The Mapping Distance – a Generalization of the Edit Distance – and its Application to Trees

Kilho Shin[1] and Taro Niiyama[2]
[1]*University of Hyogo, Kobe, Japan*
[2]*NTT DoCoMo, Tokyo, Japan*

Keywords: Edit Distance, Kernel, Mapping, Tree.

Abstract: The edit distances has been widely used as an effective method to analyze similarity of compound data, which consist of multiple components, such as strings, trees and graphs. For example, the Levenshtein distance for strings is known to be effective to analyze DNA and proteins, and the Taï distance and its variations are attracting wide attention of researchers who study tree-type data such as glycan, HTML-DOM-trees, parse trees of natural language processing and so on. The problem that we recognize here is that the way of engineering new edit distances was ad-hoc and lacked a unified view. To solve the problem, we introduce the concept of the mapping distance. The mapping distance framework can provide a unified view over various distance measures for compound data focusing on partial one-to-one mappings between data. These partial one-to-one mappings are a generalization of what are known as traces in the legacy study of edit distances. This is a clear contrast to the legacy edit distance framework, which define distances between compound data through edit operations and edit paths. Our framework enables us to design new distance measures consistently, and also, various distance measures can be described using a small number of parameters. In fact, in this paper, we take rooted trees as an example and introduce three independent dimensions to parameterize mapping distance measures. As a result, we define 16 mapping distance measures, 13 of which are novel. In experiments, we discover that some novel measures outperform the others including the legacy edit distances in accuracy when used with the *k*-NN classifier.

1 INTRODUCTION

Edit distances have proven to be effective to measure similarity of compound data such as strings, trees and graphs. By a compound datum, we mean a datum that consists of one or more components: a string consists of letters, and a tree and a graph consist of vertices and edges.

The Levenshtein distance for strings (Levenshtein, 1966) is a well-known example of edit distance measures. Taï extended the Levenshtein distance to trees and introduced the first instance of edit distance measures that measure similarity between trees (Taï, 1979). Since computing Taï distances requires heavy computation, a number of its variations have been proposed in the literature including the *constrained* distance (Zhang, 1995), the *less-constrained* distance (Lu et al., 2001) and the *degree-two* distances (Zhang et al., 1996). Their definitions are all stemmed from the Taï distance, and they have succeeded in reducing computational complexity of the Taï distance. On the other hand, Wang and Zhang (Wang and Zhang, 2001) introduced the *alignment* distance to extend the concept of string alignments to trees. In fact, the alignment distance has turned out to be identical to the less constrained distance (Kuboyama et al., 2005). For graphs, a definition of edit distances is given in (Neuhaus and Bunke, 2007).

When we survey the study history of the tree edit distance, we see that many different definitions have been introduced in the literature, but the ways to introduce them appeared *ad-hoc* rather than being amenable to discipline. Therefore, we cannot deny the possibility that we have missed instances of the edit distance measure that have good performance in accuracy or time-efficiency or both.

Two of the important contributions of this paper are to introduce the notion of the *mapping distance*, which generalizes the legacy edit distance with a consistent view, and to engineer new distance measures for trees through three novel parameters obtained by leveraging the mapping distance framework.

In the following sections, we introduce the notion of mapping distances and clarify their advantages. To

Shin, K. and Niiyama, T.
The Mapping Distance – a Generalization of the Edit Distance – and its Application to Trees.
DOI: 10.5220/0006721902660275
In *Proceedings of the 10th International Conference on Agents and Artificial Intelligence (ICAART 2018) - Volume 2*, pages 266-275
ISBN: 978-989-758-275-2

illustrate, we develop our discussion focusing on application to trees. In fact, we introduce 16 instances of mapping distance measures for trees. Although three of them are well-known in the literature, the remainder are novel and are not investigated in the literature. In addition, we report the results of experiments that we run to compare these mapping distance measures. As a result, we have discovered that the distance measures that exhibit the best accuracy performance are novel measures.

2 LEGACY EDIT DISTANCES FOR TREES

Just for convenience of explanation, we mean *rooted trees* by "trees". Therefore, in this paper, a tree has always a *root* vertex, and all of the other vertices are its *descendants*.

In the traditional way, edit distances are defined based on *edit operations*, *edit paths* and *edit costs*. To illustrate, we let X and Y be two trees. An edit path from X to Y is a sequence of edit operations, which is one of (1) to substitute a vertex y of Y for a vertex x of X (denoted by (x,y)); (2) to delete a vertex x of X (denoted by $(x,\perp)$); the children of x is re-defined as children of the parent of x; (3) to insert a vertex y of Y below a vertex in the relevant tree as a child (denoted by $(\perp,y)$); an arbitrary subset of the child vertices of the vertex below which y is inserted can be selected and re-defined as child vertices of y.

Example 1. Fig. 1 exemplifies an edit path for the Taï distance. The leftmost tree is X, while the rightmost tree is Y. We first delete the vertex x_b (the vertex with label "b") from X. The children of x_b is re-defined as children of the root x_a. Next, we substitute the vertices y_a, y_c, y_d and y_g of Y for the vertices x_a, x_c, x_d and x_e, and obtain X_2. Finally, we insert the vertex y_f below the root y_a of X_2. To determine children of the new vertex y_f, we select y_d and y_g. Hence, the edit path here is represented by

$$(x_b,\perp)(x_a,y_a)(x_c,y_c)(x_d,y_d)(x_e,y_g)(\perp,y_f).$$

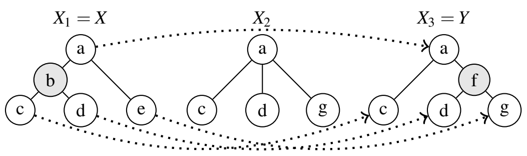


Figure 1: An edit path and a trace (dotted arrows) of the Taï distance: $(x_b,\perp)(x_a,y_a)(x_c,y_c)(x_d,y_d)(x_e,y_g)(\perp,y_f)$.

