

# Optimal Decomposition Strategy For Tree Edit Distance

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# Ordered Labelled Tree

An ordered labelled tree is a tree in which the nodes are labeled and the left-to-right order among siblings is significant.

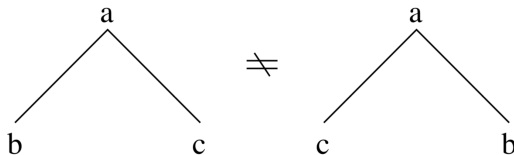


Figure: Ordered Labelled Tree

The ordered labelled tree can represent:

- an XML document
- a natural language parse
- RNA secondary structure
- and so on...

# Tree Edit Distance

- The string edit distance is the minimum cost to transform one string to another.

- Align two sequences of nucleotides

```
AGGCTATCACCTGACCTCCAGGCCGATGCCC
TAGCTATCACGACCGCGGTTCGATTGCCCCGAC
```

- Resulting alignment

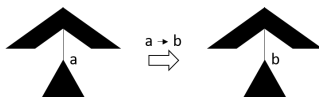
```
-AGGCTATCACCTGACCTCCAGGCCGA--TGCCC---
TAG-CTATCAC--GACCGC--GGTCGATTGCCCCGAC
```

- The tree edit distance is introduced by Tai as a generalization of the string edit distance.
- The edit distance between two trees  $P$  and  $D$  is the minimum cost to change  $P$  to  $D$  via a sequence of basic edit operations.

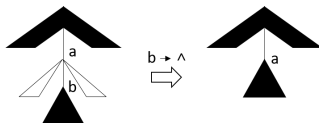
# Edit Operations

- Three valid edit operations supported:

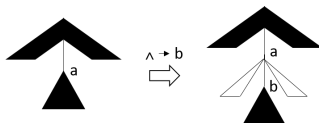
- Substitution.** replace a label of a node by another label.



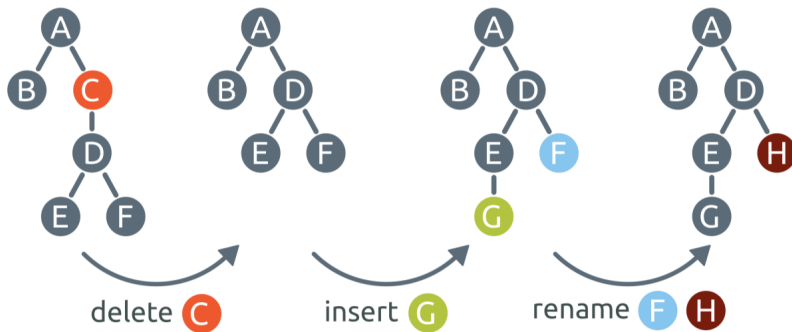
- Deletion.** deletion of a node



- Insertion.** insertion of a node.



# Edit Operations



# Cost of Edit Operations

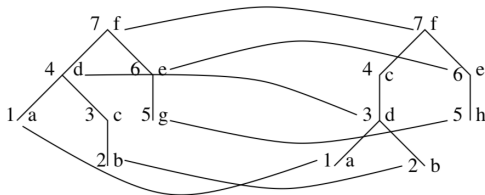
- Each edit operations has a cost.
- Let  $\gamma$  be a cost function of each operations. The cost function  $\gamma$  is a distance metric.
  - $\gamma(a \rightarrow b)$  can be 1 or other user defined value.

-	A	G	C	U	AA	AG	AC	AU	GA	GG	GC	GU	CA	CG	CC	CU	UA	UG	UC	UU
A	1	0																		
G	1	1	0																	
C	1	1	1	0																
U	1	1	1	1	0															
AA	1	1	1	1	1	0														
AG	1	1	1	1	1	1	0													
AC	1	1	1	1	1	1	1	0												
AU	1	1	1	1	1	1	1	1	0											
GA	1	1	1	1	1	1	1	1	1	0										
GG	1	1	1	1	1	1	1	1	1	1	0									
GC	1	1	1	1	1	1	1	1	1	1	1	0								
GU	1	1	1	1	1	1	1	1	1	1	1	1	0							
CA	1	1	1	1	1	1	1	1	1	1	1	1	1	0						
CG	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0					
CC	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0				
CU	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0			
UA	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0		
UG	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	
UC	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0
UU	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

- The edit distance is the sum of the cost of the minimum cost sequence.

# Mapping in Trees

- Mapping between trees.
- The cost of a mapping is the sum of its insertion, deletion and substitutions.



