j, rl_Y(j)] = \bar{y}_j$. Therefore, we have

$$D(X[i, rl_X(i)], Y[j, rl_Y(j)]) := \min_{\delta \in \Delta_X} \left\{ C(\delta, \bar{x}_i) \middle| \delta(\bar{x}_i) = \bar{y}_j \right\}$$

which corresponds exactly to the definition of $d_c(\bar{x}_i, \bar{y}_j)$.

Finally, we can go on to prove the arguably most important theorem for the TED, namely the recursive decomposition of the subforest edit distance:

Theorem 8. Let $X$ and $Y$ be non-empty forests over some alphabet $\mathcal{X}$ that is non-negative, self-equal, and conforms to the triangular inequality, let $\bar{x}_k$ be an ancestor of $\bar{x}_i$ in $X$, and let $\bar{y}_k$ be an ancestor of $\bar{y}_j$ in $Y$. Then it holds:

$$D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = \min \left\{ \begin{array}{ll}
c(x_i, -) + D_c(X[i + 1, rl_X(k)], Y[j, rl_Y(l)]), \\
c(-, y_j) + D_c(X[i, rl_X(k)], Y[j + 1, rl_Y(l)]), \\
\end{array} \right. \tag{13}$$

Further it holds:

$$d_c(\bar{x}_i, \bar{y}_j) = \min \{c(x_i, -) + D_c(X[i + 1, rl_X(i)], Y[j, rl_Y(j)]), \right. \tag{14}$$

Proof. We first show that an intermediate decomposition holds. In particular, we show that:

$$D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = \min \left\{ \begin{array}{ll}
c(x_i, -) + D_c(X[i + 1, rl_X(k)], Y[j, rl_Y(l)]), \\
c(-, y_j) + D_c(X[i, rl_X(k)], Y[j + 1, rl_Y(l)]), \\
\end{array} \right. \tag{15}$$

Now, because we require that $c$ is non-negative, self-equal, and conforms to the triangular inequality, we know that Theorem 7 holds, that is, we know that we can replace the cost of a cheapest edit script with the cost of a cheapest mapping. Let $M$ be a cheapest mapping between the subtrees $X[i, rl_X(k)]$ and $Y[j, rl_Y(l)]$. Regarding $i$ and $j$, only the following cases can occur:

1. $i$ is not part of the mapping. In that case, $x_i$ is deleted and we have $D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = c(x_i, -) + D_c(X[i + 1, rl_X(k)], Y[j, rl_Y(l)]).$

2. $j$ is not part of the mapping. In that case, $y_j$ is inserted and we have $c(-, y_j) + D_c(X[i, rl_X(k)], Y[j + 1, rl_Y(l)]).$

3. Both $i$ and $j$ are part of the mapping. Let $j'$ be the index $i$ is mapped to and let $i'$ be the index that is mapped to $j$, that is, $(i, j') \in M$ and $(i', j) \in M$. Because of the third constraint on mappings we know that $i \geq i' \iff j' \geq j$ and $i \leq i' \iff j' \leq j$. Now, consider the case that $i' > i$. In that case we know that $j' < j$. However, in that case, $j'$ is not part of the subforest
\[ Y[j, rl_Y(l)] \], because \( j \) is per definition the smallest index within the subforest. Therefore, \((i, j')\) can not be part of a cheapest mapping between our two considered subforests.

Conversely, consider the case \( i' < i \). This is also not possible because in that case \( i' \) is not part of the subforest \( X[i, rl_X(k)] \). Therefore, it must hold that \( i' = i \). However, this implies by the first constraint on mappings that \( j' = j \). Therefore, \((i, j) \in M\). So we know that \( x_i \) is replaced with \( y_j \), which implies that \( D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = c(x_i, y_j) + D_c(X[i + 1, rl_X(k)], Y[j + 1, rl_Y(l)]) \).

However, if \((i, j) \in M\), the fourth constraint on mappings implies that all descendants of \( x_i \) are mapped to descendants of \( y_j \). More specifically, for any \((i', j') \in M\) where \( x_i \) is an ancestor of \( x_{i'} \) it must hold that \( y_j \) is also an ancestor of \( y_{j'} \). Therefore, the subforest edit distance further decomposes into:

\[ D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = c(x_i, y_j) + D_c(X[i + 1, rl_X(i)], Y[j + 1, rl_Y(j)]) \]

Because we required that \( M \) is a cheapest mapping, the minimum of these three options must be the case, which yields Equation \([15]\).

Using this intermediate result, we can now go on to prove Equations \([13]\) and \([14]\). In particular, Equation \([13]\) holds because we find that:

\[
d_e(\bar{x}_i, \bar{y}_j) = D_c(X[i, rl_X(i)], Y[j, rl_Y(j)]) = \min \left\{ c(x_i, \cdot) + D_c(X[i + 1, rl_X(i)], Y[j, rl_Y(j)]), \right. \\
\left. c(\cdot, y_j) + D_c(X[i, rl_X(i)], Y[j + 1, rl_Y(j)]), \right. \\
\left. c(x_i, y_j) + D_c(X[i + 1, rl_X(i)], Y[j + 1, rl_Y(j)]), \right. \\
\left. D_c(X[rl_X(i) + 1, rl_X(k)], Y[rl_Y(j) + 1, rl_Y(l)]) \right\}
\]

where \( D_c(X[rl_X(i) + 1, rl_X(k)], Y[rl_Y(j) + 1, rl_Y(l)]) = 0 \) because the two input forests are empty.

With respect to Equation \([13]\), we observe that one way to transform the subforest \( X[i, rl_X(k)] \) into the subforest \( Y[j, rl_Y(l)] \) is to transform the subforest \( X[i, rl_X(i)] \) into the subforest \( Y[j, rl_Y(j)] \), and then the subforest \( X[rl_X(i) + 1, rl_X(k)] \) into the subforest \( Y[rl_Y(j) + 1, rl_Y(l)] \). Therefore, we obtain:

\[
D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) \leq D_c(X[i, rl_X(i)], Y[j, rl_Y(j)]) + D_c(X[rl_X(i) + 1, rl_X(k)], Y[rl_Y(j) + 1, rl_Y(l)]) = d_e(\bar{x}_i, \bar{y}_j) + D_c(X[rl_X(i) + 1, rl_X(k)], Y[rl_Y(j) + 1, rl_Y(l)]),
\]

Further, we observe that:

\[
d_e(\bar{x}_i, \bar{y}_j) \leq c(x_i, y_j) + D_c(X[i + 1, rl_X(i)], Y[j + 1, rl_Y(j)]),
\]

because this is only one of the three cases in Equation \([14]\).

Now, note that the first two cases in Equations \([13]\) and \([15]\) are the same. Finally, consider that the last case of Equation \([15]\). In that case, we can conclude that:

\[
d_e(\bar{x}_i, \bar{y}_j) + D_c(X[rl_X(i) + 1, rl_X(k)], Y[rl_Y(j) + 1, rl_Y(l)]) \leq c(x_i, y_j) + D_c(X[i + 1, rl_X(i)], Y[j + 1, rl_Y(j)] + \\
D_c(X[rl_X(i) + 1, rl_X(k)], Y[rl_Y(j) + 1, rl_Y(l)]) \leq D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) \leq d_e(\bar{x}_i, \bar{y}_j) + D_c(X[rl_X(i) + 1, rl_X(k)], Y[rl_Y(j) + 1, rl_Y(l)])
\]

which implies that Equation \([13]\) holds.
Figure 5: An illustration of the decompositions in Equation 13 and 14.

we obtain the distance $c(b, -) + D_c(c, d, e, f)$ for the deletion, $D_c(b, c, d, f(g)) + D_c(e, e)$ for the replacement, and $c(-, f) + D_c c(d, c, d, e, g)$ for the insertion (also refer to Figure 5).

Now, consider the replacement option. According to Equation 14, we can decompose the TED $d_c(b, c, d, f(g))$ in three ways, corresponding to the options to delete $b$, replace $b$ with $f$, and insert $f$. In particular, we obtain the distance $c(b, -) + D_c(d, e, f(g))$ for the deletion, $c(b, f) + D_c(d, e, g)$ for the replacement, and $c(-, f) + D_c(b, c, d, g)$ for the insertion (also refer to Figure 5).

For an efficient algorithm for the TED, we are missing only one last ingredient, namely a valid base case for empty forests. This is easy enough to obtain:

**Theorem 9.** Let $X$ and $Y$ be forests over some alphabet $X$, let $c$ be a cost function $X$ that is non-negative, self-equal, and conforms to the triangular inequality, let $x_k$ be an ancestor of $x_i$ in $X$, and let $y_j$ be an ancestor of $y_i$ in $Y$. Then it holds:

$$D_c(e, e) = 0$$
$$D_c(X[i, rlX(k)], e) = c(x_i, e) + D_c(X[i + 1, rlX(k)], e)$$
$$D_c(e, Y[j, rlY(l)]) = c(-, y_j) + D_c(e, Y[j + 1, rlY(l)])$$

**Proof.** Because $c$ non-negative and self-equal, the cheapest script to transform an empty forest into an empty forest is to do nothing. Further, because $c$ conforms to the triangular inequality, the cheapest script to transform a non-empty forest into an empty forest is to delete all nodes. Finally, the cheapest script to transform an empty forest into a non-empty one is to insert all nodes.

Now, we are able to construct an efficient algorithm for the TED. We just need to iterate over all possible pairs of subtrees in both input trees and compute the TED between these subtrees. For this, we require the subforest edit distance for all pairs of subforests in these subtrees. We store intermediate results for the subforest edit distance in an array $D$ and intermediate results for the subtree edit distance in an array $d$. Finally, the edit distance between the whole input trees will be in the first entry of $d$.

**Theorem 10.** The output of Algorithm 3 is the TED. Further, Algorithm 3 runs in $O(m^2 \cdot n^2)$ time and in $O(m \cdot n)$ space complexity where $m$ and $n$ are the sizes of the input trees.

**Proof.** Each computational step is justified by one of the equations proven before (refer to the comments in the pseudo-code). Therefore, the output of the algorithm is correct. Finally, the algorithm runs in $O(m^2 \cdot n^2)$ because two of the nested for-loops run at most $m$ times and two of the loops run
at most \( n \) times. Note that this bound is tight because the worst case does occur for the trees shown in Figure 6. Regarding space complexity, we note that we maintain two matrices, \( d \) and \( D \), each with \( \mathcal{O}(m \cdot n) \) entries.