To each edit operation is assigned a *cost*, which is usually a non-negative real number. We let $\gamma(v,w)$, $\gamma(v,\perp)$ and $\gamma(\perp,w)$ denote the costs of substituting w for v, deleting v and inserting w. When $\ell(v)$ denotes the label of a vertex v, the most common setting of costs is:

$$\gamma(v,w) = \begin{cases} 0, & \text{if } \ell(v) = \ell(w); \\ 1, & \text{if } \ell(v) \neq \ell(w). \end{cases}$$
$$\gamma(v,\perp) = \gamma(\perp,w) = 1. \tag{1}$$

Then, the cost of an edit path is the sum of the costs of the operations that comprise the path: for example, the cost of the path of Fig. 1 is 3. The *Taï distance* $d_T(X,Y)$ is the minimum cost across all possible edit paths from X to Y (Taï, 1979).

Many variations of the Taï distance are known in the literature. The degree-two distance (Zhang et al., 1996) is an example and poses the constraint that only vertices with degree one and two can be deleted and inserted. The degree of a vertex is the number of edges that the vertex has, and the degree-two distance is the minimum cost of edit paths under this constraint.

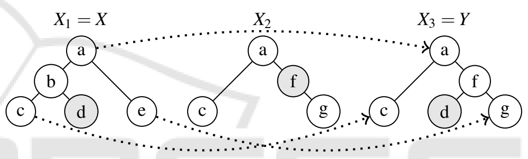


Figure 2: An edit path and a trace of the degree-two distance: $(x_d,\perp)(x_b,\perp)(\perp,y_f)(x_a,y_a)(x_c,y_c)(x_e,y_g)(\perp,y_d)$.

Example 2. In Fig. 2, the vertex x_d is of degree one, and hence, we can delete it. The degree of x_b has changed from three to two after deleting x_d, we can delete it. On the other hand, we can insert y_f between x_a and x_c, because its degree is two. In the same way as Example 1, we substitute the vertices y_a, y_c and y_g of Y for the vertices x_a, x_c and x_e. Then, we obtain X_2. Finally, we insert y_d, whose degree is one. The corresponding edit script is

$$(x_d,\perp)(x_b,\perp)(\perp,y_f)(x_a,y_a)(x_c,y_c)(x_e,y_g)(\perp,y_d),$$

and its cost is five.

The *trace* of an edit path is a partial one-to-one mapping between the vertex sets of X and Y, determined by the substitution operations included in the path. For the edit path of Example 1, the trace determines $(x_a \to y_a, x_c \to y_c, x_d \to y_d, x_e \to y_g)$, while that of Example 2 does $(x_a \to y_a, x_c \to y_c, x_e \to y_g)$. The domain and the range of a trace τ are those of τ as a partial mapping. For example, when we denote the trace of Example 1 by τ, the domain $\mathrm{Dom}(\tau)$ and the range $\mathrm{Ran}(\tau)$ are $\{x_a,x_c,x_d,x_e\}$ and $\{y_a,y_c,y_d,y_g\}$, respectively.

The constrained distance (Zhang, 1995), on the other hand, poses a constrain on traces.

In the remainder of this paper, we denote the *nearest common ancestor* (NCA) of vertices v and w in a tree X by $v \smile w$. More generally, for a set S of vertices of X, $S^{\smile}$ denotes the nearest common ancestor of all of the vertices of S.

Definition 1. Two sets S and T of vertices are *separable*, iff $S^{\smile}$ and $T^{\smile}$ are not in the ancestor-descendent relation.

Definition 2. A trace τ of an edit path is said to be *separable*, when $S \subseteq \mathrm{Dom}(\tau)$ and $T \subseteq \mathrm{Dom}(\tau)$ are separable in X, iff $\tau(S)$ and $\tau(T)$ are separable in Y.

The constrained distance requires that traces are always separable and is the minimum cost of edit paths under this constraint.

Example 3. The trace of the edit path of Example 1 is not separable. In fact, we let $S = \{x_c, x_d\}$ and $T = \{x_e\}$. Since $S^{\smile} = x_b$ and $T^{\smile} = x_e$, S and T are separable in X. By contrast, $\tau(S)^{\smile} = y_a$ is the root of Y, and hence, $\tau(S)$ and $\tau(T)$ are not separable.

3 MAPPING DISTANCES

The conditions that determine the edit paths of the Taï and degree-two distances can be equivalently described as constraints on their associated traces. To be specific, an edit path complies to the Taï or degree-two distance, if, and only if, its associated trace meets the following condition.

Taï: A trace preserves the relation of ancestors and descendants: x_1 is an ancestor of x_2 in $\mathrm{Dom}(\tau) \subseteq X$, iff $\tau(x_1)$ is an ancestor of $\tau(x_2)$ in Y.

Degree-two: A trace preserves the relation of NCA: if x_1 and x_2 are in $\mathrm{Dom}(\tau) \subseteq X$, then $x_1 \smile x_2 \in \mathrm{Dom}(\tau)$ and $\tau(x_1 \smile x_2) = \tau(x_1) \smile \tau(x_2)$ hold.

These constraints on traces require that traces as mappings preserve particular intrinsic *structures* of trees.