Edit sequence:  $(c \rightarrow \lambda), (g \rightarrow h), (\lambda \rightarrow c)$

Figure: The Edit Sequence and its Cost

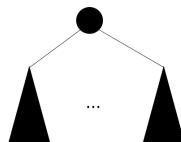


- **Tree**

- $l(f)$



- $l(A_1 \circ A_2 \circ \dots \circ A_n)$



Let  $T$  be a tree,

- $r(T)$

the root of  $T$

- $T^\circ$

$$T - r(T)$$

- $lr(T)$

the root of the leftmost tree in the forest  $T^\circ$

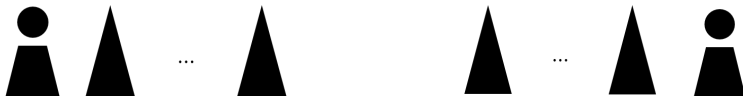
- $rr(T)$

the root of the rightmost tree in the forest  $T^\circ$

- **Forest**

- $l(f) \circ t$

- $t \circ l(f)$



Let  $F$  be a forest,

- $|F|$  the number of nodes in the forest  $F$
- $\#leaves(F)$  the number of leaves in the forest  $F$
- $F(i)$  the sub-tree of  $F$  rooted at node  $i$
- $F - i$  the forest after deleting node  $i$
- $lr(F)$  the root of the leftmost tree in the forest  $F$
- $rr(F)$  the root of the rightmost tree in the forest  $F$

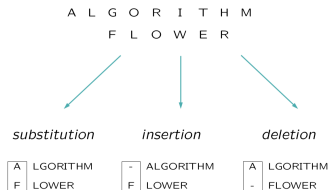
# String Edit Distance and its Recursive Solution

- String edit distance is the minimum cost to change one string to another via a sequence of basic edit operations.
- The recursive solution of the string edit problem  $d(S_1, S_2)$  is

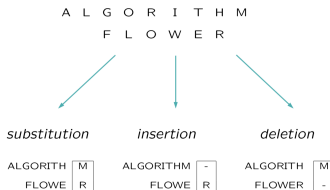
$$d(S_1, S_2) = \min \begin{cases} d(S_1 - u, S_2) + \delta(u, \emptyset) \\ d(S_1, S_2 - v) + \delta(\emptyset, v) \\ d(S_1 - u, S_2 - v) + \delta(u, v) \end{cases}$$

# String Edit Distance and its Recursive Solution

- If  $u$  and  $v$  is both the first element of string  $S_1$  and  $S_2$ , then it is a leftmost decomposition.



- If  $u$  and  $v$  is both the last element of string  $S_1$  and  $S_2$ , then it is a rightmost decomposition.



# Tree Edit Distance and its Recursive Solution

For tree-to-tree distance, Let  $T_1$  and  $T_2$  are both trees of the form  $l(f)$  and  $l'(f')$ ,

$$d(l(f), l'(f')) = \min \begin{cases} d(f, l'(f')) + \delta(l, \emptyset) \\ d(l(f), l'(f')) + \delta(\emptyset, l') \\ d(f, f') + \delta(l, l') \end{cases}$$

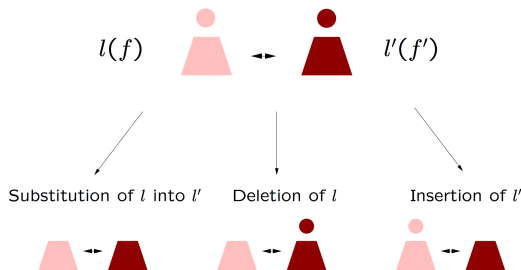


Figure: Tree-to-Tree Edit Distance

# Tree Edit Distance and its Recursive Solution

For forest-to-forest distance, Let  $F_1$  and  $F_2$  are both trees of the form  $l(f) \circ t$  and  $l'(f') \circ t'$ ,

$$d(l(f) \circ t, l'(f') \circ t') = \min \begin{cases} d(f \circ t, l'(f') \circ t') + \delta(l, \emptyset) \\ d(l(f) \circ t, f' \circ t') + \delta(\emptyset, l') \\ d(t, t') + d(l(f), l'(f')) \end{cases}$$



Leftmost decomposition

Substitution of  $l$  into  $l'$

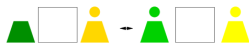


$\text{Distance}(l(f), l'(f'))$

+

$\text{Distance}(t, t')$

Deletion of  $l$



$\text{Distance}(f \circ t, l'(f') \circ t') + \text{del}(l)$

Insertion of  $l'$



$\text{Distance}(l(f) \circ t, f' \circ t') + \text{ins}(l')$

# Tree Edit Distance and its Recursive Solution

For forest-to-forest distance, Let  $F_1$  and  $F_2$  are both trees of the form  $l(f) \circ t$  and  $l'(f') \circ t'$ ,

$$d(t \circ l(f), t' \circ l'(f')) = \min \begin{cases} d(t \circ f, t' \circ l'(f')) + \delta(l, \emptyset) \\ d(t \circ l(f), t' \circ f') + \delta(\emptyset, l') \\ d(t, t') + d(l(f), l'(f')) \end{cases}$$



Rightmost decomposition

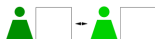
Substitution of  $l$  into  $l'$



$\text{Distance}(l(f), l'(f'))$

+

$\text{Distance}(t, t')$



Deletion of  $l$



$\text{Distance}(t \circ f, t' \circ l'(f')) + \text{del}(l)$

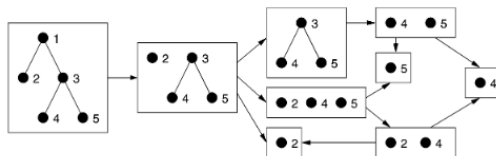
Insertion of  $l'$



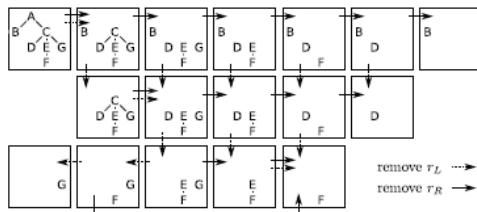
$\text{Distance}(t \circ l(f), t' \circ f') + \text{ins}(l')$