**Algorithm 3** An efficient algorithm for the TED. Note that this algorithm is not yet the most efficient one, but a proto-version of the actual TED algorithm of Zhang and Shasha (1989) which is shown later as Algorithm 5. The algorithm iterates over all subtrees of \( \bar{x} \) and \( \bar{y} \) and computes the tree edit distance for them based on the forest edit distances between all subforests of the respective subtrees.

```plaintext
function TREE-EDIT-DISTANCE(Two input trees \( \bar{x} \) and \( \bar{y} \), a cost function \( c \))
    \( m \leftarrow |\bar{x}|, n \leftarrow |\bar{y}|. \)
    \( d \leftarrow m \times n \) matrix of zeros.
    \( D \leftarrow (m + 1) \times (n + 1) \) matrix of zeros.

    for \( k \leftarrow m, \ldots, 1 \) do
        for \( l \leftarrow n, \ldots, 1 \) do
            \( D_{rlX(k)+1, rlY(l)+1} \leftarrow 0. \)
            for \( i \leftarrow rlX(k), \ldots, k \) do
                \( D_{i, rlY(l)+1} \leftarrow D_{i+1, rlY(l)+1} + c(x_i, \cdot). \)
                end for
            for \( j \leftarrow rlY(l), \ldots, l \) do
                \( D_{rlX(k)+i, j} \leftarrow D_{rlX(k)+1, j+1} + c(\cdot, y_j). \)
                end for
            end for
            if \( rlX(i) = rlX(k) \land rlY(j) = rlY(l) \) then
                \( D_{i, j} \leftarrow \min\{D_{i+1, j} + c(x_i, \cdot), \)
                \( D_{i+1, j+1} + c(x_i, y_j), \)
                \( D_{i+1, j+1} + c(\cdot, y_j)\}. \)
                \( d_{i, j} \leftarrow D_{i, j}. \)
                end if
        end for
    end for

return \( d_{1, 1}. \)
end function
```

As Zhang and Shasha (1989) point out, we can be even more efficient in our algorithm if we re-use already computed subforest edit distances whenever the outermost right leaf is equal:

**Theorem 11.** Let \( X \) and \( Y \) be forests over some alphabet \( \mathcal{X} \), let \( c \) be a cost function over \( \mathcal{X} \), let \( \bar{x}_k \) be an ancestor of \( \bar{x}_{k'} \) in \( X \) such that \( rlX(k) = rlX(k') \), and let \( \bar{y}_l \) be an ancestor of \( \bar{y}_{l'} \) such that \( rlY(l) = rlY(l') \). Then it holds for all \( i \) such that \( \bar{x}_k \) is an ancestor of \( \bar{x}_i \) and all \( j \) such that \( \bar{y}_l \) is an ancestor of \( \bar{y}_j \):

\[
D_c(X[i, rlX(k)], Y[j, rlY(l)]) = D_c(X[i, rlX(k')], Y[j, rlY(l')])
\]

(21)

**Proof.** Because we required that \( rlX(k) = rlX(k') \) and \( rlY(l) = rlY(l') \), this follows directly. □

Therefore, we can make our algorithm faster by letting the two outer loops only run over nodes for which we can not re-use the subforest edit distance. Those nodes are the so-called keyroots of our input trees.
Figure 6: An example tree structure which yields the worst-case runtime of $O(m^2 \cdot n^2)$ in Algorithm 3 as well as Algorithm 5.

**Definition 14** (keyroots). Let $X$ be a forest over some alphabet $\mathcal{X}$ and let $\bar{x}_i$ be a leaf in $X$. We define the keyroot of $\bar{x}_i$ as

$$k_X(i) = \min\{k | rl_X(k) = i\}$$

(22)

We define the keyroots of $X$, denoted as $\mathcal{K}(X)$ as the set of keyroots for all leaves of $X$.

For example, if we inspect tree $\bar{x} = a(b(c, d), e)$ from Figure 2 our leaves are $\bar{x}_3 = c$, $\bar{x}_4 = d$, and $\bar{x}_5 = e$. The corresponding key roots are $k_3(3) = 3$, $k_4(4) = 2$, and $k_5(5) = 1$. Accordingly, the set of keyroots $\mathcal{K}(\bar{x})$ is $\{1, 2, 3\}$.

Computing the keyroots is possible using Algorithm 4.

**Algorithm 4** An algorithm to compute the key roots of a forest.

```plaintext
function keyroots(A forest $X$)
    $m \leftarrow |X|$.
    $R \leftarrow \emptyset$.
    $\mathcal{K} \leftarrow \epsilon$.
    for $i \leftarrow 1, \ldots, m$ do
        $rl \leftarrow rl_X(i)$.
        if $rl \notin R$ then
            $R \leftarrow R \cup \{rl\}$.
            $\mathcal{K} \leftarrow \mathcal{K} \oplus i$.
        end if
    end for
    return $\mathcal{K}$.
end function
```

This yields the TED Algorithm 5 of Zhang and Shasha (1989).

**Theorem 12.** Algorithm 5 computes the TED. Further, Algorithm 5 runs in $O(m^2 \cdot n^2)$ and has $O(m \cdot n)$ space complexity.

**Proof.** The runtime proof is simple: Because we use a subset of outer loop iterations compared to Algorithm 3 we are at most as slow. Still, the runtime bound is tight, because the set of keyroots is per definition as large as the set of leaves of a tree, and the number of leaves of a tree can grow linearly with the size of a tree, as is the case in Figure 6. The space requirements are the same as for Algorithm 3.

Further, Algorithm 5 still computes the same result as Algorithm 3 because according to Theorem 11 the same subforest edit distances are computed as before.

As an example, consider the trees $\bar{x} = a(b(c, d), e)$ and $\bar{y} = f(g)$ from Figure 2 and the trivial cost function $c(x, y) = 0$ if $x = y$ and 1 otherwise. The TED algorithm first considers the edit distance
Algorithm 5 The $O(m^2 \cdot n^2)$ TED algorithm of Zhang and Shasha [1989]. The algorithm iterates over all subtrees of $\bar{x}$ and $\bar{y}$ rooted at key roots and computes the TED for them based on the forest edit distances between all subforests of the respective subtrees. Refer to our project web site for a reference implementation.

function TREE-EDIT-DISTANCE(Two input trees $\bar{x}$ and $\bar{y}$, a cost function $c$.)

$m \leftarrow |\bar{x}|$, $n \leftarrow |\bar{y}|$.

$K(\bar{x}) \leftarrow \text{KEYROOTS}(\bar{x})$.

$K(\bar{y}) \leftarrow \text{KEYROOTS}(\bar{y})$.

$d \leftarrow m \times n$ matrix of zeros.

$D \leftarrow (m + 1) \times (n + 1)$ matrix of zeros.

$\triangleright d_{i,j} = d_c(\bar{x}_i, \bar{y}_j)$.

$\triangleright D_{i,j} = D_c(X[i, rl_x(k)], Y[j, rl_y(l)])$.

for $k \in K(\bar{x})$ in descending order do

for $l \in K(\bar{y})$ in descending order do

$D_{rl_x(k)+1, rl_y(l)+1} \leftarrow 0$.

$\triangleright \text{Equation 18}$

end for

for $j \leftarrow rl_y(l)$, $\ldots$, $l$ do

for $i \leftarrow rl_x(k)$, $\ldots$, $k$ do

$D_{rl_x(k)+1, j} \leftarrow D_{rl_x(k)+1, j+1} + c(-, y_j)$.

$\triangleright \text{Equation 20}$

end for

end for

for $i \leftarrow rl_x(k)$, $\ldots$, $k$ do

for $j \leftarrow rl_y(l)$, $\ldots$, $l$ do

if $rl_x(i) = rl_y(k) \land rl_y(j) = rl_y(l)$ then

$D_{i,j} \leftarrow \min\{D_{i+1,j} + c(x_i, -),$

$D_{i,j+1} + c(-, y_j)$,

$D_{i+1,j+1} + c(x_i, y_j)\}$.

$\triangleright \text{Equation 14}$

else

$D_{i,j} \leftarrow \min\{D_{i+1,j} + c(x_i, -),$ $D_{i,j+1} + c(-, y_j),$ $D_{rl_x(i)+1, rl_y(j)+1} + d_{i,j}\}$.

$\triangleright \text{Equation 13}$

end if

end for

end for

end for

end for

return $d_{1,1}$.

end function
Figure 7: An illustration of the TED Algorithm of Zhang and Shasha (1989) for the two input trees from Figure 2. Nodes with the same right outermost leaf are shown in the same color. For these nodes, the subforest edit distance is re-used. Top right: The TED between all subtrees of the input trees. Bottom: The subforest edit distances for all key root pairs. All entries which correspond to a subtree edit distance are highlighted in color and linked with dashed arrows to the corresponding entries in the subtree edit distance table at the top right. Co-optimal mappings are indicated by solid lines linking the entries of the dynamic programming table to the distances they are decomposed into.
Definition 15 (Co-Optimal Mappings)  

We start by phrasing more precisely what we are looking for: Which edit script corresponds to the TED?  

Zhang and Shasha (1989) only hint at an answer in their own paper. Here, we shall rephrase the question: Which edit script corresponds to the TED? We have answered this question in part in Algorithm 1, which transforms a mapping into an edit script with the same cost. Therefore, we can rephrase the question: Which edit script corresponds to the TED? 

Now that we have computed the TED, the next question is: Which edit script corresponds to the TED?  

Listing all co-optimal mappings is infeasible in general, as the following theorem demonstrates:  

Theorem 13. Let $\bar{a}(1)$ be the tree $a$ over the alphabet $X = \{1\}$ and let $\bar{a}(m) = a(\bar{a}(m-1))$. Then, for any metric cost function $c$ over $X$ and any $m \in \mathbb{N}$ which is divisible by 2 it holds: There are $m!/[(m/2)!]^2$ co-optimal mappings between the trees $\bar{x} = \bar{a}(m)$ and $\bar{y} = \bar{a}(m/2)$. Further, this number is larger than $\frac{m^2}{2^m} \cdot \frac{3^{m+1}}{\sqrt{m}}$.  

Proof. Because $c$ is metric, we have $c(a, a) = 0$ and $c(a, -) > 0$. Therefore, we want to replace as many $a$ with $\bar{a}$ as possible to reduce the cost. At most, we can replace $m/2$ $a$ with $\bar{a}$, because...
\[ |\bar{a}(m/2)| = m/2. \] Therefore, this corresponds to choosing \( m/2 \) nodes from \( \bar{x} \) which are mapped to the \( m/2 \) nodes from \( \bar{y} \). As we know from combinatorics, there are

\[
\binom{m}{m/2} = \frac{m!}{(m/2)!^2}
\]

ways to choose \( m/2 \) from \( m \) elements. Using Stirling’s approximation we then obtain the following lower bound:

\[
\frac{m!}{(\frac{m}{2})^2} \geq \sqrt{2\pi} \cdot \frac{m^{m+\frac{1}{2}} \cdot e^{-m}}{(e \cdot (\frac{m}{2})^{\frac{m}{2}+\frac{1}{2}} \cdot e^{-\frac{m}{2}})^2} = \frac{m^{m+\frac{1}{2}}}{e^2} \cdot \frac{e^{-m}}{e^{-m}} = \frac{2m+\frac{1}{2}}{\sqrt{2}} \cdot \sqrt{\frac{2\pi}{e^2}} = \frac{2m+1}{\sqrt{m}}
\]

While it is therefore infeasible to list all co-optimal mappings, it is still possible to return some of the co-optimal mappings. In particular, it turns out that constructing a co-optimal mapping corresponds to finding a path in a graph which we call the co-optimal edit graph. First, we define a general graph as follows:

**Definition 16 (Directed Acyclic Graph (DAG)).** Let \( V \) be some set, and let \( E \subseteq V \times V \). Then we call \( G = (V, E) \) a graph, \( V \) the nodes of \( G \) and \( E \) the edges of \( G \). We call \( G \) a directed acyclic graph (DAG) if there exists a total ordering relation \(<\) on \( V \), such that for all edges \((u, v) \in E\) it holds: \( u < v \), i.e. edges occur only from lower nodes to higher nodes in the ordering.