Taï: If a vertex v is an ancestor of a vertex w in a tree X, we denote $v > w$. This makes X a *partial ordered set* (poset). Hence, the condition stated above requires $v > w \Leftrightarrow \tau(v) > \tau(w)$. In other words, τ and τ^{-1} are *homomorphisms* of posets.

Degree-two: A tree X can be defined as an algebraic structure $(X, \smile)$ so that $v^{\smile}v = v$, $v^{\smile}w = w^{\smile}v$, $(v^{\smile}w)^{\smile}u = v^{\smile}(w^{\smile}u)$ and $v^{\smile}w^{\smile}u \in \{v^{\smile}w, w^{\smile}u, u^{\smile}v\}$ hold for any $\{v,w,u\} \subseteq X$. The condition stated above means that τ and τ^{-1} are homomorphisms, that is, $\tau(v^{\smile}w) = \tau(v)^{\smile}\tau(w)$ holds for any $\{v,w\} \subseteq \mathrm{Dom}(\tau) \subseteq X$.

On the other hand, given an edit path π and the associated trace τ, the cost $\gamma(\pi)$ is calculated by

$$\gamma(\pi) = \sum_{v \in X \setminus \mathrm{Dom}(\tau)} \gamma(v, \perp) + \sum_{w \in X \setminus \mathrm{Ran}(\tau)} \gamma(\perp, w) + \sum_{v \in \mathrm{Dom}(\tau)} \gamma(v, \tau(v)).$$

Since the left-hand side is a function of τ, we also denote it by $\gamma(\tau)$.

To determine a *mapping distance* $d(X,Y)$ between X and Y, we first determine a set $M_{X,Y}$ per pair (X,Y) that consists of partial one-to-one mappings from X to Y, and then, we let $d(X,Y) = \min_{\mu \in M_{X,Y}} \gamma(\mu)$.

Furthermore, we let $\mathcal{X}$ be a set of trees for which distances are to be computed and assume that a set of mapping $M_{X,Y}$ is uniquely assigned to each pair $(X,Y) \in \mathcal{M}^2$. By requiring $\mu \in M_{X,Y} \Rightarrow \mu^{-1} \in M_{Y,X}$ and symmetry of the cost function γ, that is, $\gamma(v,w) = \gamma(w,v)$ and $\gamma(v,\perp) = \gamma(\perp,v)$, the resulting distance measure has symmetry. Hence, $d(X,Y) = d(Y,X)$ holds. Regarding the triangle inequality $d(X,Y) + d(Y,Z) \geq d(X,Z)$, we have the following theorem.

Theorem 1. *If a family of sets of partial mappings $\mathcal{M} = \{M_{X,Y} \mid (X,Y) \in \mathcal{X}^2\}$ is* transitive*, that is, if $\mu \in M_{X,Y}$ and $\nu \in M_{Y,Z}$, $\nu \circ \mu \in M_{X,Z}$, the triangle inequality holds for the resulting mapping distance.*

4 PARAMETERIZING TRACES

The framework of the mapping distance also suits parameterizing mapping distance measures. In this section, we introduce a set of parameters that describe a certain class of mapping distances for trees. Once such parameters are given, by testing all of the combinations of parameter values, we can find the distance measure that fits to the relevant application the best.

For simplicity, we pose two premises on the partial mappings (traces) to investigate.

- We focus on rooted trees: the relation of ancestor and descendants is given among vertices.
- Traces preserve the relation of ancestors and descendants: $v > w \Leftrightarrow \tau(v) > \tau(w)$ always holds.

The parameters we introduce below are *shape type*, *inter-vertex gap* and *exact label match*.

4.1 Shape Type

This parameter determines domains and ranges of traces. In this paper, we determine five possible values for this parameter, namely, `Forest`, `Tree`, `Agreement`, `Path` and `Separable`.

Forest: This value specifies that $\mathrm{Dom}(\tau)$ and $\mathrm{Ran}(\tau)$ can be arbitrary subsets of trees X and Y, and

τ does not require anything more than that τ is a homomorphism of posets with respect to the ancestor-descendent order. This value applies to the Taï edit distance.

Tree: This value specifies that $\mathrm{Dom}(\tau)$ and $\mathrm{Ran}(\tau)$ have the maximum vertices with respect to the ancestor-descendent relation, and τ does not require anything more than that τ is a homomorphism of posets with respect to the ancestor-descendent order.

Agreement: This value specifies that $\mathrm{Dom}(\tau)$ and $\mathrm{Ran}(\tau)$ are closed under the NCA operation, and τ is a homomorphism of algebraic structures with respect to the NCA operator. This value applies to the degree-two edit distance.

Path: This value specifies that $\mathrm{Dom}(\tau)$ and $\mathrm{Ran}(\tau)$ are totally ordered sets with respect to the ancestor-descendent relation, and τ is a homomorphism of posets.

Separable: Definition 2 defines this value. $\mathrm{Dom}(\tau)$ and $\mathrm{Ran}(\tau)$ can be arbitrary subsets of trees X and Y, and τ is separable. This value applies to the constrained edit distance.

4.2 Inter-vertex Gap

The parse-tree kernel (Collins and Duffy, 2001) counts the number of so-called *co-rooted subtrees* shared between two trees. The basic idea of the kernel is that, the more co-rooted subtrees the trees share, the more similar are the trees. What we should note here is that a co-rooted subtree does not allow gaps between their vertices: If two vertices are in the relation of parent and child in a co-rooted subtree, they are also a parent and a child in the original tree.

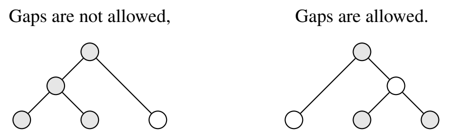


Figure 3: Inter-vertex gaps: vertices in gray determines a subtree.