# Relevant Sub-forests and Full Decomposition

- Relevant sub-forests



- Full decomposition



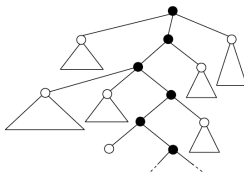


# Root-leaf Path and Relevant Sub-trees

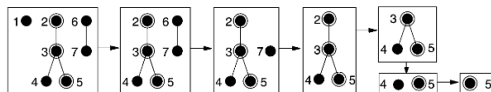
- Root-leaf path



- Relevant sub-trees



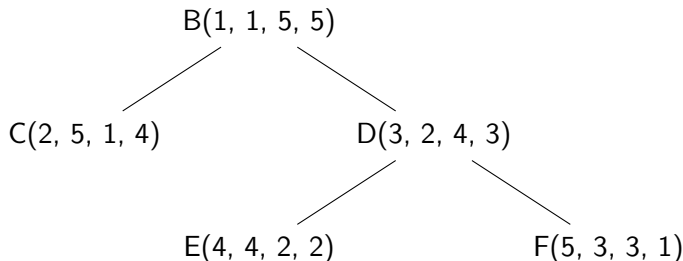
- Path decomposition



# Tree Indexing

- $preOrder\_left\_to\_right \rightarrow preL$
- $preOrder\_right\_to\_left \rightarrow preR$
- $postOrder\_left\_to\_right \rightarrow postL$
- $postOrder\_right\_to\_left \rightarrow postR$

Consider a tree  $T(preL, preR, postL, postR)$



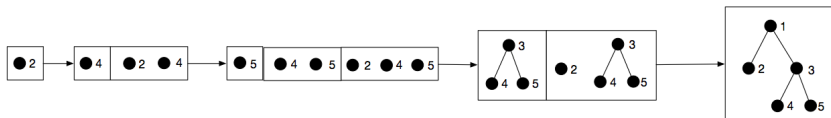
## Note:

- $preL + postR = treeSize + 1$
- $preR + postL = treeSize + 1$

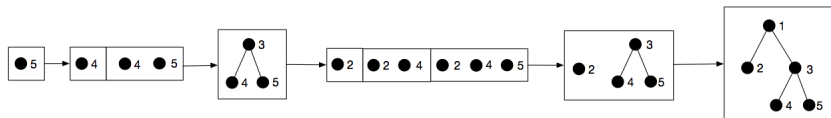
# Bottom-up Enumeration

Two orders of the enumeration of the full decomposition:

- Prefix-suffix order



- Suffix-prefix order



# A Simple Algorithm

## Main Idea:

Enumerate each pairs of sub-forests in tree A and B in prefix-suffix post order or suffix-prefix post order.

## Pseudocode:

---

**Algorithm 1:** Compute tree edit distance by enumerating all pairs in  $O(m^2n^2)$  time.

---

**inputs:**  $(T_1, T_2)$ , with  $|T_1| = m$  and  $|T_2| = n$

**output:**  $d(T_1[i], T_2[j])$  for  $1 \leq i \leq m$  and  $1 \leq j \leq n$

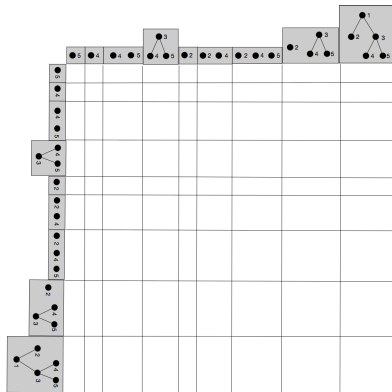
```
1  $L_1 \leftarrow \text{POSTORDER}(T_1);$ 
2  $L_2 \leftarrow \text{POSTORDER}(T_2);$ 
3 for  $i = 1$  to  $|L_1|$  do
4   for  $j = 1$  to  $|L_2|$  do
5      $\mid$  compute  $d(L_1[i], L_2[j])$  as in Equation 2.3
6   end
7 end
8  $d(T_1[i], T_2[j]) \leftarrow d(L_1[[i]], L_2[[j]]);$ 
9 return  $d(T_1[i], T_2[j]);$ 
```

---

# A Simple Algorithm

## Implementation:

- Implemented in dynamic programming.
- Runs in  $\mathcal{O}(m^2 n^2)$  time using  $\mathcal{O}(m^2 n^2)$  space.

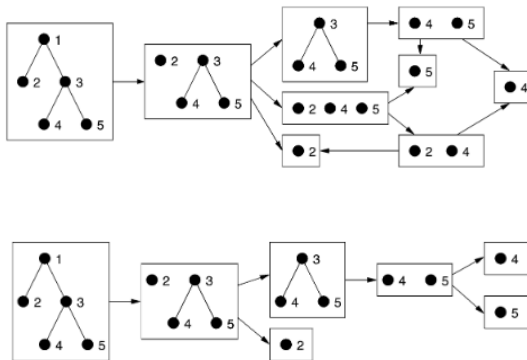


- The upper bound of the post-order enumeration method for the tree edit distance problem is  $\mathcal{O}(n^4)$

# Improved Algorithmic Path Strategies

## Key Ideas:

- Different path decomposition creates different number of relevant sub-forests.
- Take advantage of the overlap among sub-forests that are contained in the same sub-tree, and the overlap of sub-trees as well.



