### Algorithms for the Edit Distance Between Trees

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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.

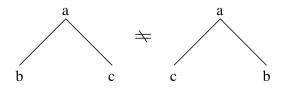


Figure: Ordered Labelled Tree

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
TAGCTATCACGACCGCGGTCGATTTGCCCGAC

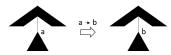
Resulting alignment

```
-AGGCTATCACCTGACCTCCAGGCCGA--TGCCC---
TAG-CTATCAC--GACCGC--GGTCGATTTGCCCGAC
```

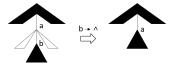
- The tree edit distance is introduced by Tai as a generalization of the string edit distance.
- The edit distance between two trees *P* and *D* is the minimum cost to change *P* to *D* via a sequence of basic edit operations.

# **Edit Operations**

- Three valid edit operations supported:
  - **Substitution.** replace a label of a node by another label.



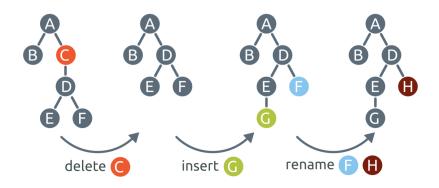
• **Deletion.** deletion of a node



• 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.
  - $\gamma(a \to b)$  can be 1 or other user defined value.

 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.

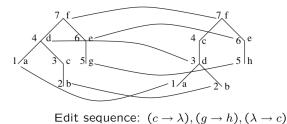


Figure: The Edit Sequence and its Cost

### **Notation**

#### Tree

I(f)



• 
$$I(A_1 \circ A_2 \circ \cdots \circ A_n)$$



Let T be a tree,

- r(T)
- T°
- Ir(T)
- rr(T)

the root of T

$$T - r(T)$$

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

### Notation

#### Forest

- *l*(*f*) ∘ *t* 
  - **Å** Å ...

•  $t \circ I(f)$ 







Let F be a forest,

- |F|
- #leaves(F)
- F(i)
- F − i
- Ir(F)
- rr(F)

the number of nodes in the forest F the number of leaves in the forest F the sub-tree of F rooted at node i the forest after deleting node i the root of the leftmost tree in the forest F

the root of the rightmost tree in the forest F

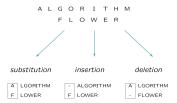
# String Edit Distance and its Recursive Solution

- 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

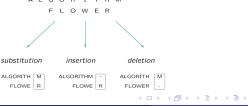
$$d(S_1, S_2) = min \begin{cases} d(S_1 - u, S_2) + \delta(u, \emptyset) \\ d(S_1, S_2 - v) + \delta(\emptyset, v) \\ d(S_1 - u, S_2 - v) + \delta(u, v) \end{cases}$$

### 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 I(f) and I'(f'),

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

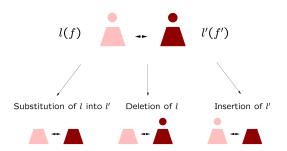


Figure: Tree-to-Tree Edit Distance

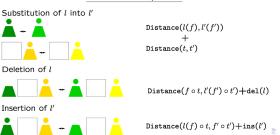
#### Tree Edit Distance and its Recursive Solution

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

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

$$l(f) \circ t$$
  $l'(f') \circ t$ 

#### Leftmost decomposition



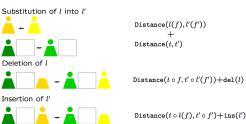
### Tree Edit Distance and its Recursive Solution

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

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

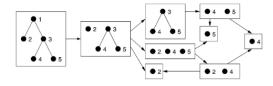


#### Rightmost decomposition

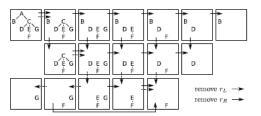


### Relevant Sub-forests and Full Decomposition

Relevant sub-forests



Full decomposition

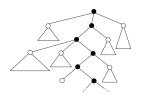


### Root-leaf Path and Relevant Sub-trees

Root-leaf path



Relevant sub-trees



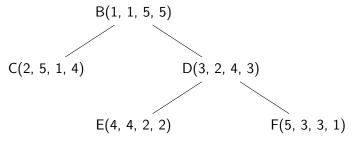
Path decomposition



### Tree Indexing

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

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



#### Note:

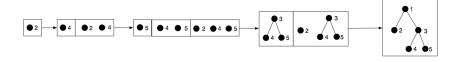
- preL + postR = treeSize + 1
- preR + postL = treeSize + 1