By contrast, the distances that we saw in Section 1 all allow gaps. Hence, the second parameter *inter-vertex gap* determines whether $\mathrm{Dom}(\tau)$ and $\mathrm{Ran}(\tau)$ allow gaps between their adjacent vertices.

4.3 Exact Label Match

In (Shin, 2015), a method to convert edit distance problems into pattern extraction problems is shown. In particular, the author of the paper has derived *Mostly Adjusted Agreement Sub-Tree* (*MAAST*) problem from the degree-two distance, which relaxes the constraint of exact match of labels of the well-known MAST problem (Kao et al., 2007).

First, we briefly review MAST problem. To make the explanation simple, we take two rooted trees X_1 and X_2 and consider *agreement subtrees* between them. In Fig. 4, Y is an agreement subtree with embeddings $\varepsilon_1 : Y \to X_1$ and $\varepsilon_2 : Y \to X_2$. The embeddings are required to preserve the relation of ancestors and descendants, the NCA relation and vertex labels. The MAST problem is a problem to find the largest agreement subtree in size. In other words, the objective function of optimization is the size $|Y|$.

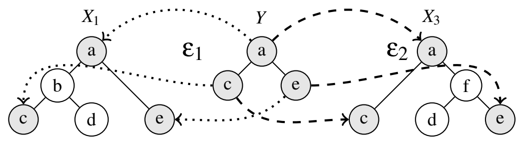


Figure 4: An agreement subtree and the MAST problem.

On the other hand, Fig. 5 depicts a trace τ of the edit path of Fig. 2. Actually, $\varepsilon_2 \circ \varepsilon_1^{-1}$ is comparable with τ, and the only difference is that τ does not necessarily preserve labels of vertices. In fact, in Fig. 5, τ maps the vertex labeled "e" of X_1 to the vertex labeled "g" of X_2.

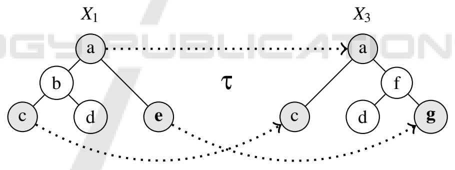


Figure 5: A trace of the degree-two distance.

In (Shin, 2015), a non-negative penalty function p is introduced, and the MAAST problem is defined as a problem to maximize the objective function of the form of $|\mathrm{Dom}(\tau)| - p(\tau)$. $p(\tau) = 0$, iff τ preserves vertex labels.

The author has also proven that the τ that maximizes this objective function also yields the degree-two distance.

The significance of (Shin, 2015) consists in defining a new type of pattern extraction problems relaxing the constraint of the exact label match and having shown the equivalence between solving the MAAST problem and computing the degree-two distance.

Reversely, this inspires us to introduce a new class of edit distances by requiring exact label match for traces. Thus, the last parameter that we introduce determines whether or not exact label match is required for traces.

Table 1: Possible combinations of parameters. In the SHAPE column: F = Forest; T = Tree; S = Separable; A = Agreement; P = Path; In the GAP and MATCH columns: T = True; F = False.

SHAPE	GAP	MATCH	DESCRIPTION
F	T	F	Taï (Taï, 1979)
F	T	T	
F	F	F	
F	F	T	
T	T	F	Identical to Taï distance.
T	T	T	
T	F	F	Identical to A-F-F.
T	F	T	Identical to A-F-T.
S	T	F	Constrained (Zhang, 1995)
S	T	T	
S	F	F	
S	F	T	
A	T	F	Degree-two (Zhang et al., 1996)
A	T	T	
A	F	F	Identical to T-F-F.
A	F	T	Identical to T-F-T.
P	T	F	
P	T	T	
P	F	F	
P	F	T	

4.4 Combinations of Parameters

Table 1 shows the possible combinations of parameter values. For convenience of expression, we represent each combination by the three capitals of the parameter values selected. For example, F-F-T represents the combination of SHAPE_TYPE = Forest, INTER_VERTEX_GAP = False and EXACT_LABEL_MATCH = True.

Three of the distances in Table 1 are known in the literature: F-T-F represents the Taï distance (Taï, 1979); S-T-F represents the constrained distance (Zhang, 1995); A-T-F represents the degree-two distance (Zhang et al., 1996). The remainder are novel edit distances first introduced in this paper.

Also, some of them are identical to each other. To be precise, since trees that do not allow inter-vertex gaps are always agreement trees, T-F-F and T-F-T are identical to A-F-F and A-F-F, respectively.

5 A COMPREHENSIVE COMPARISON OF THE MAPPING DISTANCE MEASURES

5.1 Rooted Ordered Trees

To compute mapping distances efficiently, we further assume that trees are *rooted ordered trees*.

When an total order is given to the children of every parent vertex of a tree, the tree is called an *rooted ordered tree*. The order is called a *sibling order*. The sibling order can be easily extended to a left-right order so that, given two vertices in a rooted ordered tree, they are either in the ancestor-descendant relation or the left-right relation (Fig. 6).

When considering mapping distances between rooted ordered trees, partial one-to=one mappings (traces) that we consider must preserve not only the ancestor-descendant order but also the left-right order: x_1 is located left to x_2 in $\mathrm{Dom}(\tau) \subseteq X$, iff $\tau(x_1)$ is located left to $\tau(x_2)$ in Y.