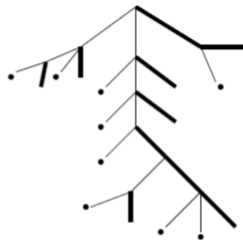
# Zhang and Shasha's Algorithm

## Key Ideas:

- Fixed direction in each recursive calls.
  - Recursive right decomposition - leftmost paths.
  - Recursive left decomposition - rightmost paths.



(a) leftmost paths



(b) rightmost paths

## Implementation:

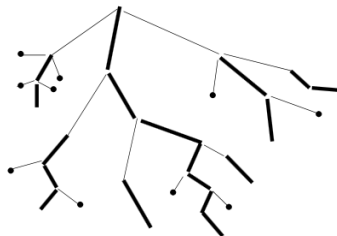
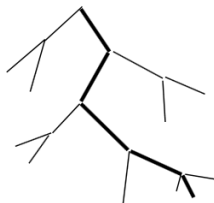
- Implemented via dynamic programming.
- Enumerates sub-trees pairs rooted at key roots.
  - Leftmost paths: either tree root or has a left sibling
  - Rightmost paths: either tree root or has a right sibling
- Uses two memorized tables to store intermediate results:
  - a temporary table to store forest-forest distance.
  - a permanent table to store tree-tree distance.
- Runs in  $\mathcal{O}(|A| * |B| * \min\{\text{depth}(A), \text{leaves}(A)\} * \min\{\text{depth}(B), \text{leaves}(B)\})$  time and  $\mathcal{O}(|A| * |B|)$  space.



# Klein's Algorithm

## Key Ideas:

- Zhang and Shasha's algorithm depends on shapes of trees.
- Heavy node.
- Heavy paths generate the least number of sub-forests on one tree.



## Implementation:

- Implemented via dynamic programming.
- applies heavy paths to the larger tree and fully decomposes the smaller tree.
- Uses temporary tables to store forest-forest distance and a permanent tables to store tree-tree distance.
- Runs in  $\mathcal{O}(|A| \log(|A|) * |B|^2)$  time using  $\mathcal{O}(|A| * |B|)$  space.

## Key Ideas:

- Klein's algorithm consider the shape of one tree with no consideration on the other tree.
- Heavy paths can be applied on both trees.
- Always applies heavy paths on the larger tree.

## Implementation:

- Implemented via dynamic programming.
- Runs in  $\mathcal{O}(|A| |B|^2 (1 + \log(\frac{|A|}{|B|})))$  time using  $\mathcal{O}(|A| * |B|)$  space.

# Conclusion

	Time	Space	Comments
Simple Algorithm	$\mathcal{O}(n^4)$	$\mathcal{O}(n^4)$	first algorithm
Zhang	$\mathcal{O}(n^2 \log^2(n))$	$\mathcal{O}(n^2)$	efficient for balanced trees
Klein	$\mathcal{O}(n^3 \log(n))$	$\mathcal{O}(n^2)$	no consider smaller trees
Demaine	$\mathcal{O}(n^3)$	$\mathcal{O}(n^2)$	worse case is frequent

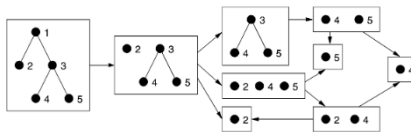
**Table:** State-of-the-Art Algorithms in the Tree Edit Distance Problem

## Key Idea:

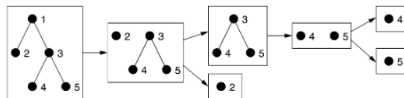
- heavy paths is a kind of greedy algorithm which usually lead to the local optimum rather than global optimum.
- quantifies each possible paths and selects the path with the least number of sub-problems is selected
- implemented via dynamic programming.
- Preprocessing time is bounded by  $\mathcal{O}(|A| |B|)$

# Relevant Leftmost/Rightmost/Special Sub-forests

- Path decomposition  $\rightarrow$  relevant sub-forests
- Recursive leftmost path decomposition  $\rightarrow$  relevant leftmost sub-forests



- Recursive rightmost path decomposition  $\rightarrow$  relevant rightmost sub-forests



- Full decomposition  $\rightarrow$  relevant special sub-forests

# Relevant Leftmost/Rightmost/Special Sub-forests

Let  $T$  be a tree of the form  $I(T_1 \circ \cdots \circ T_n)$  and the size of  $T$  is  $n$ ,