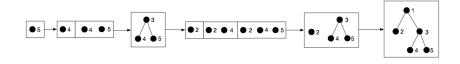
### Bottom-up Enumeration

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 \le i \le m and 1 \le j \le 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 | compute d(L_1[i], L_2[j]) as in Equation 2.3

6 | end

7 end

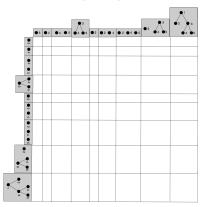
8 d(T_1[i], T_2[j]) \leftarrow d(L_1[|L_1|][|L_2|]);

9 return d(T_1[i], T_2[j]);
```

# A Simple Algorithm

### Implementation:

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

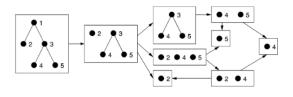


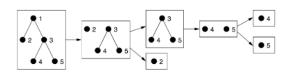
• The upper bound of the post-order enumeration method for the tree edit distance problem is  $\mathcal{O}(n^4)$ 

### 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.





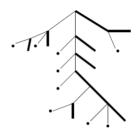
### Zhang and Shasha's Algorithm

#### **Key Ideas:**

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



(a) leftmost paths



(b) rightmost paths

# Zhang and Shasha's Algorithm

#### 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\{depth(A), leaves(A)\}*min\{depth(B), 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.





### Klein's Algorithm

#### 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.

# Demaine's Algorithm

#### **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	` '	$\mathcal{O}(n^4)$	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

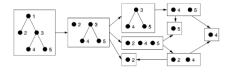
### Optimal Root-leaf Path

#### Key Idea:

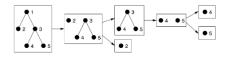
- heavy paths is a kind of greedy algorithm which usually lead to the local optimum rather than global optimum.
- quantifies each possible paths and selects the path with the least number of sub-problems is selected
- implemented via dynamic programming.
- Preprocessing time is bounded by  $\mathcal{O}(|A||B|)$

### Relevant Leftmost/Rightmost/Special Sub-forests

- ullet Path decomposition o relevant sub-forests
- ullet Recursive leftmost path decomposition o relevant leftmost sub-forests



ullet Recursive rightmost path decomposition o relevant rightmost sub-forests



Full decomposition → 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))

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

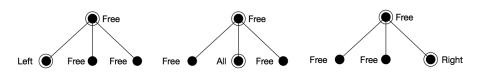
Relevant Special Sub-forests(#special(T))

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

#### 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.



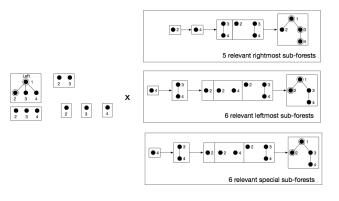
- Seven memorized tables to store intermediate results.
  - Free
  - LeftA
  - RightA
  - AllA
  - LeftB
  - RightB
  - AIIB
- Dynamic programming.

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



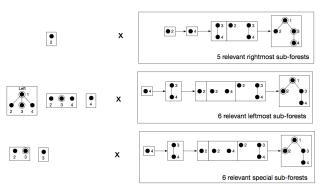


Let A be a tree with a root-leaf path and B be another tree.



#leftA(1,1) = Free(3,1) + Free(4,1) + LeftA(2,1)  
+ 
$$|A - A(2)| * #left(B)$$
  
=  $#left(B) + #left(B) + #left(B) + 3 * #left(B)$ 