We then define our co-optimal edit graph as follows.

**Definition 17 (Co-optimal Edit Graph).** Let \( X \) and \( Y \) be forests over some alphabet \( X \) and let \( c \) be a cost function over \( X \). Then, we define the co-optimal edit graph between \( X \) and \( Y \) according to \( c \) as the graph \( G_{c,X,Y} = (V, E) \) with nodes \( V \) and edges \( E \) as follows.

If \( X = \epsilon \) and \( Y = \epsilon \) we define \( V := \{(1, 1, 1)\} \) and \( E := \emptyset \).

If \( X = \epsilon \) but \( Y \neq \epsilon \) we define \( V := \{(1, 1, 1, j) | j \in \{1, \ldots, |Y|+1\}\} \) and \( E := \{((1, 1, 1, j), (1, 1, 1, j+1)) | j \in \{1, \ldots, |Y|\}\} \).

If \( X \neq \epsilon \) but \( Y = \epsilon \) we define \( V := \{(1, i, 1, 1) | i \in \{1, \ldots, |X|+1\}\} \) and \( E := \{((1, i, 1, 1), (1, i+1, 1, 1)) | i \in \{1, \ldots, |X|\}\} \).
If neither forest is empty, we define:

\[ V := \{(k, i, l, j) | k \in \mathcal{K}(X), i \in \{k, \ldots, rl_X(k) + 1\}, l \in \mathcal{K}(Y), j \in \{l, \ldots, rl_Y(l) + 1\} \} \]  
(23)

\[ E := \left\{ \left(k, i, l, j, (k, i + 1, l, j) \right) \mid D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = c(x_i, -) + D_c(X[i + 1, rl_X(k)], Y[j, rl_Y(l)]) \right\} \cup \]  
\[ \left\{ \left(k, i, l, j, (k, i, l, j + 1) \right) \mid D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = c(-, y_j) + D_c(X[i, rl_X(k)], Y[j + 1, rl_Y(l)]) \right\} \cup \]  
\[ \left\{ \left(k, i, l, j, (k, i + 1, l, j + 1) \right) \mid D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = c(x_i, y_j) + D_c(X[i + 1, rl_X(k)], Y[j + 1, rl_Y(l)]) \right\} \cup \]  
\[ \left\{ \left(k, i, l, j, (k, i, l, j) \right) \mid D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = c(x_i, y_j) + D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) \right\} \cup \]  
(24)

\[ \left\{ \left(k, i, l, j, (k, i + 1, l, j) \right) \mid D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = c(x_i, y_j) + D_c(X[i + 1, rl_X(k)], Y[j + 1, rl_Y(l)]) \right\} \cup \]  
\[ \left\{ \left(k, i, l, j, (k, i, l, j + 1) \right) \mid D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = c(x_i, y_j) + D_c(X[i + 1, rl_X(k)], Y[j + 1, rl_Y(l)]) \right\} \cup \]  
\[ \left\{ \left(k, i, l, j, (k, i, l, j) \right) \mid D_c(X[i, rl_X(k)], Y[j, rl_Y(l)]) = c(x_i, y_j) + D_c(X[i + 1, rl_X(k)], Y[j + 1, rl_Y(l)]) \right\} \cup \]  
(25)

\[ \left\{ \left(k, rl_X(k) + 1, l, rl_Y(l) + 1 \right), (k, X, rl_X(k) + 1, rl_X(k) + 1, Y, rl_Y(l) + 1, Y) \right\} \cup \]  
\[ \left\{ \left(k, rl_X(k) + 1, l, rl_Y(l) + 1 \right), (k, X, rl_X(k) + 1, rl_X(k) + 1, Y, rl_Y(l) + 1, Y) \right\} \cup \]  
\[ \left\{ \left(k, rl_X(k) + 1, l, rl_Y(l) + 1 \right), (k, X, rl_X(k) + 1, rl_X(k) + 1, Y, rl_Y(l) + 1, Y) \right\} \cup \]  
(26)

As this definition is quite extensive, we shall explain it in a bit more detail. The nodes of the co-optimal edit graph are, essentially, the entries of the dynamic programming matrix \( D \) of Algorithm 5. Given that this matrix needs to be computed for every combination of keyroots \((k, l) \in \mathcal{K}(X) \times \mathcal{K}(Y)\), we need four indices to identify a position in the dynamic programming matrix \( D \) uniquely, namely the keyroot indices and the matrix indices, leading to a quintuple \((k, i, l, j)\). Now, with respect to the edges, Equation 24 defines the edges corresponding to deletions (the first case in Equations 13 and 14). Equation 25 defines the edges corresponding to insertions (the second case in Equations 13 and 14). Equation 26 defines the edges corresponding to replacements within a subtree (the third case in Equation 14), and Equation 27 defines the edges corresponding to replacements of entire subtrees (the third case in Equation 13).

The remaining edges cover special cases. In particular, Equation 27 covers the case where all options, deletion, insertion, and replacement are co-optimal, and Equations 28, 29, and 30 cover cases where we are at the end of the dynamic programming matrix for a subtree and need to continue the computation in the dynamic programming matrix for a larger subtree which includes the current subtree.

An example, consider the co-optimal edit graph between the trees \( \bar{x} = a(b(c, d), e) \) and \( \bar{y} = f(g) \) from Figure 2. An excerpt of this graph is shown in Figure 9.

An important insight regarding the co-optimal edit graph is that it is acyclic.

**Theorem 14.** Let \( X \) and \( Y \) be forests over some alphabet \( \mathcal{X} \), let \( c \) be a cost function over \( \mathcal{X} \), and let \( \mathcal{G}_{c,X,Y} \) be the co-optimal edit graph with respect to \( X, Y, \) and \( c \). Then, \( \mathcal{G}_{c,X,Y} \) is a directed acyclic graph with the ordering relation \((k, i, l, j) < (k', i', l', j')\) if and only if \( i < i' \), or \( i = i' \) and \( j < j' \), or \( i = i' \) and \( j = j' \) and \( k > k' \), or \( i = i' \) and \( j = j' \) and \( k = k' \) and \( l < l' \).
Figure 9: An excerpt of the co-optimal edit graph between the trees $\bar{x}$ and $\bar{y}$ from Figure 2. The figure only shows nodes which are reachable from $(1, 1, 1, 1)$. Further, to support clarity, the nodes are labelled with indices and with the corresponding subforest edit distance. The indices in blue mark the order according to the ordering relationship $<$ as defined in Theorem [13].
Proof. Follows directly from the definition of the edges.

The ordering for the example graph in Figure 2 is displayed as blue indices.

Each edge in the co-optimal edit graph corresponds to an edit which could be used in a co-optimal edit script. Accordingly, we should be able to join edges in the co-optimal edit graph together, such that we obtain a complete, co-optimal edit script. This notion of joining edges is captured by the notion of a path.

Definition 18 (path). Let $\mathcal{G} = (V, E)$ be a graph. A path $p$ from $u \in V$ to $v \in V$ is defined as a sequence of nodes $p = v_0, \ldots, v_T$, such that $v_0 = u$, $v_T = v$, and for all $t \in \{1, \ldots, T\}$ : $(v_{t-1}, v_t) \in E$.

If a path from $u$ to $v$ exists, we call $v$ reachable from $u$.

Note that our definition permits trivial paths of length $T = 0$ from any node to itself. Next, we define the corresponding mapping to a path in the co-optimal edit graph:

Definition 19 (corresponding mapping). Let $X$ and $Y$ be forests over some alphabet $\mathcal{X}$, let $c$ be a cost function over $\mathcal{X}$, and let $\mathcal{G}_{c,X,Y} = (V, E)$ be the co-optimal edit graph with respect to $X,$ $Y,$ and $c$. Further, let $v_0, \ldots, v_T$ be a path from 1 to $|V|$ in $\mathcal{G}_{c,X,Y}$. Then, we define the corresponding mapping $M_{X,Y}(v_0, \ldots, v_T)$ for path $v_0, \ldots, v_T$ as $M = \emptyset$ if $X$ or $Y$ are empty and as follows otherwise:

$$M_{X,Y}(v_0, \ldots, v_T) = \{(i, j)|v_i = (k, i, l, j), v_{i+1} = (k', i + 1, l', j + 1) \text{ for any } k, l, k', l'\} \quad (32)$$

Consider the example path $p = (1, 1, 1, 1), (1, 2, 1, 2), (1, 3, 1, 2), (3, 4, 1, 3), (2, 4, 1, 3), (2, 5, 1, 3), (1, 5, 1, 3), (1, 6, 1, 3)$ in Figure 3. The corresponding mapping $M_{c, (b,c,d), f} (p)$ would be $\{ (1,1), (3,2) \}$, corresponding to the replacement edges on the path.

Given these definitions, we can go on to show our key theorem for backtracing, namely that the corresponding mapping for every path through the co-optimal edit graph is a co-optimal mapping, and that every co-optimal mapping corresponds to a path through the co-optimal edit graph.

Theorem 15. Let $X$ and $Y$ be forests over some alphabet $\mathcal{X}$, let $c$ be a cost function over $\mathcal{X}$ that is non-negative, self-equid, and conforms to the triangular inequality, and let $\mathcal{G}_{c,X,Y}$ be the co-optimal edit graph with respect to $X,$ $Y,$ and $c$. Then it holds:

1. For all paths $p$ from $(1,1,1,1)$ to $(1,|X|+1,1,|Y|+1)$ in $\mathcal{G}_{c,X,Y}$, the corresponding mapping $M_{X,Y}(p)$ is a co-optimal mapping between $X$ and $Y$.

2. For all co-optimal mappings $M$ between $X$ and $Y$, there exists at least one path $p$ from $(1,1,1,1)$ to $(1,|X|+1,1,|Y|+1)$ in $\mathcal{G}_{c,X,Y}$ such that $M_{X,Y}(p) = M$.

Proof. As a shorthand, we will call a path from $(1,1,1,1)$ to $(1,|X|+1,1,|Y|+1)$ in a co-optimal edit graph $\mathcal{G}_{c,X,Y}$ a path through that graph.

We start by considering the trivial cases of empty forests. If $X = \epsilon$ or $Y = \epsilon$, the only co-optimal mapping is $M = \emptyset$. It remains to show that, in these cases, the co-optimal edit graph contains only paths which correspond to this mapping.

$X = \epsilon$ and $Y = \epsilon$: In this case, we obtain $V = \{(1,1,1,1)\}$ and $E = \emptyset$. Accordingly, the trivial path $p = (1,1,1,1)$ is the only possible path through $\mathcal{G}_{c,X,Y}$ and it does indeed hold $M_p = \emptyset$.

$X = \epsilon$ and $Y \neq \epsilon$: In this case, we obtain $V = \{(1,1,1,j)|j \in \{1,\ldots,|Y|+1\}\}$ and $E = \{((1,1,1,j),(1,1,1,j+1))|j \in \{1,\ldots,|Y|\}\}$.