- The Number of Relevant Leftmost Sub-forests( $\#left(T)$ )

$$\#left(T) = |T| - |T_1| + \sum_{i=1}^n \#left(T_i)$$

- The Number of Relevant Rightmost Sub-forests( $\#right(T)$ )

$$\#right(T) = |T| - |T_n| + \sum_{i=1}^n \#right(T_i)$$

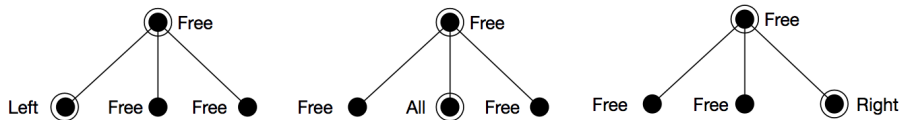
- Relevant Special Sub-forests( $\#special(T)$ )

$$\#spec(T) = \frac{n(n+3)}{2} - \sum_{i \in T} |T(i)|$$

# Status of a Node in a Tree

Let  $T$  be a tree with a root-leaf path,

- Free node: the node is the root of  $T$ , or is not on the root-leaf path.
- Left node: the node is on the root-leaf path and is the leftmost child of its parent.
- Right node: the node is on the root-leaf path and is the rightmost child of its parent.
- All node: the node is on the root-leaf path and is neither the leftmost child nor the rightmost child of its parent.



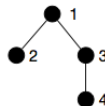


# Quantify the Number of Sub-Problem

- Seven memorized tables to store intermediate results.
  - Free
  - LeftA
  - RightA
  - AllA
  - LeftB
  - RightB
  - AllB
- Dynamic programming.

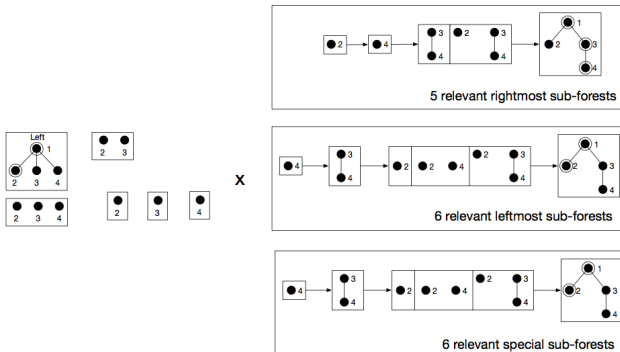
# Quantify the Number of Sub-Problem

Let  $A$  be a tree with a root-leaf path and  $B$  be another tree,



# Quantify the Number of Sub-Problem

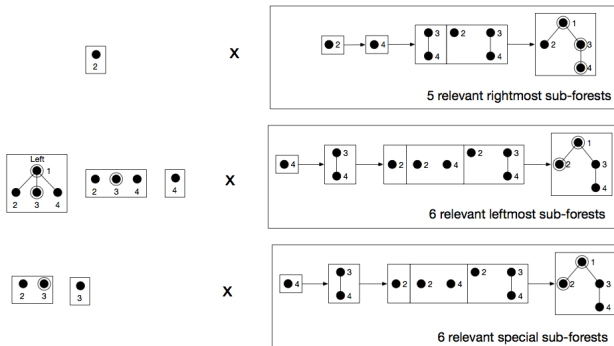
Let A be a tree with a root-leaf path and B be another tree.



$$\begin{aligned}
 \#leftA(1, 1) &= Free(3, 1) + Free(4, 1) + LeftA(2, 1) \\
 &+ |A - A(2)| * \#left(B) \\
 &= \#left(B) + \#left(B) + \#left(B) + 3 * \#left(B)
 \end{aligned}$$

# Quantify the Number of Sub-Problem

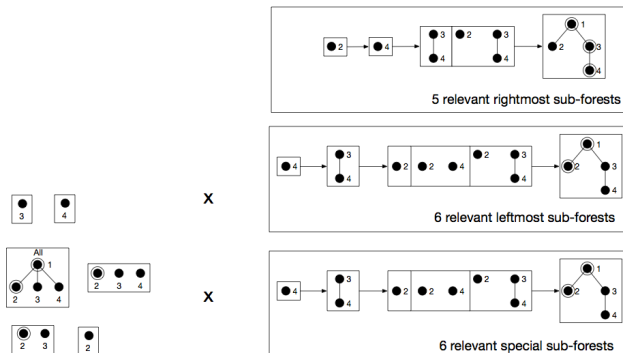
Let A be a tree with a root-leaf path and B be another tree.



$$\begin{aligned}
 \#leftA(1, 1) &= Free(2, 1) + Free(4, 1) + AllA(3, 1) \\
 &+ |1 + A(4)| * \#left(B) + |A(2)| * \#special(B) \\
 &= \#right(B) + \#left(B) + \#special(B) \\
 &+ \#special(B) + 2 * \#left(B)
 \end{aligned}$$

# Quantify the Number of Sub-Problem

Let  $A$  be a tree with a root-leaf path and  $B$  be another tree.



$$\begin{aligned}
 \#AllA(1, 1) &= Free(3, 1) + Free(4, 1) + AllA(2, 1) \\
 &+ |A - A(2)| * \#special(B) \\
 &= \#left(B) + \#left(B) + \#special(B) + 3 * \#special(B)
 \end{aligned}$$

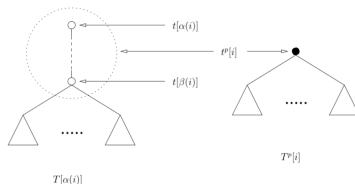
# Vertical Reduction on Trees

## Key Ideas:

- A large number of non-branching nodes can be compressed into one node.