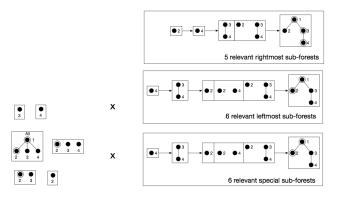
Let A be a tree with a root-leaf path and B be another tree.



#leftA(1,1) = Free(2,1) + Free(4,1) + AllA(3,1)  
+ 
$$|1 + A(4)| * \#left(B) + |A(2)| * \#special(B)$$
  
=  $\#right(B) + \#left(B) + \#special(B)$   
+  $\#special(B) + 2 * \#left(B)$ 

## Quantify the Number of Sub-Problem

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

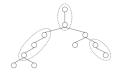


$$\#AIIA(1,1) = Free(3,1) + Free(4,1) + AIIA(2,1) + |A - A(2)| * #special(B) = #left(B) + #left(B) + #special(B) + 3 * #special(B)$$

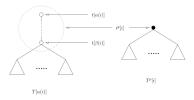
#### Vertical Reduction on Trees

#### **Key Ideas:**

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

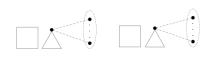


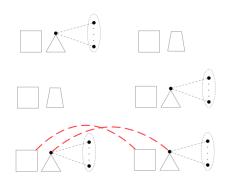
• The compact representation of the original tree can aid in improving the running time for computing the tree edit distance.



# Algorithm

#### Forest-to-Forest Distance:

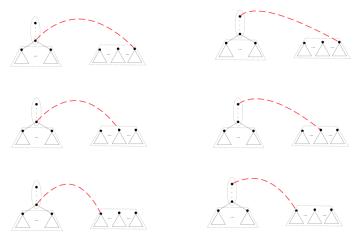




## Algorithm

#### Tree-to-Tree Distance:

• Compute  $d(\widetilde{T_1}, \widetilde{T_2}^{\circ})$ 

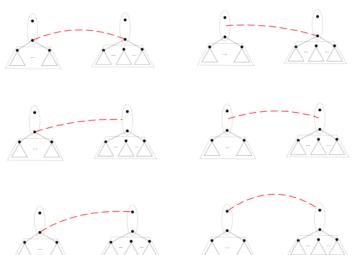


ullet The computation of  $d(\widetilde{T_1}^{\circ},\widetilde{T_2})$  is symmetric.

# 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.

  - $\widetilde{D}_t$ : a  $(\left|\widetilde{T}_1\right|+1)*(\left|\widetilde{T}_2\right|+1)$  two dimensional permanent array.  $\widetilde{D}_f$ : a  $(\left|\widetilde{T}_1\right|+1)*(\left|\widetilde{T}_2\right|+1)$  two dimensional temporary array.
- Dynamic programming.

#### **RNA**

- 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 UCGCCCGGCG
  - 151 GGAAGGGUGA AACGCGGUAA CCUCCACCUG GAGCAAUCCC AAAUAGGCAG
  - 201 GCGAUGAAGC GGCCCGCUGA GUCUGCGGGU AGGGAGCUGG AGCCGGCUGG
  - 251 HAACAGCCGG CCHAGAGGAA HGGHHGHCAC GCACCGHHHG CCGCAAGGCG
  - 251 Official Cook of C
  - 301 GGCGGGGCGC ACAGAAUCCG GCUUAUCGGC CUGCUUUGCU U
- RNA is unstable.

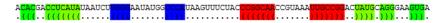
## RNA Secondary Structure

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

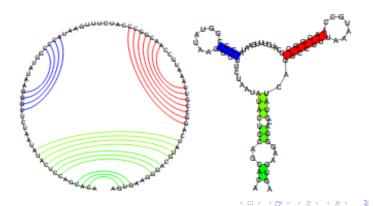
(	1)	1	337	10
(	2)	11	326	1
(	3)	12	278	7
(	4)	20	45	2
(	5)	23	42	8
(	6)	59	183	4
(	7)	71	179	5
(	8)	77	89	4
(	9)	91	105	1
(	10)	92	103	4
(	11)	106	174	2
(	12)	111	172	2
(	13)	127	156	4
(	14)	132	151	8
(	15)	187	235	4
(	16)	197	226	6
(	17)	206	220	5
(	18)	242	261	8
(	19)	281	308	2
(	20)	284	305	9

## RNA Secondary Structure Representation

String representation



Graph representation



## Tree Representation of the RNA Secondary Structure

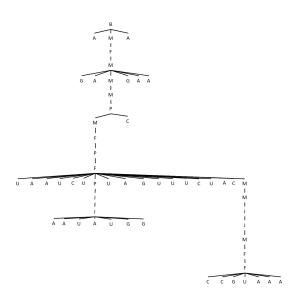
Base pair labelling

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

Table: The Label of Base Pair

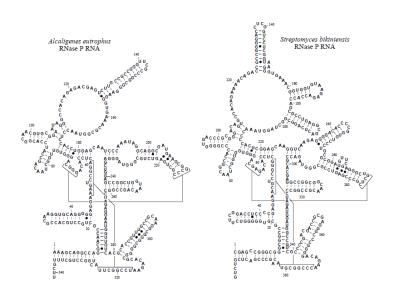
Tree representation

## Tree Representation of the RNA Secondary Structure



## **Experiment**

## **Experiment**



## **Experiment Result**