Accordingly, the only possible path through $\mathcal{G}_{c,X,Y}$ is $p = (1,1,1,1), (1,1,1,2), \ldots, (1,1,1,|Y|+1)$. And indeed it holds $M_p = \emptyset$.

$X \neq \epsilon$ and $Y = \epsilon$: In this case, we obtain $V = \{(1,i,1,1)|i \in \{1,\ldots,|X|+1\}\}$ and $E = \{((1,i,1,1),(1,i+1,1,1))|i \in \{1,\ldots,|X|\}\}$.

Accordingly, the only possible path through $\mathcal{G}_{c,X,Y}$ is $p = (1,1,1,1), (1,2,1,1), \ldots, (1,|X|+1,1,1)$. And indeed it holds $M_p = \emptyset$.
It remains to show both claims for the case of non-empty forests. For both claims, we apply an induction over the added size of both input forests, for which the base case is already provided by our considerations above. For the induction, we assume that both claims hold for inputs forests $X$ and $Y$ with $|X| + |Y| \leq k$.

Now, we consider two input forests $X$ and $Y$ with $m + n = k + 1$, where $m = |X|$ and $n = |Y|$.

Regarding the first claim, let $p = v_0, \ldots, v_{T'}$ be a path through $G_{c,X,Y}$, let $X' := X[2,|X|]$, let $Y' := Y[2,|Y|]$, and consider the following cases regarding $v_1$.

$v_1 = (1,2,1,1)$: In this case, it must hold $D_c(X,Y) = c(x_1, -) + D_c(X',Y')$, otherwise $(v_0,v_1) \not\in E$. Now, if $X'$ is empty, then $p$ must have the form $p = (1,1,1,1),(1,2,1,2), \ldots, (1,2,1,|X'| + 1)$, and $\emptyset$ must be a co-optimal mapping between $X'$ and $Y'$. Accordingly, $\emptyset = \emptyset$. Now, if $X'$ is non-empty, the path $v_1, \ldots, v_{T'}$ is isomorphic to a path from $(1,1,1,1)$ to $(1,|X'| + 1,1,|Y'| + 1)$ in $G_{c,X',Y'}$. Accordingly, by virtue of our induction hypothesis, $M_{p'}$ is a co-optimal mapping between $X'$ and $Y'$. Further, we obtain per construction $M_p = \{(i + 1,j)|(i,j) \in M_{p'}\}$. Accordingly, it holds: $C(M_{p'},X,Y) = c(x_1, -) + C(M_{p'},X',Y') = c(x_1, -) + D_c(X',Y') = D_c(X,Y)$.

$v_1 = (1,1,2,1)$: In this case, it must hold $D_c(X,Y) = c(x_1, y_1) + D_c(X',Y')$, otherwise $(v_0,v_1) \not\in E$. Now, if $Y'$ is empty, then $p$ must have the form $p = (1,1,1,1),(1,2,1,2), \ldots, (1,|X'| + 1,2)$, and $\emptyset$ must be a co-optimal mapping between $X$ and $Y'$. Accordingly, $\emptyset = \emptyset$. Now, if $Y'$ is non-empty, the path $v_1, \ldots, v_{T'}$ is isomorphic to a path from $(1,1,1,1)$ to $(1,|X'| + 1,1,|Y'| + 1)$ in $G_{c,X,Y'}$. Accordingly, by virtue of our induction hypothesis, $M_{p'}$ is a co-optimal mapping between $X$ and $Y'$. Further, we obtain per construction $M_p = \{(i,j + 1)|(i,j) \in M_{p'}\}$. Accordingly, it holds: $C(M_{p'},X,Y) = c(\emptyset, x_1) + C(M_{p'},X',Y') = c(x_1, -) + D_c(X',Y') = D_c(X,Y)$.

$v_1 = (1,2,1,2)$: In this case, it must hold $D_c(X,Y) = c(x_1, 1) + D_c(X',Y')$. Now, if $X'$ is empty, then $p$ must have the form $p = (1,1,1,1),(1,2,1,2), \ldots, (1,|X'| + 1,2)$, and $\emptyset$ must be a co-optimal mapping between $X'$ and $Y'$. Accordingly, $\emptyset = \emptyset$. Now, if $X'$ is non-empty, the path $v_1, \ldots, v_{T'}$ is isomorphic to a path from $(1,1,1,1)$ to $(1,|X'| + 1,1,|Y'| + 1)$ in $G_{c,X,Y'}$. Accordingly, by virtue of our induction hypothesis, $M_{p'}$ is a co-optimal mapping between $X'$ and $Y'$. Further, we obtain per construction $M_p = \{(i,1)|\{i\} \cup \{(i + 1,j + 1)|(i,j) \in M_{p'}\}\}$. Accordingly, it holds: $C(M_{p'},X,Y) = c(x_1, 1) + C(M_{p'},X',Y') = c(x_1, 1) + D_c(X',Y') = D_c(X,Y)$, which means that $M_p$ is co-optimal, as claimed.

Other cases can not occur such that our induction is concluded.

Regarding the second claim, let $M$ be a co-optimal mapping between $X$ and $Y$, i.e. $C(M,X,Y) = D_c(X,Y)$, and distinguish the following cases.

$I \in I(M,X,Y)$: In this case it holds $C(M,X,Y) = c(x_1, -) + C(M',X',Y')$ with $M' = \{(i - 1,j)|\{i\} \in M\}$. It must hold that $M'$ is a co-optimal mapping between $X'$ and $Y$. Otherwise, we would obtain $D_c(X,Y) \leq D_c(X',Y') + c(x_1, -) < C(M',X',Y') + c(x_1, -)$, which is a contradiction. This also implies that $D_c(X,Y) = c(x_1, -) + D_c(X',Y')$, which in turn implies that $\{(i - 1,1,1),(i,2,1,1)\} \in E$.

Now, if $X' = \emptyset$, $M$ must be $\emptyset$, and we can construct the path $p = (1,1,1,1),(1,2,1,1), \ldots, (1,2,1,|Y'| + 1)$, which is a path through $G_{c,X,Y}$ such that $M_p = \emptyset$. 28
If \( X' \) is not empty, our induction hypothesis implies that there exists a path \( p' \) from \((1,1,1,1)\) to \((1,|X'|+1,1,|Y'|+1)\) in \( G_{c,X,Y} \) such that \( M_{p'} = M' \). Therefore, we can construct an isomorphic path \( \tilde{p} \) between \((1,2,1,1)\) and \((1,|X|+1,1,|Y|+1)\) in \( G_{c,X,Y} \). Accordingly, \( p := (1,1,1,1) \), \( \tilde{p} \) must be a path through \( G_{c,X,Y} \), and per construction it must hold that \( M_p = M \).

\[ 1 \in J(M,X,Y) : \text{In this case it holds } C(M,X,Y) = c(-,y_1) + C(M',X,Y') \text{ with } M' = \{(i,j-1)\} \in M \}. \text{ It must hold that } M' \text{ is a co-optimal mapping between } X \text{ and } Y'. \text{ Otherwise, we would obtain } D_c(X,Y) \leq D_c(X,Y') + c(-,y_1) < C(M',X,Y') + c(-,y_1) = C(M,X,Y) = D_c(X,Y), \text{ which is a contradiction. This also implies that } D_c(X,Y) = c(-,y_1) + D_c(X,Y'), \text{ which in turn implies that } ((1,1,1,1), (1,1,1,2)) \in E. \]

Now, if \( Y' = \epsilon \), \( M \) must be \( \emptyset \), and we can construct the path \( p = (1,1,1,1), (1,2,1,2), \ldots, (1,|X|+1,1,2) \), which is a path through \( G_{c,X,Y} \) such that \( M_p = \emptyset \).

If \( X' \) is not empty, our induction hypothesis implies that there exists a path \( p' \) from \((1,1,1,1)\) to \((1,|X|+1,1,|Y'|+1)\) in \( G_{c,X,Y} \) such that \( M_{p'} = M' \). Therefore, we can construct an isomorphic path \( \tilde{p} \) between \((1,2,1,1)\) and \((1,|X|+1,|Y'|+1)\) in \( G_{c,X,Y} \). Accordingly, \( p := (1,1,1,1) \), \( \tilde{p} \) must be a path through \( G_{c,X,Y} \), and per construction it must hold that \( M_p = M \).

\[ \exists (1,j), (i,1) \in M : \text{In this case, } i = j = 1, \text{ which we can show as follows. Consider the case } j > 1. \text{ In that case, } i < 1, \text{ which is impossible. Similarly, if } i > 1, \text{ it must hold } j < 1, \text{ which is impossible. Therefore } i = 1 \text{ and } j = 1. \]

In this case it holds \( C(M,X,Y) = c(x_1,y_1) + C(M',X',Y') \text{ with } M' = \{(i-1,j-1)\} \in M \setminus \{(1,1)\} \}. \text{ It must hold that } M' \text{ is a co-optimal mapping between } X' \text{ and } Y'. \text{ Otherwise, we would obtain } D_c(X,Y) \leq D_c(X',Y') + c(x_1,y_1) < C(M',X',Y') + c(x_1,y_1) = C(M,X,Y) = D_c(X,Y), \text{ which is a contradiction. This also implies that } D_c(X,Y) = c(x_1,y_1) + D_c(X',Y'), \text{ which in turn implies that } ((1,1,1,1), (1,2,1,2)) \in E. \]

Now, if \( X' = \epsilon \), \( M \) must be \( \{(1,1)\} \), and we can construct the path \( p = (1,1,1,1), (1,2,1,2), \ldots, (1,|X|+1,1,2) \), which is a path through \( G_{c,X,Y} \) such that \( M_p = \{(1,1)\} \).

If \( Y' = \epsilon \), \( M \) must be \( \{(1,1)\} \), and we can construct the path \( p = (1,1,1,1), (1,2,1,2), \ldots, (1,|X|+1,1,2) \), which is a path through \( G_{c,X,Y} \) such that \( M_p = \{(1,1)\} \).

If neither \( X' \) nor \( Y' \) is empty, our induction hypothesis implies that there exists a path \( p' \) through \( G_{c,X,Y'} \) such that \( M_{p'} = M' \). Therefore, we can construct an isomorphic path \( \tilde{p} \) between \((1,2,1,2)\) and \((1,|X|+1,|Y'|+1)\) in \( G_{c,X,Y} \). Accordingly, \( p := (1,1,1,1) \), \( \tilde{p} \) must be a path through \( G_{c,X,Y} \), and per construction it must hold that \( M_p = M \).

As no other cases can occur, this concludes the proof.

\[ \square \]

### 4.1 Finding a single co-optimal mapping

Now that we have proven that finding a co-optimal mapping is equivalent to finding a path through the co-optimal edit graph, it is relatively simple to construct an algorithm which identifies one such mapping.

**Theorem 16.** Given two input trees \( \tilde{x} \) and \( \tilde{y} \) as well as a cost function \( c \) that is non-negative, self-equal, and conforms to the triangular inequality, Algorithm 6 computes a co-optimal mapping \( M \) between \( \tilde{x} \) and \( \tilde{y} \). Further, Algorithm 6 runs in \( \mathcal{O}(m + n) \cdot m \cdot n \) time complexity and \( \mathcal{O}(m \cdot n) \) space complexity.