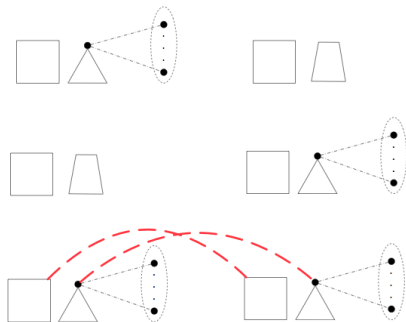
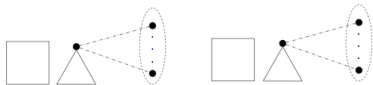


- The compact representation of the original tree can aid in improving the running time for computing the tree edit distance.



•  $T \rightarrow \tilde{T}$

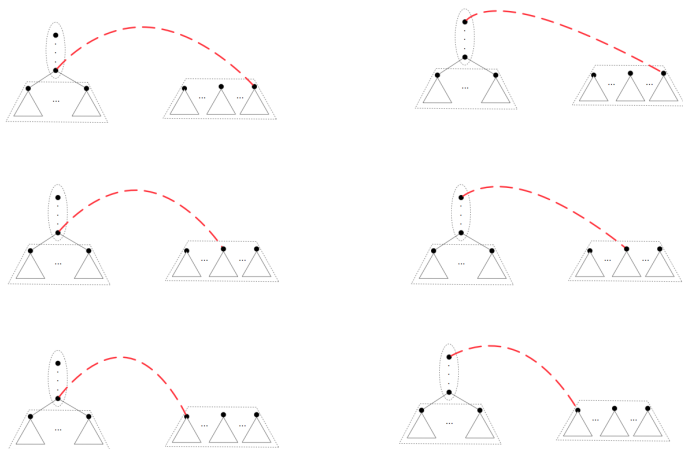
## Forest-to-Forest Distance:



# Algorithm

## Tree-to-Tree Distance:

- Compute  $d(\widetilde{T}_1, \widetilde{T}_2^\circ)$



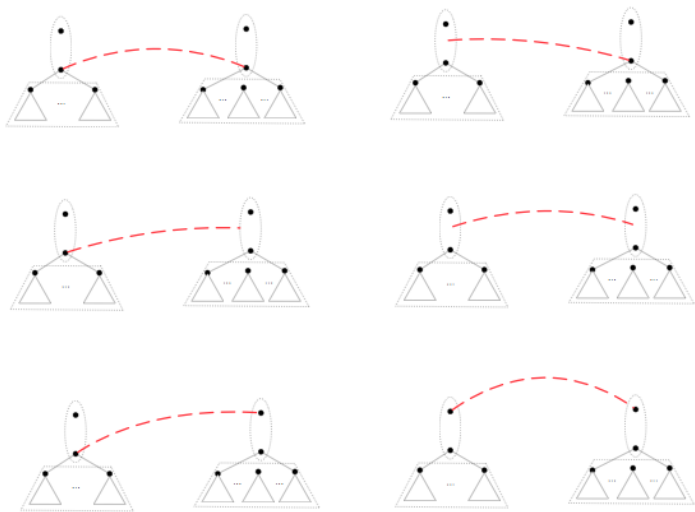
- The computation of  $d(\widetilde{T}_1, \widetilde{T}_2)$  is symmetric.



# Algorithm

## Tree-to-Tree Distance:

- Compute  $d(\widetilde{T}_1, \widetilde{T}_2)$



# Implementation

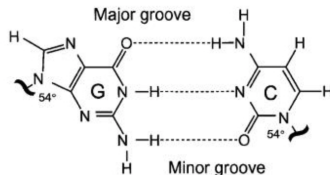
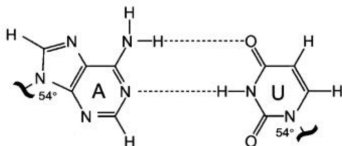
- three memorized tables to store intermediate results:
  - $D_t$ : a  $(|T_1| + 1) * (|T_2| + 1)$  two dimensional permanent array.
  - $\tilde{D}_t$ : a  $(|\tilde{T}_1| + 1) * (|\tilde{T}_2| + 1)$  two dimensional permanent array.
  - $\tilde{D}_f$ : a  $(|\tilde{T}_1| + 1) * (|\tilde{T}_2| + 1)$  two dimensional temporary array.
- Dynamic programming.

- RNA is an essential molecule in organisms.
  - Cellular organisms
  - Viruses
- RNA is assembled as a chain of nucleotides.

```

1  AAAGCAGGCC AGGCAACCGC UGCCUGCACC GCAAGGUGCA GGGGGAGGAA
51  AGUCCGGACU CCACAGGGCA GGGUGUUGGC UAACAGCCAU CCACGGCAAC
101 GUGCGGAAUA GGGCCACAGA GACGAGUCUU GCCGCCGGGU UGCCCCGGCG
151 GGAAGGGUGA AACGCGGUAA CCUCCACCUG GAGCAAUCCC AAAUAGGCAG
201 GCGAUGAAGC GGCCCGCUGA GUCUGCGGGU AGGGAGCUGG AGCCGGCUGG
251 UAACAGCCGG CCUAGAGGAA UGGUUGUCAC GCACCGUUUG CCGCAAGGCG
301 GGCGGGGCGC ACAGAAUCCG GCUUAUCGGC CUGCUUUGCU U
    
```

- RNA is unstable.