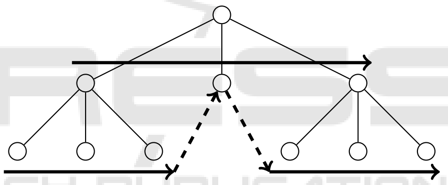


Figure 6: A rooted ordered tree: A sibling order (solid arrows) and an extended left-right order (dashed arrows).

When trees are not ordered, in other words, when they are rooted but *unordered trees*, it is known that computing their edit distances is not necessarily tractable (Yamamoto et al., 2014).

On the other hand, when we assume that trees are ordered, for all of the edit distances listed in Table 1, there are efficient algorithms to compute them.

In the literature, the problem of computing Taï edit distances has been known to have heavy computational complexity, and much effort has been made to improve efficiency. Zhang and Shasha (Zhang and Shasha, 1989) proposed an algorithm of $O(|X||Y|\min\{w(X),h(X)\}\min\{w(Y),h(Y)\})$-time, where $|X|$, $w(X)$ and $h(X)$ denote the number of vertices, the width (the number of leaves) and the height (the length of the longest path from the root to a leaf) of X. Klein (Klein, 1998) improved the efficiency to $O(|X|^2|Y|\log|Y|)$-time by taking advantage of *decomposition strategies* (Dulucq and Touzet, 2003). Demaine et al. (Demaine et al., 2006) further optimized this technique and presented an algorithm of $O(|X|^3)$-time. When we only look at the asymptotic evaluations, Demaine's algorithm looks the fastest, but it easily lapses into the worst case. Therefore, the algorithm of Zhang and Shasha in fact outperforms Demaine's algorithm in many practical cases. In this regard, *RTED*, an algorithm that Pawlik and Augsten (Pawlik and Augsten, 2011) have developed, not only has the same asymptotic complexity as Demaine's algorithm but also almost always outperforms the competitors in practice.

For the constrained distance (Zhang, 1995) and the degree-two distance (Zhang et al., 1996), efficient algorithms to compute them in $O(|X||Y|)$-time are presented in their original papers.

5.2 Algorithms

Fig. 7 to 11 give algorithms to compute the edit distances listed in Table 1 except for those already known.

The function $c(x,y)$ for trees x and y is defined as follows:

$$c(x,y) = \begin{cases} 0, & \text{if } \ell(\mathrm{rt}(x)) = \ell(\mathrm{rt}(y)); \\ 1, & \text{if } \ell(\mathrm{rt}(x)) \neq \ell(\mathrm{rt}(y)) \\ & \quad \text{and } \texttt{ELM = False}; \\ \infty, & \text{if } \ell(\mathrm{rt}(x)) \neq \ell(\mathrm{rt}(y)) \\ & \quad \text{and } \texttt{ELM = True}. \end{cases}$$

$\ell(\mathrm{rt}(x))$ denotes the label of the root of x and `ELM` stands for `EXACT_LABEL_MATCH`.

In the diagrams of the figures, for a tree, the method `.children` takes the children of the root of the tree and return as an array of trees. The order in the array is identical to the sibling order.

The algorithm is expressed as pseudo-codes using an imaginary programming language similar to SCALA (https://scala-lang.org). For example, for an array of trees the method `.head` returns the first tree of the array, while the method `.tail` returns the new array of trees after eliminating the first tree. Also, the operator ++ indicates a simple concatenation of arrays. The function `ff*` computes edit distances of the types of `F-F-F` and `F-F-T`. The difference between them as algorithms is only the value of $c(x,y)$ used when the labels $\ell(\mathrm{rt}(x))$ and $\ell(\mathrm{rt}(y))$ are different.

The asymptotic estimations of the time complexity of these algorithms are $O(|X|^2|Y|^2)$ for `ff*`, `tt*` and `tf*` and $O(|X||Y|)$ for the others. These complexities might be improved taking advantages of the method used in (Pawlik and Augsten, 2011) and (Kimura and Kashima, 2012). In (Kimura and Kashima, 2012), a linear-time algorithm to compute subpath kernels is presented. The algorithm leverages a list of all the suffixes ordered in the lexicographical order: A suffix

```
ff*(x: Array[Tree], y: Array[Tree]): Int = {
 if(x.isEmpty) return y.size
 if(y.isEmpty) return x.size
 t = x.head; u = y.head
 v0 = c(t, u) + sub(t.children, u.children)
  + ff*(x.tail, y.tail)
 v1 = ff*(t.children ++ x.tail, y) + 1
 v2 = ff*(x, u.children ++ y.tail) + 1
 return min(v0, v1, v2)
}
sub(x: Array[Tree], y: Array[Tree]): Int = {
 if(x.isEmpty) return y.size
 if(y.isEmpty) return x.size
 t = x.head; u = y.head
 v0 = c(t, u) + sub(t.children, u.children)
  + ff*(x.tail, y.tail)
 v1 = e(x.tail, y) + t.size
 v2 = e(x, y.tail) + u.size
 return min(v0, v1, v2)
}
```

Figure 7: Algorithms for `F-F-F` and `F-F-T`.

```
tt*(x: Tree, y: Tree) => Int = {
  v0 = c(x, y) + tt*(x.children, y.children)
  v1 = x.children.map(t => sub(t, y) + x.size - t.size)
  v2 = y.children.map(t => sub(x, t) + y.size - t.size)
  v3 = x.size + y.size
  return min(v0, min(v1), min(v2), v3)
}
sub(x: Array[Tree], y: Array[Tree]): Int = {
  if(x.isEmpty) return y.size
  if(y.isEmpty) return x.size
  t = x.head; u = y.head
  v0 = c(t, u) + sub(t.children, u.children)
    + sub(x.tail, y.tail)
  v1 = sub(t.children ++ x.tail, y) + 1
  v2 = sub(x, u.children ++ y.tail) + 1
  return min(v0, v1, v2).min
}
```