**Proof.** Note: This is only a sketch of a proof. For a rigorous proof, we would have to properly match the actions of Algorithm 6 with the co-optimal edit graph.

Algorithm 6 starts at \((1,1,1,1)\) and then travels along the co-optimal edit graph, implicitly constructing it as needed. In particular, lines 29-33 cover the (replacement) edges defined in Equations 29 and 27 and lines 35-39 cover the (subtree replacement) edges defined via Equation 28. Lines 41-42 cover the (deletion) edges defined via Equation 24 and lines 43-45 cover the (insertion) edges defined via Equation 23. The backwards connections defined via Equations 29 30 31 are taken when returning from a recursive call in line 36. Importantly, note that the update in lines 7-25 always ensures that we consider to correct subforest edit distance matrix \( D \) when stepping into a new level of recursion.
Algorithm 6 A recursive backtracing algorithm for the TED, which infers a co-optimal mapping between the input trees \( \bar{x} \) and \( \bar{y} \). Refer to our project website for a reference implementation.

1: function BACKTRACE(\( \bar{x} \) and \( \bar{y} \), the matrices \( d \) and \( D \) after executing Algorithm 5 and a cost function \( c \))
2: \( M \leftarrow \emptyset \).
3: BACKTR(\( \bar{x} \), \( \bar{y} \), \( d \), \( D \), \( c \), \( M \), 1, 1).
4: return \( M \).
5: end function
6: function BACKTR(\( \bar{x} \) and \( \bar{y} \), \( d \), \( D \), \( c \), partial mapping \( M \), node indices \( k \) and \( l \))
7: if \( k > 1 \vee l > 1 \) then \( \triangleright \) Update \( D \)
8: for \( i \leftarrow rl_{x}(k), \ldots, k \) do
9: \( D_{i,rl_{y}(l)+1} \leftarrow D_{i+1,rl_{y}(l)+1} + c(x_{i}, -) \).
10: end for
11: for \( j \leftarrow rl_{y}(l), \ldots, l \) do
12: \( D_{i,rl_{x}(k)+1,j} \leftarrow D_{rl_{x}(k)+1,j+1} + c(\bar{y}_{j}) \).
13: end for
14: for \( i \leftarrow rl_{x}(k), \ldots, k \) do
15: for \( j \leftarrow rl_{y}(l), \ldots, l \) do
16: if \( rl_{x}(i) = rl_{x}(k) \land rl_{y}(j) = rl_{y}(l) \) then
17: \( D_{i,j} \leftarrow d_{i,j} + D_{rl_{x}(k)+1,rl_{y}(l)+1} \).
18: else
19: \( D_{i,j} \leftarrow \min\{D_{i+1,j} + c(x_{i}, -), \)
20: \( D_{i,j+1} + c(-, y_{j}), \)
21: \( D_{rl_{x}(i)+1,rl_{y}(j)+1} + d_{i,j}\} \).
22: end if
23: end for
24: end for
25: \( i \leftarrow k, j \leftarrow l \). \( \triangleright \) Start finding a path through the edit graph between \( \bar{x}_{k} \) and \( \bar{y}_{l} \).
26: while \( i \leq rl_{x}(k) \land j \leq rl_{y}(l) \) do
27: if \( \{rl_{x}(i) = rl_{x}(k) \land rl_{y}(j) = rl_{y}(l)\} \lor \{c(x_{i}, y_{j}) = c(x_{i}, -) + c(-, y_{j})\} \) then
28: if \( D_{i,j} = D_{i+1,j+1} + c(x_{i}, y_{j}) \) then
29: \( M \leftarrow M \cup \{(i,j)\} \). \( \triangleright \) replacement is optimal
30: \( i \leftarrow i + 1, j \leftarrow j + 1. \)
31: continue.
32: end if
33: else
34: if \( D_{i,j} = D_{rl_{x}(i)+1,rl_{y}(j)+1} + d_{i,j} \) then
35: BACKTR(\( \bar{x} \), \( \bar{y} \), \( d \), \( D \), \( c \), \( M \), \( i, j \)). \( \triangleright \) Recursively edit subtree \( \bar{x}_{i} \) into \( \bar{y}_{j} \).
36: \( i \leftarrow rl_{x}(i) + 1, j \leftarrow rl_{y}(j) + 1. \)
37: continue.
38: end if
39: end if
40: end if
41: if \( D_{i,j} = D_{i+1,j} + c(x_{i}, -) \) then
42: \( i \leftarrow i + 1. \) \( \triangleright \) deletion is optimal
43: else if \( D_{i,j} = D_{i,j+1} + c(-, y_{j}) \) then
44: \( j \leftarrow j + 1. \) \( \triangleright \) insertion is optimal
45: end if
46: end while
47: end function
Further note that Algorithm 6 directly constructs a co-optimal mapping from the path via line 30 which adds a tuple \((i, j)\) to the mapping whenever we use a replacement edge, as suggested by Theorem 15.

Regarding space complexity, the only data structures we require are the matrices \(D\) and \(d\) from before, as well as the trees \(\bar{x}\) and \(\bar{y}\), the cost function \(c\), and the (partial) mapping \(M\) which results in \(O(m \cdot n)\) space complexity. Regarding runtime, we note that each iteration of the while loop in lines 27-46 of Algorithm 6 advances either \(i\) or \(j\). Accordingly, the while loop can run at most \(O(m + n)\) times. At worst, we need to perform a recursion in each step, in which case a section of the matrix \(D\) is updated. Each of these updates takes at worst \(O(m \cdot n)\) operations, such that we obtain \(O((m + n) \cdot m \cdot n)\) overall.

As an example, consider the co-optimal edit graph in Figure 8 corresponding to the subforest edit graph, specifically.

As we have already seen, it is infeasible to list all co-optimal mappings in general (see Theorem 13). Interestingly, though, we can still count the number of such mappings efficiently. We will first consider the problem of counting the number of paths in a general DAG, and then return to the co-optimal edit graph, specifically.

**Theorem 17.** Let \(G = (V, E)\) be a DAG with ordering relation \(<\) and let \(v_1, \ldots, v_n\) be the nodes in \(V\) as ordered according to \(<\). Then, Algorithm 7 returns a \(n \times 1\) vector \(\bar{\alpha}\), such that \(\alpha_i\) is exactly the number of paths leading from \(v_1\) to \(v_i\). Further, Algorithm 7 runs in \(O(n)\) time and space complexity.

**Proof.** To prove this result, we first show two lemmata:

1. Algorithm 7 visits all reachable nodes from \(v_1\) in ascending order, and no other nodes.
2. When Algorithm 7 visits node \( v_i \), \( \alpha_i \) contains exactly the number of paths from \( v_1 \) to \( v_i \).

We call a note visited, if it is pulled from \( Q \). We proof both lemmata by induction over \( i \).

1. Our base case is \( v_1 \), which is indeed visited first.

Now, assume that the claim holds for all reachable nodes \( \leq v \). Consider the smallest node \( u > v \) which is reachable from \( 1 \). Then, there is a path \( u_0, \ldots, u_T \) with \( u_0 = v_1 \) and \( u_T = u \). Because \( G \) is a DAG, \( u_{T-1} < u \). Further, because \( u_0, \ldots, u_{T-1} \) is a path from \( v_1 \) to \( u_{T-1} \), \( u_{T-1} \) is reachable from \( v_1 \). Because \( u \) is per definition the smallest node larger than \( v \) which is reachable from \( v_1 \), it must hold \( u_{T-1} \leq v \). Therefore, per induction, \( u_{T-1} \) has been visited before. This implies that \( u \in Q \). Because we select the minimum from \( Q \) in each iteration, and because all elements smaller than \( u \) have been visited before (and are not visited again due to the DAG property), \( u \) will be visited next. Therefore, still all reachable nodes from \( v_1 \) are visited in ascending order, and all nodes that are visited are reachable nodes.

2. Again, our base case is \( v_1 \), which is visited first. As it is visited, \( \alpha_1 = 1 \). Indeed, there is only one path from \( v_1 \) to \( v_1 \), which is the trivial path.

Now, assume that the claim holds for all reachable nodes \( \leq v \). Then, consider the smallest node \( v_1 > v \) which is reachable from \( v_1 \). Further, let \( v_1, \ldots, v_m \) be all nodes which are reachable from \( v_1 \), such that \( (v_1, v_j) \in E \). Because \( G \) is a DAG, \( v_1 < v_j \). Further, because \( v_1 \) is reachable from \( 1 \) and \( v_j \) is per definition the smallest node larger than \( v \) which is reachable from \( v_1 \), it must hold \( v_{j-1} \leq v \). Therefore, per induction, \( \alpha_{j-1} \) is equal to the number of paths from \( v_1 \) to \( v_{j-1} \). For any such path \( p \), the concatenation \( p \oplus v_1 \) is a path from \( v_1 \) to \( v_1 \). Conversely, we can decompose any path \( p' \) from \( v_1 \) to \( v_1 \) as \( p' = p \oplus v_i \), where \( p \) is a path from \( v_1 \) to some node \( v_{j-1} \).

Accordingly, the number of paths from \( v_1 \) to \( v_{j-1} \) is exactly \( \sum_{j=1}^m \alpha_{j-1} \).

Finally, because of the first lemma, we know that all \( v_j \) have been visited already (without duplicates), and that on each of these visits, \( \alpha_{j-1} \) has been added to \( \alpha_i \). Therefore, we obtain \( \alpha_i = \sum_{j=1}^m \alpha_{j-1} \).

Because Lemma 1 implies that we do not visit any node smaller than \( v_i \) after \( v_i \) has been visited, the value \( \alpha_i \) does not change after \( v_i \) is visited. Therefore, \( \alpha_i \) still contains the number of paths from \( v_1 \) to \( v_i \) at the end of the algorithm.

Regarding runtime, it follows from the first lemma that, per iteration, exactly one reachable node is processed and will not be visited again. In the worst case, all nodes in the graph are reachable, which yields \( O(n) \) iterations. In each iteration we need to retrieve the minimum of \( Q \) and insert all \( v \) into \( Q \), for which \( (u, v) \in E \). Both is possible in constant time if a suitable data structure for \( Q \) is used. If one uses a tree structure for \( Q \), the runtime rises to \( O(n \cdot \log(n)) \). The space complexity is \( O(n) \) because \( \alpha_i \) has \( n \) entries and \( Q \) can not exceed \( n \) entries.