```
Alcaligenes eutrophus ~ Streptomyces bikiniens
deletion: 1 insertion: 1 substitution: 1 distance: 134
AAAG-CAGGCAGCAACCGCUGCCUGCACCG-CAAGGUGCAGGGGGGGAGGAAAGUCCGGACUCCACAGGGCAGG-GUGU-UGGCUAACAGCCAU-CCAC
CGAGCC-GGGCGGCCGCCGCGLGGGG-GLICULCG-GAC-CLICCCCGAGGAACGLICCGGGCLICCACAGAGCA-GGGLIG-GLIGGCLIAACGGCCA-CCCGG
ĠGCAAĆĠÚĠCĠĠÀAUAĠĠGCCACAGAGA-CGAGUCUUĠĊĊĠĊĠ-ĠĠ--UUCĠ--ĆĆ-ĆĠĠĆ--ĠĠGAAGG-GU----------G-AA-A------
GGLIGACCC GC GGGAC AGLIGCC AC AGAAAAC -AG----ACC GCC GGGGAC C LIC GGLIC C LIC GGLICAAGGG-----LIGAAAC GGLIGGLIGLIAAGAGAC C ACC AGC
GCC LIGAGGC GAC UC AGGC GGC LIAGGLIAAAC C C C AC LIC – GGAGC AAGGLIC AAGAGGGGAC AC C C C GGLIGLIC C C LIGC GC GGALIGLILIC GAGGGC LIGC LIC GC C
CGAGUCCGCGGGUAGACCGCACGAGGCCGGC-GGCAAC-GCCGGCCCUAGAUGGA-UGGCCGUCG-CC-CCG---ACGACCGCGAGGUC---CCGG-GG
GCACAGAAUCCGGCUUAUCGGCCUG-CUUUGCUU
```

-- ACAGAACCCGGCGUACAGCCC-GACUCGUCUG

### **Evaluation**

Tree size: 246 and 282

#Rel.sub	Time[sec]
849282	0.08
2039089	0.13
7175224	0.65
553526	0.04
428766	0.05
686562	0.05
291329	0.03
	849282 2039089 7175224 553526 428766 686562

### **Evaluation**

Tree size: 1041 and 1012

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

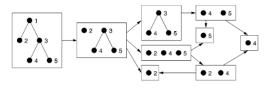
#### Conclusion

- 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.

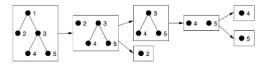
Thank you. Questions?

## Path Decomposition

• Leftmost path decomposition



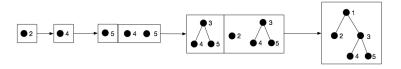
• Rightmost path decomposition



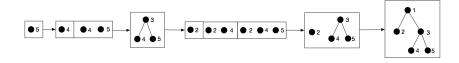
## Bottom-up Enumeration

Two orders of the enumeration of the path decomposition:

• LR-postorder enumeration

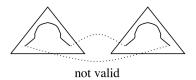


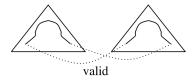
RL-postorder enumeration



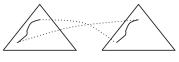
## Matching in Trees

- **Input:** Two labelled ordered trees T and P.
- Constraints:
  - One-to-one relationship
  - Sibling order is preserved.

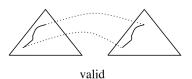




Ancestor order is preserved.



not valid



• Output: Mapping between T and P.