Figure 8: Algorithms for `T-T-F` and `T-T-T`.

```
tf*(x: Tree, y: Tree) => Int = {
 v0 = c(x, y) + sub (x.children, y.children)
 v1 = x.children.map(t => tf*(t, y) + x.size - t.size)
  ++ Array(x.size + y.size)
 v2 = y.children.map(t => tf*(x, t) + y.size - t.size)
  ++ Array(x.size + y.size)
 return min(v0, min(v1), min(v2))
}
sub(x: Array[Tree], y: Array[Tree]): Int = {
 if(x.isEmpty) return y.size
 if(y.isEmpty) return x.size
 t = x.head; u = y.head
 v0 = c(t, u) + sub(t.children, u.children)
  + sub(x.tail, y.tail)
 v1 = d(x.tail, y) + t.size
 v2 = d(x, y.tail) + u.size
 return min(v0, v1, v2)
}
```

Figure 9: Algorithms for `T-F-F` and `T-F-T`.

```
pt*(x: Tree, y: Tree) => Int = {
 v0 = c(x, y) + x.size + y.size - 2 +
  (Array(0) +: x.children.flatMap(t =>
   y.children.map(u => pt*(t, u) - t.size - u.size)))
 v1 = x.children.map(t => pttf(t, y) + x.size - t.size)
  ++ Array(x.size + y.size)
 v2 = y.children.map(t => pttf(x, t) + y.size - t.size)
  ++ Array(x.size + y.size)
 return min(min(v0), min(v1), min(v2))
}
```

Figure 10: Algorithms for `P-T-F` and `P-T-T`.

```
pf*: (x: Tree, y: Tree): Int = {
 v0 = sub(x, y)
 v1 = x.children.map(t => pf*(t, y) + x.size - t.size)
 v2 = y.children.map(t => pf*(x, t) + y.size - t.size)
 v3 = x.size + y.size
return min(v0, min(v1), min(v2), v3)
}
sub(x: Tree, y: Tree): Int = {
 return c(x, y) + x.size + y.size - 2 +
  min((Array(0) ++ x.children.flatMap(t =>
   y.children.map(u => sub(t, u) - t.size - u.size))))
```

Figure 11: Algorithms for `P-F-F` and `P-F-T`.

is a string of labels of a contiguous path from a vertex to the root of the tree.

5.3 Comparison Results

In the following, we see the results of experiments using six datasets. We ran five-fold cross validation with the *k*-NN algorithm changing *k* from 1 to 10, and then, measured accuracy scores ($\frac{\text{TP+TN}}{\text{TP+FP+FN+TN}}$). The edit distance measures whose `SHAPE_TYPE` parameter is `PATH` did not show good results for all the datasets tested, we exclude them from the explanation.

5.3.1 Colon-Cancer Dataset

The COLON-CANCER dataset was retrieved from the KEGG/GLYCAN database (Hashimoto et al., 2006), and specifies 134 glycan trees annotated relating to the disease of colon cancer. As Fig. 12 (a) shows, although the `T-T-T`, `A-T-T`, `A-T-F` (degree-two) and `S-T-F` (constrained) distances show the highest accuracy, the novel two outperform the known two on average across all *k*.

5.3.2 Cystic-Fibrosis Dataset

This dataset was also retrieved from the KEGG/GLYCAN database. It contains 160 glycan trees annotated relating to the disease of cystic-fibrosis. As Fig. 12 (b) shows, the `T-F-T` distance shows the highest accuracy, which is novel introduced in this paper.

5.3.3 Leukemia Dataset

This dataset was also retrieved from the KEGG/GLYCAN database. It contains 422 trees annotated relating to the disease of leukemia. As Fig. 12 (c) shows, the `A-T-T`, `T-T-T` and `L-T-T` distances show the highest accuracy. All of them require exact label match, and therefore, are novel.

5.3.4 Syntactic Dataset

This dataset is the dataset PropBank provided in (Moschitti,). It contains 225 parse trees labeled with two syntactic role classes for modeling the syntactic/semantic relation between a predicate and the semantic roles of its arguments in a sentence. As Fig. 12 (d) shows, the `F-T-F` (Taï) distance shows the highest accuracy, and the `S-T-F` (constrained) and `A-T-F` (degree-two) distances follow. All of them are known in the literature.

5.3.5 Web Access Dataset

This dataset was the one used in (Zaki and Aggarwal, 2006), and consists of 810 trees representing webpage accesses by users, and the annotation is based on whether the user is from a .edu site or not. As Fig. 12 (e) shows, the `A-T-T` distance outperforms the others in terms of both the highest accuracy and the average. The `A-T-T` distance has been introduced in this paper.

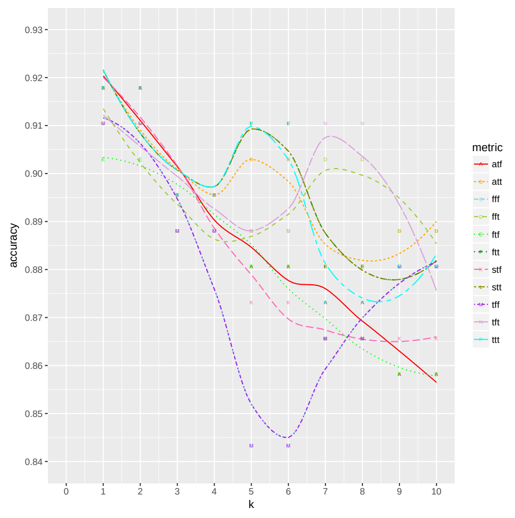
5.3.6 Phishing Dataset

We generated this dataset for this experiment. We collected 73 URL of phishing sites from PhishTank, (https://www.phishtank.com/), and 65 URL of authentic sites independently. From the collected URL, we generated DOM trees to form this dataset. As Fig. 12 (f) shows, the `F-T-F` (Taï) distance shows the highest accuracy, and the `F-F-F` and `T-T-T` distances follow.