**Algorithm 7** An algorithm to count the number of paths between \( v_1 \) and \( v_i \) in a DAG \( G = (\{v_1, \ldots, v_n\}, E) \) with ordering relation \(<\).

```plaintext
function COUNT-PATHS-FORWARD(A DAG \( G = (\{v_1, \ldots, v_n\}, E) \) with ordering relation \(<\))
  \( \tilde{\alpha} \leftarrow 0^n \).
  \( \alpha_1 \leftarrow 1 \).
  \( Q \leftarrow \{v_1\} \).
  while \( Q \neq \emptyset \) do
    \( v_i \leftarrow \min_{\leq Q} Q \).
    \( Q \leftarrow Q \setminus \{v_i\} \).
    for \( (v_j, v_i) \in E \) do
      \( \alpha_i \leftarrow \alpha_i + \alpha_j \).
      \( Q \leftarrow Q \cup \{v_j\} \).
    end for
  end while
  return \( \tilde{\alpha} \).
end function
```

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As an example, consider the DAG in Figure 9 with the ordering indices shown in blue. Assuming a sorted set for \( Q \), Algorithm 3 would initialize \( \alpha_1 \leftarrow 1 \) and \( Q \leftarrow \{(1,1,1,1)\} \) and would then behave as follows.

1. \( v_i = v_1 = (1,1,1,1) \), \( \alpha_2 \leftarrow 1 \), \( \alpha_3 \leftarrow 1 \), \( Q \leftarrow \{(1,2,1,1),(1,2,1,2)\} \).
2. \( v_i = v_2 = (1,2,1,1) \), \( \alpha_4 \leftarrow 1 \), \( Q \leftarrow \{(1,2,1,2),(2,3,1,2)\} \).
3. \( v_i = v_3 = (1,2,1,2) \), \( \alpha_5 \leftarrow 1 \), \( \alpha_6 \leftarrow 1 \), \( Q \leftarrow \{(2,3,1,2),(1,3,1,2),(2,3,1,3)\} \).
4. \( v_i = v_4 = (2,3,1,2) \), \( \alpha_7 \leftarrow 1 \), \( \alpha_9 \leftarrow 1 \), \( Q \leftarrow \{(1,3,1,2),(2,3,1,3),(2,4,1,2),(3,4,1,3)\} \).
5. \( v_i = v_5 = (1,3,1,2) \), \( \alpha_8 \leftarrow 1 \), \( \alpha_9 \leftarrow 1+1 \), \( Q \leftarrow \{(2,3,1,3),(2,4,1,2),(1,4,1,2),(3,4,1,3)\} \).
6. \( v_i = v_6 = (2,3,1,3) \), \( \alpha_{10} \leftarrow 1 \), \( Q \leftarrow \{(2,4,1,2),(1,4,1,2),(3,4,1,3),(2,4,1,3)\} \).
7. \( v_i = v_7 = (2,4,1,2) \), \( \alpha_{12} \leftarrow 1 \), \( Q \leftarrow \{(1,4,1,2),(3,4,1,3),(2,4,1,3),(2,5,1,3)\} \).
8. \( v_i = v_8 = (1,4,1,2) \), \( \alpha_{11} \leftarrow 1 \), \( \alpha_{13} \leftarrow 1 \), \( Q \leftarrow \{(3,4,1,3),(2,4,1,3),(1,5,1,2),(2,5,1,3),(1,5,1,3)\} \).
9. \( v_i = v_9 = (3,4,1,3) \), \( \alpha_{10} \leftarrow 1+2 \), \( Q \leftarrow \{(2,4,1,3),(1,5,1,2),(2,5,1,3),(1,5,1,3)\} \).
10. \( v_i = v_{10} = (2,4,1,3) \), \( \alpha_{12} \leftarrow 1+3 \), \( Q \leftarrow \{(1,5,1,2),(2,5,1,3),(1,5,1,3)\} \).
11. \( v_i = v_{11} = (1,5,1,2) \), \( \alpha_{14} \leftarrow 1 \), \( Q \leftarrow \{(2,5,1,3),(1,5,1,3),(1,6,1,3)\} \).
12. \( v_i = v_{12} = (2,5,1,3) \), \( \alpha_{13} \leftarrow 1+4 \), \( Q \leftarrow \{(1,5,1,3),(1,6,1,3)\} \).
13. \( v_i = v_{13} = (1,5,1,3) \), \( \alpha_{14} \leftarrow 1+5 \), \( Q \leftarrow \{(1,6,1,3)\} \).
14. \( v_i = v_{14} = (1,6,1,3) \), \( Q \leftarrow \emptyset \).

The resulting \( \alpha \)-values for all nodes are indicated in Figure 10.

Interestingly, we can also invert this computation to compute the number of paths which lead from any node \( v \) to the last node in a DAG.
Theorem 18. Let \( G = (V, E) \) be a DAG with ordering relation \(<\) and let \( v_1, \ldots, v_n \) be the nodes in \( V \) as ordered according to \(<\). Then, Algorithm \[ \text{\ref{alg:dynamic}} \] returns a \( n \times 1 \) vector \( \tilde{\beta} \), such that \( \beta_i \) is exactly the number of paths leading from \( v_i \) to \( v_n \). Further, Algorithm \[ \text{\ref{alg:dynamic}} \] runs in \( O(n) \) time and space complexity.

Proof. Note that the structure of this proof is exactly symmetric to Theorem 17.

To prove this result, we first show two lemmata:

1. Algorithm \[ \text{\ref{alg:dynamic}} \] visits all nodes from which \( v_n \) is reachable in descending order, and no other nodes.

2. When Algorithm \[ \text{\ref{alg:dynamic}} \] visits node \( v_i \), \( \beta_i \) contains exactly the number of paths from \( v_i \) to \( v_n \).

We call a note visited, if it is pulled from \( Q \). We proof both lemmata by induction over \( i \) in descending order.

1. Our base case is \( v_n \), which is indeed visited first.

Now, assume that the claim holds for nodes \( \geq v \) such that \( v_n \) is reachable from \( v \). Consider now the largest \( v \), such that \( v > v_i \) and \( v_n \) is reachable from \( v_i \). Then, there is a path \( u_0, \ldots, u_T \) with \( u_0 = v_i \) and \( u_T = v_n \). Because \( G \) is a DAG, \( u_1 > v_i \). Further, because \( u_1, \ldots, u_T \) is a path from \( u_1 \) to \( v_n \), \( v_n \) is reachable from \( u_1 \). Because \( v_i \) is per definition the largest node smaller than \( v \) from which \( v_n \) is reachable, \( u_1 \geq v \). Therefore, per induction, \( u_1 \) has been visited before. This implies that \( v_i \in Q \). Because we select the maximum from \( Q \) in each iteration, and because all elements larger than \( v_i \) have been visited before (and are not visited again due to the DAG property), \( v_i \) will be visited next. Therefore, still all nodes from which \( v_n \) is reachable are visited in descending order, and all nodes which are visited are nodes from which \( v_n \) is reachable.

2. Again, our base case is \( v_n \), which is visited first. As it is visited, we have \( \beta_n = 1 \). And indeed there is only one path from \( v_n \) to \( v_n \), namely the trivial path.

Now, assume that the claim holds for all nodes \( \geq v \) from which \( v_n \) is reachable. Then, consider the largest node \( v_i < v \) from which \( v_n \) is reachable. Further, let \( v_{i_1}, \ldots, v_{i_m} \) be all nodes from which \( v_n \) is reachable, such that \( (v_{i_j}, v_{i_j}) \in E \). Because \( G \) is a DAG, \( v_{i_j} > v_i \) for all \( j \). Further, because \( v_n \) is reachable from \( v_{i_j} \), and \( v_i \) is the largest node smaller than \( v \) from which \( v_n \) is reachable, it must hold \( v_{i_j} \geq v \). Therefore, per induction, \( \beta_{i_j} \) is the number of paths from \( v_{i_j} \) to \( v_n \). For any such path \( p \), the concatenation \( v_i \oplus p \) is a path from \( v_i \) to \( v_n \). Conversely, we can decompose any path \( p' \) from \( v_i \) to \( v_n \) as \( p' = v_i \oplus p \) where \( p \) is a path from \( v_{i_j} \) to \( v_n \) for some \( j \).

Accordingly, the number of paths from \( v_i \) to \( v_n \) is exactly \( \sum_{j=1}^{m} \beta_{i_j} \).

Finally, because of the first lemma, we know that all \( v_{i_j} \) have been visited already (without duplicates), and that on each of these visits, \( \beta_{i_j} \) has been added to \( \beta_i \). Therefore, we obtain \( \beta_i = \sum_{j=1}^{m} \beta_{i_j} \).

Because Lemma 1 implies that we do not visit any node larger than \( v_i \) after \( v_i \) has been visited, the value \( \beta_i \) does not change after \( i \) is visited. Therefore, \( \beta_i \) still contains the number of paths from \( v_i \) to \( v_T \) at the end of the algorithm.

Regarding runtime, it follows from the first lemma that, per iteration, exactly one reachable node is processed and will not be visited again. In the worst case, all nodes in the graph are reachable, which yields \( O(n) \) iterations. In each iteration we need to retrieve the maximum of \( Q \) and insert all \( u \) into \( Q \), for which \( (u, v) \in E \). Both is possible in constant time if a suitable data structure for \( Q \) is used. If one uses a tree structure for \( Q \), the runtime rises to \( O(n \cdot \log(n)) \). The space complexity is \( O(n) \) because \( \beta \) has \( n \) entries and \( Q \) can not exceed \( n \) entries.

As an example, consider the DAG on the right in Figure 9. The resulting \( \beta \)-values for all nodes are indicated in Figure 10.

Beyond the utility of counting the number of paths in linear time, the combination of both algorithms also permits us to compute how often a certain edge of the graph occurs in paths from \( v_1 \) to \( v_n \).

Theorem 19. Let \( G = (V = \{v_1, \ldots, v_n\}, E) \) be a DAG with ordering relation \(<\) where \( v_1, \ldots, v_n \) are ordered according to \(<\). Further, let \( \alpha \) be the result of Algorithm \[ \text{\ref{alg:dynamic}} \] for \( G \), and let \( \beta \) be the result of Algorithm \[ \text{\ref{alg:dynamic}} \] for \( G \). Then, for any edge \((v_i, v_j) \in E \) it holds: \( \alpha_i \cdot \beta_j \) is precisely the number of paths
Further, the second output argument of Algorithm 11 is the number of co-optimal mappings. Finally, we obtain
\[ m = \alpha \]
\[ v \]
\[ \leq \]
\[ m \]

Therefore, we obtain
\[ m \]
\[ \alpha \]

negative, self-equal, and conforms to the triangular inequality. Further, let
\[ \text{Theorem 17} \]
\[ \text{that the number of paths from} \]
\[ \text{DAG} \]
\[ \text{characterize the number of co-optimal mappings rather than the number of co-optimal paths.} \]

This results in a new forward-counting-
\[ \text{overcounting by covering this special case explicitly.} \]
\[ \text{These paths correspond to the same co-optimal mapping, leading to overcounting.} \]
\[ \text{We can avoid} \]
\[ \text{a replacement, and one which uses an insertion first and then a deletion. The first and last of} \]
\[ \text{Algorithm 9, a new backward-counting-Algorithm 10, and a forward-backward Algorithm 11 which} \]
\[ \text{correspond to the same co-optimal mapping.} \]

For the example DAG from Figure 9 we show all possible paths from \((1,1,1,1)\) to \((1,6,1,3)\) in Figure 10. For every edge in this DAG you can verify that, indeed, the number of traversing paths is equivalent to the \(\alpha\) value of the source node times the \(\beta\) value of the target node.