# RNA Secondary Structure

- a list of base pairs satisfies the following constraints:
  - A base cannot participate in more than one base pair,
  - No two base pairs cross.

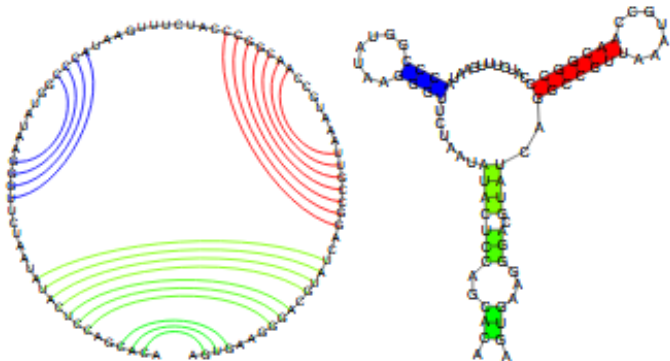
( 1)	1	337	10
( 2)	11	326	1
( 3)	12	278	7
( 4)	20	45	2
( 5)	23	42	8
( 6)	59	183	4
( 7)	71	179	5
( 8)	77	89	4
( 9)	91	105	1
( 10)	92	103	4
( 11)	106	174	2
( 12)	111	172	2
( 13)	127	156	4
( 14)	132	151	8
( 15)	187	235	4
( 16)	197	226	6
( 17)	206	220	5
( 18)	242	261	8
( 19)	281	308	2
( 20)	284	305	9

# RNA Secondary Structure Representation

- String representation

ACACGACCUCUAUAAUUCUUGGSAUAUUGGCCCAUAAGUUUCUACCCGGCAACCGUAAAUUGCCGGACUAUGCAGGGAAGUGA  
((

- Graph representation



# Tree Representation of the RNA Secondary Structure

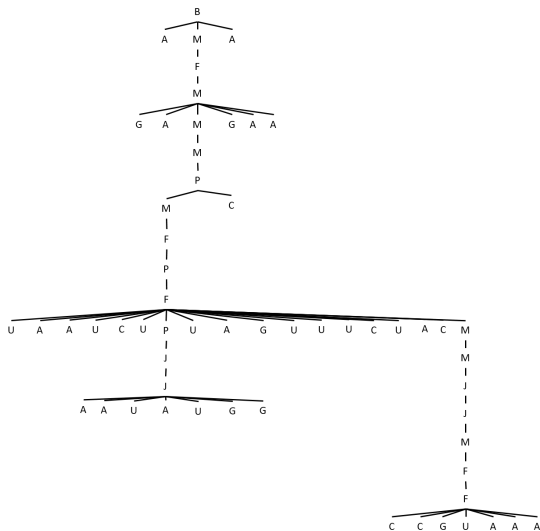
- Base pair labelling

Base Pairs	Label
$A = U$	F
$G \equiv C$	J
$U = A$	P
$C \equiv G$	M

Table: The Label of Base Pair

- Tree representation

# Tree Representation of the RNA Secondary Structure



## Experiment

RNAName: Alcaligenes-eutrophus-pb-b

RNASize: 343

[illegible]

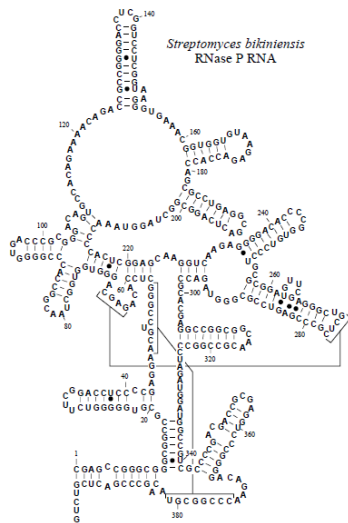
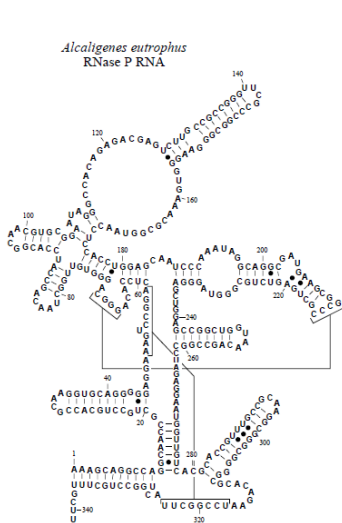
RNAName: Streptomyces-bikiniensis-gpb-h

RNASize: 400

[illegible]



# Experiment



## Experiment Result

Alcaligenes eutrophus ~ Streptomyces bikiniensis

```
deletion: 1 insertion: 1 substitution: 1 distance: 134
```

[illegible]