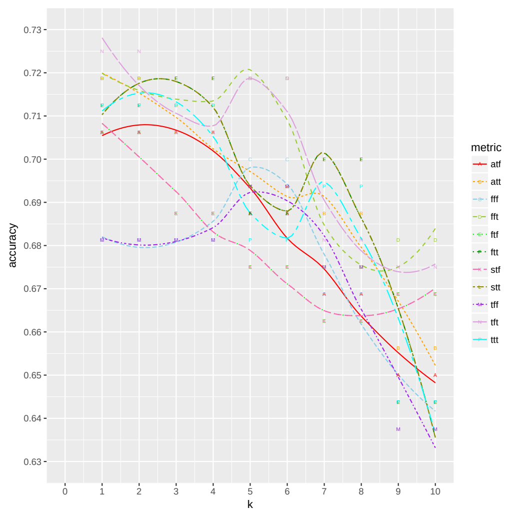
5.4 Summary

The table below shows the averaged ranks with respect to the highest accuracy scores across the six datasets.

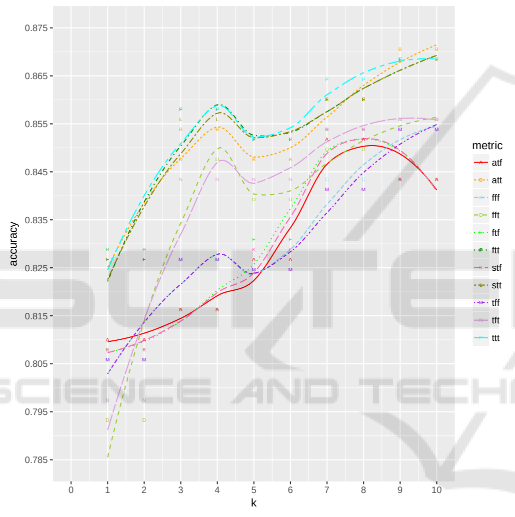
We should remark that the distances of the `*-T-T` type monopolize the top four. Hence, distances with traces that allow gaps between vertices and require exact match between labels can be more accurate. Of



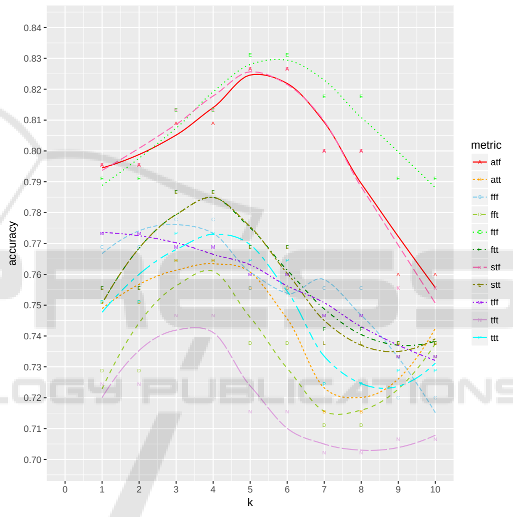
(a) COLON-CANCER



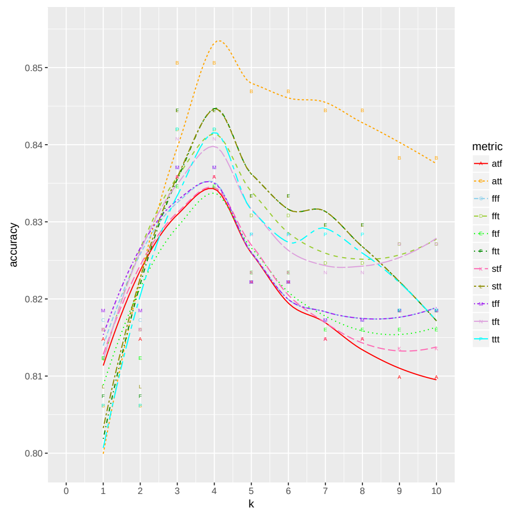
(b) CYSTIC-FIBROSIS



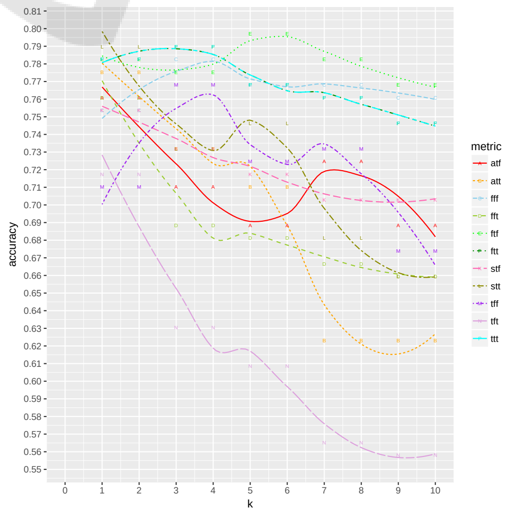
(c) Leukemia



(d) Syntactic



(e) Web-Access



(f) Phishing

Figure 12: Comparison in accuracy.