Note that the number of paths which traverses a certain edge reveals crucial information about the co-optimal mappings. In particular, if we consider an edge of the form \(\langle k, i, l, j \rangle, \langle k', i+1, l', j+1 \rangle\), the number of paths from \((1,1,1,1)\) to \((1,|X|+1,1,|Y|+1)\) which traverse this edge is an estimate of the number of co-optimal mappings which contain the tuple \((i,j)\). Unfortunately, this estimate is not necessarily exact, because there may be multiple paths through the co-optimal edit graph which correspond to the same co-optimal mapping.

In particular, excessive paths occur whenever \(c(x_i,-) + c(-,y_j) = c(x_i,y_j)\). In these cases, deletion, replacement, and insertion are all co-optimal, and thus there exist three paths from \((k,i,l,j)\) to \((k,i+1,j+1)\), one which uses a deletion first and then an insertion, one which uses only a replacement, and one which uses an insertion first and then a deletion. The first and last of these paths correspond to the same co-optimal mapping, leading to overcounting. We can avoid this overcounting by covering this special case explicitly. This results in a new forward-counting-Algorithm 8, a new backward-counting-Algorithm 10 and a forward-backward Algorithm 11 which characterize the number of co-optimal mappings rather than the number of co-optimal paths.

**Theorem 20.** Let \(\bar{x}\) and \(\bar{y}\) be trees over some alphabet \(X\) and let \(c\) be a cost function that is non-negative, self-equal, and conforms to the triangular inequality. Further, let \(G_{\bar{x},\bar{y},c} = (V,E)\) be the co-optimal edit graph corresponding to \(\bar{x},\bar{y}\), and \(c\). Then, the first output argument of Algorithm 11 is a \(|\bar{x}| \times |\bar{y}|\) matrix \(\Gamma\) such that \(\Gamma_{i,j}\) is exactly the number of co-optimal mappings which contain \((i,j)\). Further, the second output argument of Algorithm 11 is the number of co-optimal mappings. Finally, Algorithm 11 has \(O(|\bar{x}|^6 \cdot |\bar{y}|^6)\) time and \(O(|\bar{x}|^2 \cdot |\bar{y}|^2)\) space complexity.

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**Algorithm 8** An algorithm to count the number of paths between each node \(v_i\) and node \(v_n\) in a DAG \(G = (\{v_1, \ldots, v_n\}, E)\), where \(v_1, \ldots, v_n\) is the ordered node list according to the DAGs ordering relation <.

```plaintext
function COUNT-PATHS-BACKWARD(A DAG \(G = (\{v_1, \ldots, v_n\}, E)\), an ordering relation <.)
    \(\beta \leftarrow n \times 1\) vector of zeros.
    \(\beta_n \leftarrow 1.\)
    \(Q \leftarrow \{v_n\}.\)
    \(\text{while } Q \neq \emptyset \text{ do}\)
        \(v_j \leftarrow \max_{v \in Q} Q.\)
        \(Q \leftarrow Q \setminus \{v_j\}.\)
        \(\text{for } (v_i, v_j) \in E \text{ do}\)
            \(\beta_i \leftarrow \beta_i + \beta_j.\)
            \(Q \leftarrow Q \cup \{v_i\}.\)
        \(\text{end for}\)
    \(\text{end while}\)
    \(\text{return } \beta.\)
end function
```

from \(v_1\) to \(v_n\) which contain \(v_i, v_j\), that is, paths \(p = u_1, \ldots, u_T\) such that an \(t \in \{1, \ldots, T-1\}\) exists for which \(u_t = v_i\) and \(u_{t+1} = v_j\).

**Proof.** Let \((v_i, v_j) \in E\) and let \(m\) be the number of paths from \(v_1\) to \(v_n\) which traverse \((u,v)\). Further, let \(u_1, \ldots, u_T\) be a path from \(v_1\) to \(v_i\) and let \(u_T+1, \ldots, u_T\) be a path from \(v_j\) to \(v_n\). Then, because \((v_i, v_j) \in E\), \(u_1, \ldots, u_T\) is a path from \(v_1\) to \(v_n\) in \(G\) which traverses \((v_i, v_j)\). We know by virtue of Theorem 17 that the number of paths from \(v_1\) to \(v_i\) is \(\alpha_i\), and we know by virtue of Theorem 18 that the number of paths from \(v_i\) to \(v_n\) is \(\beta_j\). Now, as we noted before, any combination of a path counted in \(\alpha_i\) and a path counted in \(\beta_j\) is a path from \(v_1\) to \(v_n\), and any of these combinations is unique. Therefore, we obtain \(m \geq \alpha_u \cdot \beta_v\).

Further, we note that we can decompose any path from \(v_1\) to \(v_n\) as illustrated above, such that \(m \leq \alpha_u \cdot \beta_v\).
Proof. For the technical details of this proof, refer to my dissertation (Paaßen 2019). Here, I provide a sketch of the proof.

First, we observe that Algorithm 9 is analogous to Algorithm 7 and that Algorithm 10 is analogous to Algorithm 8. The latter analogy holds because we just postpone adding the contributions to $\beta_i$ to the visit of $\beta_i$ itself, but all contributions are still collected. We further speed up the process by considering only cells of the dynamic programming matrix which are actually reachable from $(1, 1, 1, 1)$. Another non-obvious part of the analogy is that we go into recursion to compute the number of co-optimal paths for a subtree replacement. In this regard, we note that we can extend any path from $(1, 1, 1, 1)$ to $(k, i, l, j)$ to a path to $(k, rl_x(i) + 1, l, rl_y(j) + 1)$ by using one of the possible paths in the co-optimal edit graph corresponding to $\hat{x}_i$ and $\hat{y}_j$. However, this would over-count the paths which delete the node $x_i$ or insert the node $y_j$, which we prevent by setting $D'_{k, 0} = D'_{k, 1} = \infty$. The same argument holds for the backwards case: We can extend any path from $(k, rl_x(i) + 1, l, rl_y(j) + 1)$ to $(1, |x| + 1, |y| + 1)$ to a path from $(i, j)$ to $(|x| + 1, |y| + 1)$ by using one of the possible paths in the co-optimal edit graph corresponding to $\hat{x}_i$ and $\hat{y}_j$.

Finally, Algorithm 11 computes the products of $\alpha$ and $\beta$-values according to Theorem 19. The only special case is, once again, the case of subtree replacements. In that case, we can again argue that, for any combination of a path which leads from $(1, 1, 1, 1)$ to $(k, i, l, j)$, and a path which leads from $(k, rl_x(i) + 1, l, rl_y(j) + 1)$ to $(1, |x| + 1, |y| + 1)$, we can construct a path from $(1, 1, 1, 1)$ to $(1, |x| + 1, |y| + 1)$ by inserting a ‘middle piece’ which corresponds to a path in the co-optimal edit graph for $\hat{x}_i$ and $\hat{y}_j$. Therefore, for $\gamma = A_{i,j} \cdot B_{\rho_{x(i)}(1), \rho_{y(j) + 1}}$, $\gamma'_{\rho'_{x}, \rho'_{y}}$ is an additional contribution to the count of $(i' + i - 1, j' + j - 1)$.

Now, consider the efficiency claims. First, we analyze Algorithm 7. In the worst case, lines 27-31 need to be executed in every possible iteration. In that case, $D'$ and $d'$ need to be computed via Algorithm 5, which requires $O(|\hat{x}|^2 \cdot |\hat{y}|^2)$ steps and $O(|\hat{x}| \cdot |\hat{y}|)$ space. Including the recursive calls, this can occur $O(|\hat{x}|^2 \cdot |\hat{y}|^2)$ times at worst such that Algorithm 7 has an overall runtime complexity of $O(|\hat{x}|^2 \cdot |\hat{y}|^2)$.

Regarding space complexity, each level of recursion needs to maintain a constant number of matrices of size $O(|x| \cdot |y|)$. A worst, there can be $O(|\hat{x}| \cdot |\hat{y}|)$ levels of recursion active at the same time, implying a space complexity of $O(|\hat{x}|^2 \cdot |\hat{y}|^2)$.

Now, note that Algorithm 8 by construction, iterates over the same elements as Algorithm 7 and has the same structure, such that the complexity results carry over.

Finally, regarding Algorithm 9 itself, we find that, in the worst case, lines 15-23 get executed in every possible iteration. These lines include a recursive call to Algorithm 5 and in each such recursive call, Algorithm 7 and Algorithm 8 get executed. With the same argument as before, we perform at most $O(|\hat{x}|^2 \cdot |\hat{y}|^2)$ of such recursive calls, yielding an overall runtime complexity of $O(|\hat{x}|^6 \cdot |\hat{y}|^6)$ in the worst case.

Regarding space complexity, each level of recursion needs to maintain a constant number of matrices of size $O(|\hat{x}| \cdot |\hat{y}|)$. A worst, there can be $O(|\hat{x}| \cdot |\hat{y}|)$ levels of recursion active at the same time, implying a space complexity of $O(|\hat{x}|^2 \cdot |\hat{y}|^2)$.

Note that the version of the algorithm presented here is dedicated to minimize space complexity. By additionally tabulating $\Gamma$ for all subtrees, space complexity rises to $O(|\hat{x}|^3 \cdot |\hat{y}|^3)$ in the worst case, but runtime complexity is reduced to $O(|\hat{x}|^3 \cdot |\hat{y}|^3)$.

Another point to note is that the worst case for this algorithm is quite unlikely. First, both input trees would have to be left- or right-heavy. Second, in every step of the computation, multiple options have to be co-optimal, which only occurs in degenerate cases where, for example, the deletion or insertion cost for all symbols is zero.

For the example TED calculation in Figure 7, the results for $A$, $B$, and $\Gamma$ according to Algorithm 11 are shown in Table 4. By comparing with the co-optimal mappings in Figure 8 you can verify that this matrix does indeed sum up all co-optimal mappings.

Interestingly, the matrix $\Gamma$ has further helpful properties. By considering the sum over all columns and subtracting it from the total number of co-optimal mappings we obtain the number of co-optimal mappings in which a certain node in $\hat{x}$ is deleted. In our example, $a$ is deleted in 2 co-optimal mappings, $b$ in 3 co-optimal mappings, $c$ in 4 co-optimal mappings, $d$ in 4 co-optimal mappings, and $e$ in 5 co-optimal mappings. Conversely, by summing up over all rows and subtracting the result from

\footnote{This is the version we implemented in our reference implementation}
Algorithm 9 A variation of the forward path-counting Algorithm 7 for the TED.

