# Similarity Search

## Token-Based Tree Distances

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## Outline

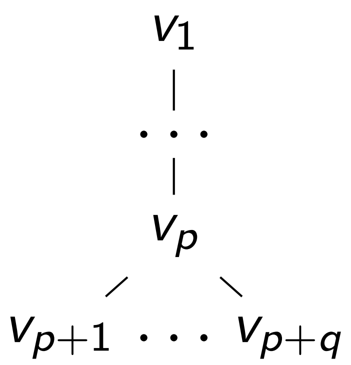
## Tokens for Trees – Intuition

- $q$-Grams for strings:
  - split string into substrings ($q$-grams) of length $q$
  - strings with many common substrings are similar
- Tokens for trees:
  - split tree into small subunits (tokens) of the same shape
  - tokens may be individual nodes, subtrees, or subgraphs
  - trees with many common tokens are similar
- Example: the so-called $pq$-gram tokens are besom-shaped subtrees with $p + q$ nodes

$$\begin{tikzcd}[arrows=-]
& v_1 \arrow[d] & \\
& \cdots \arrow[d] & \\
& v_p \arrow[dl] \arrow[dr] & \\
v_{p+1} & \cdots & v_{p+q}
\end{tikzcd}$$

## Token Profile and Label Tuples

- Token profile $P(T)$: set of all tokens of tree $T$
  - a token may be a subtree or a subgraph of the tree
  - the token profile $P(T)$ of a tree $T$ is the set of all its tokens
- A linear encoding of a token traverses all its nodes in preorder:



$$= \quad (v_1, \dots, v_p, v_{p+1}, \dots, v_{p+q})$$

- Label tuple $\lambda(t)$: tuple of the nodes labels $\lambda(\mathrm{v}_i)$ of token $t = (\mathrm{v}_1, \mathrm{v}_2, \dots, \mathrm{v}_k)$ in preorder:

$$\lambda(t) = (\lambda(\mathrm{v}_1), \lambda(\mathrm{v}_2), \dots, \lambda(\mathrm{v}_k))$$

## Token Index

### Definition (Token Index)

Let $P(T)$ be a token profile of tree $T$. The token index, $\mathcal{I}$, of tree T is the **bag of all label tuples** of T,

$$\mathcal{I}(\mathrm{T}) = \biguplus_{g \in \mathrm{P_T}} \lambda(g)$$

- Note:
  - tokens consist of nodes and are unique within a tree
  - but: different tokens may yield identical label tuples
  - thus the token index may contain duplicates

## Token-Based Distance

**Definition (Token-Based Distance)**

The token-based distance between two trees, T and T′, with token indexes $\mathcal{I}(T)$ and $\mathcal{I}(T')$, respectively, is defined as

$$\delta(T, T') = |\mathcal{I}(T) \uplus \mathcal{I}(T')| - 2|\mathcal{I}(T) \Cap \mathcal{I}(T')|$$

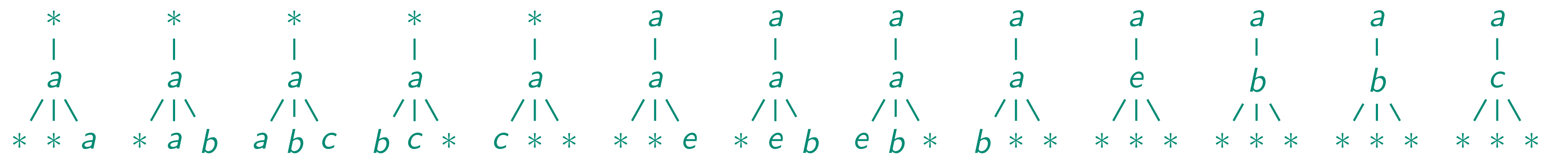
- Metric normalization to [0..1]: $\delta'_g(T, T') = \frac{\delta_g(T,T')}{|\mathcal{I}(T) \uplus \mathcal{I}(T')| - |\mathcal{I}(T) \Cap \mathcal{I}(T')|}$
- Pseudo-metric properties hold for normalization [ABG10]:
  - ✓ self-identity: $x = y \not\Leftarrow \Rightarrow \delta_g(x, y) = 0$
  - ✓ symmetry: $\delta_g(x, y) = \delta_g(y, x)$
  - ✓ triangle inequality: $\delta_g(x, z) \leq \delta_g(x, y) + \delta_g(y, z)$
- Different trees may have identical indexes.