FTT	STT	ATT	TTT	TFT	ATF
3.2	3.2	3.6	4.6	6.9	6.9
FFT	STF	FTF	FFF	TFF	
6.9	7.2	7.4	7.7	8.4	

course, all of them are novel distance measures introduced in this paper. Furthermore, the following shows the *p*-values when we perform the Hommel test letting `F-T-T` be the control.

FTT	STT	ATT	TTT	TFT	ATF
–	1.00	0.81	0.84	0.16	0.16
	FFT	STF	FTF	FFF	TFF
	0.14	0.10	0.10	0.07	0.04

We see that there is a clear line between the `*-T-T` type and the others: with the significance level of 10%, the superiority of the `F-T-T` (and `S-T-T`) distance to the `S-T-F` (constrained), `F-T-F` (Taï), `F-F-F` and `T-F-F` distances is proven statistically significant; For the `A-T-F` (degree-two) and `T-F-T` distances, although we cannot reject the null hypothesis, the *p*-values are as small as 16%, much smaller than 84% for the `T-T-T` distance.

6 CONCLUSION

We have shown that viewing edit distance measures from a view point of properties of their associated traces is useful. In particular, by using particular properties of traces as parameters to describe edit distance measures, we not only can deal with edit distances measures consistently but also can engineer new measures systematically. In fact, taking rooted trees as an example, we have introduced three independent parameters, and have shown that the parameters determine 16 edit distance measures. Surprisingly, only three among them had been known in the literature, and all the remainder were novel. Furthermore, through experiments to measure predictive accuracy of each combination of one of the 16 measures and the *k*-NN classifier, we have discovered that a certain novel class of edit distance measures can perform the best. The measures belonging to the class are significantly different from the edit distance measures known in the literature, since the cost to replace a label with a different label is set as infinity. This mandates the associated traces to preserve labels of vertices.

7 ACKNOWLEDGMENTS

This work was partially supported by the Grant-in-Aid for Scientific Research (JSPS KAKENHI Grant Number 16K12491 and 17H00762) from the Japan Society for the Promotion of Science.

REFERENCES

Collins, M. and Duffy, N. (2001). Convolution kernels for natural language. In *Advances in Neural Information Processing Systems 14 [Neural Information Processing Systems: Natural and Synthetic, NIPS 2001]*, pages 625–632. MIT Press.

Demaine, E. D., Mozes, S., Rossman, B., and Weimann, O. (2006). An optimal decomposition algorithm for tree edit distance. *ACM Trans. Algo.*, 6.

Dulucq, S. and Touzet, H. (2003). Analysis of tree edit distance algorithms. In *the 14th annual symposium on Combinatorial Pattern Matching (CPM)*, pages 83 – 95.

Hashimoto, K., Goto, S., Kawano, S., Aoki-Kinoshita, K. F., and Ueda, N. (2006). KEGG as a glycome informatics resource. *Glycobiology*, 16:63R – 70R.

Kao, M.-Y., Lam, T.-W., Sung, W.-K., and Ting, H.-F. (2007). An even faster and more unifying algorithm for comparing trees via unbalanced bipartite matchings.

Kimura, D. and Kashima, H. (2012). Fast computation of subpath kernel for trees. In *ICML*.

Klein, P. N. (1998). Computing the edit-distance between unrooted ordered trees. *LNCS*, 1461:91–102. ESA'98.

Kuboyama, T., Shin, K., Miyahara, T., and Yasuda, H. (2005). A theoretical analysis of alignment and edit problems for trees. In *Proc. of Theoretical Computer Science, The 9th Italian Conference*, Lecture Notes in Computer Science 3701, pages 323–337.

Levenshtein, V. I. (1966). Binary codes capable of correcting deletions, insertions, and reversals. *Soviet Physics Doklady*, 10(8):707 – 710.

Lu, C. L., Su, Z. Y., and Tang, G. Y. (2001). A New Measure of Edit Distance between Labeled Trees. In *LNCS*, volume 2108, pages pp. 338–348. Springer-Verlag Heidelberg.

Moschitti, A. Example data for TREE KERNELS IN SVM-LIGHT. http://disi.unitn.it/moschitti/Tree-Kernel.htm.

Neuhaus, M. and Bunke, H. (2007). *Bridging the gap between graph edit distance and kernel machines.* World Scientific.

Pawlik, M. and Augsten, N. (2011). Rted: A robust algorithm for the tree edit distance. In *Proceedings of the VLDB Endowment*, volume 5, pages 334–345.

Shin, K. (2015). Tree edit distance and maximum agreement subtree. *Inf. Process. Lett.*, 115(1):69–73.

Taï, K. C. (1979). The tree-to-tree correction problem. *journal of the ACM*, 26(3):422–433.

Wang, J. T. L. and Zhang, K. (2001). Finding similar consensus between trees: an algorithm and a distance hierarchy. *Pattern Recognition*, 34:127–137.

Yamamoto, Y., Hirata, K., and Kuboyama, T. (2014). Tractable and intractable variations of unordered tree edit distance. *Int. J. Found. Comput. Sci*, 25(3):307–330.

Zaki, M. J. and Aggarwal, C. C. (2006). XRules: An effective algorithm for structural classification of XML data. *Machine Learning*, 62:137–170.

Zhang, K. (1995). Algorithms for the constrained editing distance between ordered labeled trees and related problems. *Pattern Recognition*, 28(3):463–474.

Zhang, K. and Shasha, D. (1989). Simple fast algorithms for the editing distance between trees and related problems. *SIAM journal of Computing*, 18(6):1245 – 1262.

Zhang, K., Wang, J. T. L., and Shasha, D. (1996). On the editing distance between undirected acyclic graphs. *International Journal of Foundations of Computer Science*, 7(1):43–58.