1: function \text{forward}(\bar{x}, \bar{y}, d, D) after executing Algorithm 5 and a cost function $c$)
2: Initialize $A$ as a $(|\bar{x}| + 1) \times (|\bar{y}| + 1)$ matrix of zeros.
3: $A_{1,1} \leftarrow 1$, $Q \leftarrow \{(1,1)\}$
4: $C \leftarrow \emptyset$
5: while $Q \neq \emptyset$ do
6:   $(i, j) \leftarrow \min Q$. \hfill $\triangleright$ Lexicographic ordering
7:   $Q \leftarrow Q \setminus \{(i, j)\}$
8:   $C \leftarrow C \cup \{(i, j)\}$
9:   if $i \leq |\bar{x}| \wedge D_{i,j} = c(x_i, -) + D_{i+1,j}$ then
10:      $A_{i+1,j} \leftarrow A_{i+1,j} + A_{i,j}$.
11:      $Q \leftarrow Q \cup \{(i + 1, j)\}.$
12:   end if
13:   if $j \leq |\bar{y}| \wedge D_{i,j} = c(-, y_j) + D_{i,j+1}$ then
14:      $A_{i,j+1} \leftarrow A_{i,j+1} + A_{i,j}$.
15:      $Q \leftarrow Q \cup \{(i, j + 1)\}$.
16:   end if
17:   if $i = |\bar{x}| + 1 \vee j = |\bar{y}| + 1 \vee c(x_i, y_j) = c(x_i, -) + c(-, y_j)$ then
18:      continue
19:   end if
20:   if $rl_x(i) = rl_x(1) \wedge rl_y(j) = rl_y(1)$ then
21:      if $D_{i,j} = D_{i+1,j+1} + c(x_i, y_j)$ then
22:         $A_{i+1,j+1} \leftarrow A_{i+1,j+1} + A_{i,j}$
23:         $Q \leftarrow Q \cup \{(i + 1, j + 1)\}$.
24:      end if
25:   else
26:      if $D_{i,j} = D_{rl_x(i)+1,rl_y(j)+1} + d_{i,j}$ then
27:         Compute $D'$ and $d'$ via Algorithm 5 for the subtrees $\bar{x}^i$ and $\bar{y}^j$.
28:         $D'_{1,2} \leftarrow \infty$, $D'_{2,1} \leftarrow \infty$.
29:         $(Q', A') \leftarrow \text{forward}(\bar{x}^i, \bar{y}^j, d', D', c)$.
30:         $A_{rl_x(i)+1,rl_y(j)+1} \leftarrow A_{rl_x(i)+1,rl_y(j)+1} + A'_{|x|^i+1,|y|^j+1} \cdot A_{i,j}$.
31:         $Q \leftarrow Q \cup \{(rl_x(i) + 1, rl_y(j) + 1)\}.$
32:      end if
33:   end if
34: end while
35: return $(C, A)$.
36: end function
Algorithm 10 A variation of the backward path-counting Algorithm 8 for the TED.

1: function BACKWARD(Two trees $\bar{x}$ and $\bar{y}$, the matrices $d$ and $D$ after executing Algorithm 5 a cost function $c$, and a set of tuples $C$ as returned by Algorithm 9)
2: Initialize $B$ as a $(|\bar{x}| + 1) \times (|\bar{y}| + 1)$ matrix of zeros.
3: $B_{|\bar{x}|+1,|\bar{y}|+1} \leftarrow 1.$
4: while $C \neq \emptyset$ do
5: $(i, j) \leftarrow \max C.$  \hspace{1cm} ▶ Lexicographic ordering
6: $C \leftarrow C \setminus \{(i, j)\}$.
7: if $i \leq |\bar{x}|$ and $D_{i,j} = c(x_i,-) + D_{i+1,j}$ then
8: $B_{i,j} \leftarrow B_{i,j} + B_{i+1,j}$
9: end if
10: if $j \leq |\bar{y}|$ and $D_{i,j} = c(-,y_j) + D_{i,j+1}$ then
11: $B_{i,j} \leftarrow B_{i,j} + B_{i,j+1}$
12: end if
13: continue
14: end if
15: if $i = |\bar{x}| + 1$ or $j = |\bar{y}| + 1$ or $c(x_i,y_j) = c(x_i,-) + c(-,y_j)$ then
16: if $rl_i = rl(1)$ and $rl_j = rl(1)$ then
17: if $D_{i,j} = D_{i+1,j+1} + c(x_i,y_j)$ then
18: $B_{i,j} \leftarrow B_{i,j} + B_{i+1,j+1}$
19: end if
20: else
21: $D_{i,j} = D_{rl_i+1,j} + d_{i,j}$
22: Compute $D'$ and $d'$ via Algorithm 5 for the subtrees $\bar{x}'$ and $\bar{y}'$.
23: $D_{i,2} \leftarrow \infty.$ $D_{2,1} \leftarrow \infty.$
24: $(Q',A') \leftarrow FORWARD(\bar{x}',\bar{y}',d',D',c)$.
25: $B_{i,j} \leftarrow B_{i,j} + B_{rl_i+1,j} \cdot A'_{|\bar{x}|+1,|\bar{y}|+1}$.
26: end if
27: end if
28: end if
29: return $B$.
30: end function

| $A_{i,j}$ | $B_{i,j}$ | $\Gamma_{i,j}$ |
|----------|-----------|--------------|
| $i$ | $j$ | $x_i$ | $y_j$ | $f$ | $g$ | $i$ | $j$ | $x_i$ | $y_j$ | $f$ | $g$ | $i$ | $j$ | $x_i$ | $y_j$ | $f$ | $g$ |
| 1 | a | 1 | - | 1 | a |
| 2 | b | 1 | 1 | 1 | b |
| 3 | c | 1 | - | 2 | c |
| 4 | d | 1 | 1 | 5 | d |
| 5 | e | 1 | - | 6 | e |
| 6 | - | 1 | 1 | - | 1 |
| 1 | a | 4 | 0 |
| 2 | b | 2 | 1 |
| 3 | c | 0 | 1 + 1 |
| 4 | d | 0 | 1 + 1 |
| 5 | e | 0 | 1 |

Table 1: The forward matrix $A$, the backward matrix $B$, and the matrix $\Gamma$ for the trees $\bar{x} = a(b(c,d),e)$ and $\bar{y} = f(g)$ from Figure 4 as returned by Algorithms 9, 10, and 11 respectively. The color coding follows Figure 7.
Algorithm 11 A forward-backward algorithm to compute the number of times the tuple \((i, j)\) occurs in co-optimal mappings for paths in the co-optimal edit graphs between two input trees \(\tilde{x}\) and \(\tilde{y}\). The second output is the overall number of co-optimal mappings. Refer to our [project web site] for a reference implementation.

1: function cooptimals(Two trees \(\tilde{x}\) and \(\tilde{y}\), the matrices \(d\) and \(D\) after executing algorithm 5, and a cost function \(c\))
2: \((C, A) \leftarrow \text{forward}(\tilde{x}, \tilde{y}, d, D, c)\). \(\triangleright\) Refer to Algorithm 9
3: \(B \leftarrow \text{backward}(\tilde{x}, \tilde{y}, d, D, c, C)\). \(\triangleright\) Refer to Algorithm 10
4: Initialize \(\Gamma\) as a \(|\tilde{x}| \times |\tilde{y}|\) matrix of zeros.
5: for \((i, j) \in C\) do
6: if \(i = |\tilde{x}| + 1 \lor j = |\tilde{y}| + 1\) then continue
7: if \(\{rl_{\tilde{x}}(i) = |\tilde{x}| \land rl_{\tilde{y}}(j) = |\tilde{y}|\} \lor c(x_i, y_j) = c(x_i, -) + c(-, y_j)\) then
8: if \(D_{i,j} = D_{i+1,j+1} + c(x_i, y_j)\) then
9: \(\Gamma_{i,j} \leftarrow \Gamma_{i,j} + A_{i,j} \cdot B_{i+1,j+1}\).
10: end if
11: else
12: if \(D_{i,j} = D_{rl_{\tilde{x}}(i)+1, rl_{\tilde{y}}(j)+1} + d_{i,j}\) then
13: \(\gamma \leftarrow A_{i,j} \cdot B_{rl_{\tilde{x}}(i)+1, rl_{\tilde{y}}(j)+1}\).
14: Compute \(D'\) and \(d'\) via Algorithm 9 for the subtrees \(\tilde{x}'\) and \(\tilde{y}'\).
15: \(D'_{1,2} \leftarrow \infty, D'_{2,1} \leftarrow \infty\).
16: \((\Gamma', k) \leftarrow \text{cooptimals}(\tilde{x}', \tilde{y}', D', d', c)\).
17: for \(i' \leftarrow 1, \ldots, |\tilde{x}'|\) do
18: for \(j' \leftarrow 1, \ldots, |\tilde{y}'|\) do
19: \(\Gamma_{i'+i'-1,j'+j'-1} \leftarrow \Gamma_{i'+i'-1,j'+j'-1} + \Gamma'_{i', j'} \cdot \gamma\).
20: end for
21: end for
22: end if
23: end if
24: end if
25: end for
26: return \((\Gamma, A_{|\tilde{x}|+1,|\tilde{y}|+1})\).
27: end function
the total number of co-optimal mappings we obtain the number of co-optimal mappings in which a certain node of $\bar{y}$ is inserted. In this example, neither $f$ nor $g$ are inserted in any co-optimal mapping.

Another interesting property is that the matrix $\Gamma$ represents the frequency of certain pairings of nodes in co-optimal mappings, if we divide all entries by the total number of co-optimal mappings. This version of the matrix also offers an alternative view on the tree edit distance itself.

**Theorem 21.** Let $\bar{x}$ and $\bar{y}$ be trees over some alphabet $\mathcal{X}$, and let $c$ be a cost function over $\mathcal{X}$. Further, let $\Gamma$ and $k$ be the two outputs of Algorithm 11 for $\bar{x}$, $\bar{y}$, and $c$, and let $P_c(\bar{x}, \bar{y}) := \frac{1}{k} \cdot \Gamma$.

Then, the following equation holds:

$$d_c(\bar{x}, \bar{y}) = \sum_{i=1}^{|x|} \sum_{j=1}^{|y|} P_c(\bar{x}, \bar{y})_{i,j} \cdot c(x_i, y_j)$$

$$+ \sum_{i=1}^{|x|} p_i^{\text{del}} \cdot c(x_i, -) + \sum_{j=1}^{|y|} p_j^{\text{ins}} \cdot c(-, y_j)$$

where

$$p_i^{\text{del}} := 1 - \sum_{j=1}^{|y|} P_c(\bar{x}, \bar{y})_{i,j}$$

$$p_j^{\text{ins}} := 1 - \sum_{i=1}^{|x|} P_c(\bar{x}, \bar{y})_{i,j}$$

**Proof.** Per construction, $\Gamma$ is equivalent to the number of co-optimal mappings $M$, such that $(i, j) \in M$, and $k$ is equivalent to the number of co-optimal mappings overall. The cost of each co-optimal mapping is per definition $d_c(\bar{x}, \bar{y})$. Therefore, summing over the cost of all these mappings and dividing by the number of mappings is also equal to $d_c(\bar{x}, \bar{y})$. 

This alternative representation of the TED is particularly useful if one wishes to learn the parameters of the tree edit distance, as all the computational complexity of the tree edit distance is encapsulated in the matrix $P_c(\bar{x}, \bar{y})_{i,j}$ and all learned parameters are linearly multiplied with this matrix. This trick has been originally suggested by Bellet, Habrard, and Sebban (2012) to learn optimal parameters for the string edit distance.

This concludes our tutorial. For further reading, I recommend the robust tree edit distance by Pawlik and Augsten (2011), as well as the metric learning approaches by Bellet, Habrard, and Sebban (2012) and Paassen et al. (2018b).

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