(-----)))))--)((---((-----(((((---((-----))--)))--))--)))--  
 GGCAACGUGCGGAUAGGGCCACAGAGA-CGAGUCUUGCCGCCG-GG--UUUC--CC-CGGC--GGGAAGG-GU-----G-AA-A-  
 GGUGACCCGCGGGACAGUGCCACAGAAAC-AG----ACCGCCGGGGACUCGGUCCUCGGUAAGGG----UGAAACGGUGUGUAAGAGACCACCAAG-

-----))))))--))))--(((-----(((((-----((-----))  
 ((((((-----))))))-----C-----(((((((-----))))))-----(((((-----((-----))  
 -----CG-----C-----GGUAAACCUCCAC-----CUGGAGCAAUCCCAA-----A-----UA-----G-----GCAGGCGAU-----GA-----AGCGGCCCGCU  
 GCCUGAGGCGACUCAGGCGGCUAGGUAACCCACUC-----GGAGCAAGGUAAGAGGGGACACCCCGUGUCCUUGCGCGGAUGUUCGAGGGCGUCUCGC

[illegible]

-----)))))--))-----  
 -----)))))--))-----  
 GCACAGAAUCCGGCUUUAUCGGCCUG-  
 --ACAGAACCCGGCGUACAGCCC-GACUCGUCUG

Tree size: 246 and 282

Algorithm	# <i>Rel.sub</i>	Time[sec]
<i>Zhang – L</i>	849282	0.08
<i>Zhang – R</i>	2039089	0.13
<i>Demaine</i>	7175224	0.65
<i>Our Algorithm(Before Compression)</i>	553526	0.04
<i>Zhang – L(Compressed)</i>	428766	0.05
<i>Zhang – R(Compressed)</i>	686562	0.05
<i>Our Algorithm(After Compression)</i>	291329	0.03

Tree size: 1041 and 1012

Algorithm	#Rel.sub	Time[sec]
<i>Zhang – L</i>	41889364	3.2
<i>Zhang – R</i>	42972591	3.3
<i>Demaine</i>	273276733	20.98
<i>Our Algorithm(Before Compression)</i>	32254346	2.3
<i>Zhang – L(Compressed)</i>	17769036	0.47
<i>Zhang – R(Compressed)</i>	18154025	0.51
<i>Our Algorithm(After Compression)</i>	13546825	0.34

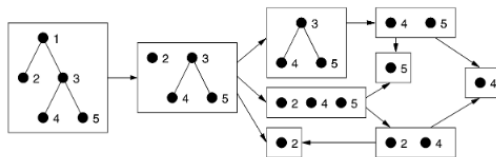
# Conclusion

- Tree edit distance quantifies the similarity between two ordered labelled trees.
- Three kinds of root-leaf path are introduced to take the advantages of the overlapping relevant sub-forests and sub-trees in different ways.
- The optimal root-leaf path can be found via dynamic programming and can be used for the tree edit distance problem.
- The vertical reduction on trees can significantly reduced the running time.
- The comparison between RNA secondary structures is an application of the tree edit distance.
- Our strategies on compressed trees are by far the best decomposition strategy, creating the least number of relevant sub-problems.

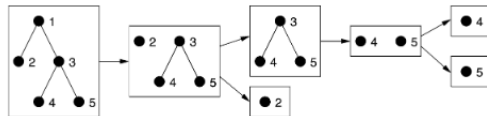
Thank you. Questions?

# Path Decomposition

- Leftmost path decomposition



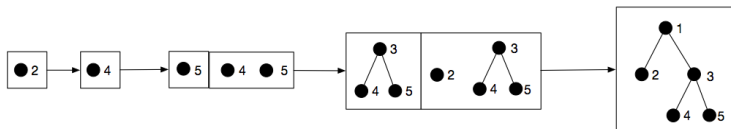
- Rightmost path decomposition



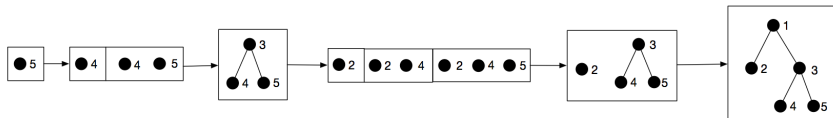
# Bottom-up Enumeration

Two orders of the enumeration of the path decomposition:

- LR-postorder enumeration



- RL-postorder enumeration



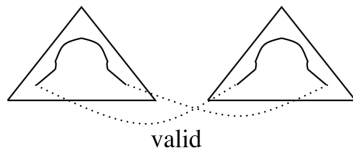
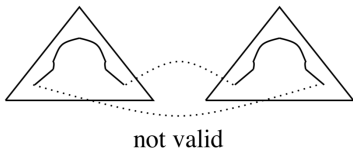


# Matching in Trees

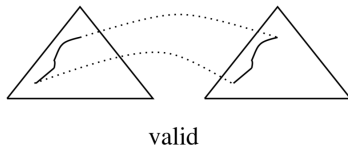
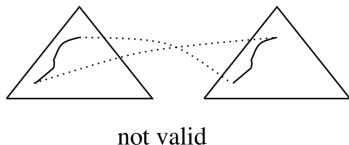
- **Input:** Two labelled ordered trees  $T$  and  $P$ .

- **Constraints:**

- One-to-one relationship
- Sibling order is preserved.



- Ancestor order is preserved.



- **Output:** Mapping between  $T$  and  $P$ .