## Storing the Token Index Efficiently

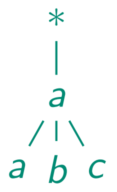
- Problem: How to store node labels efficiently?
    - Long labels: large storage overhead
    - Varying label length: in a relational database, the inefficient VARCHAR type must be used instead of the efficient CHAR type
- Solution: Hashing
    - compute fingerprint hash for labels
    - store concatenation of the hashed labels
- Fingerprint hash function (e.g., Karp-Rabin [KR87]):
    - maps a string $s$ to a hash value $h(s)$
    - $h(s)$ is of fixed length
    - $h(s)$ is unique with high probability
      (for two different strings $s_1 \neq s_2$, $h(s_1) \neq h(s_2)$ with high probability)

## Overview: Token Index

- Token profile: (so-called *pq*-grams in the example, $p = 2, q = 3$)



- Hashing: map tokens to integers:



$\xrightarrow{\textit{serialize}} (*, a, a, b, c) \xrightarrow{\textit{(shorthand)}} *aabc \xrightarrow{\textit{hash}} 03376$

| label l | h(l) |
|---|---|
| * | 0 |
| a | 3 |
| b | 7 |
| c | 6 |
| e | 4 |

Note: labels may be strings of arbitrary length!

- Token index: bag of hashed tokens

$$\mathcal{I}(T) = \{03003, 03037, 03376, 03760, 03600, 33004, 33047, 33470, 33700, 37000, 36000, 34000, 37000\}$$

Intuition: similar trees have similar token indexes.

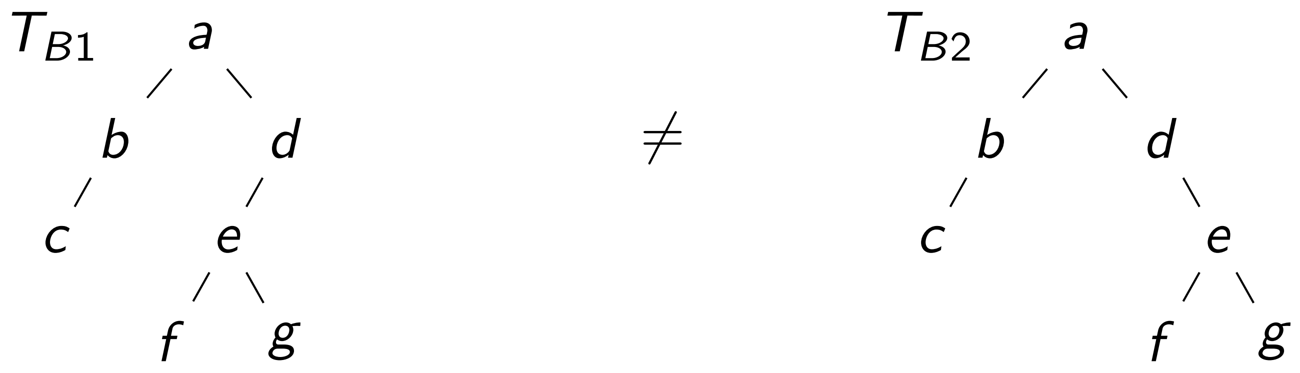
## Binary Tree

- In a binary tree
  - each node has at most two children;
  - left child and right child are distinguished:
    a node can have a right child without having a left child;
- Notation: $\mathsf{T}_B = (N, E_l, E_r)$
  - $\mathsf{T}_B$ denotes a binary tree
  - $N$ are the nodes of the binary tree
  - $E_l$ and $E_r$ are the edges to the left and right children, respectively
- Full binary tree:
  - binary tree
  - each node has exactly zero or two children.

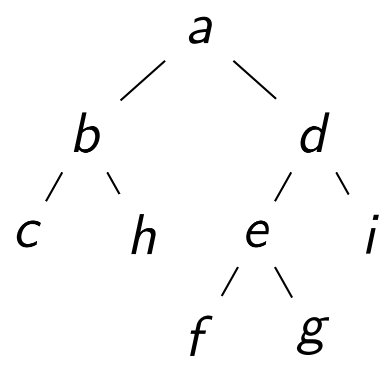
## Example: Binary Tree

- Two different binary trees: $\mathrm{T}_B = (N, E_l, E_r)$

$$\mathrm{T}_{B1} = (\{a,b,c,d,e,f,g\},\ \{(a,b),(b,c),(d,e),(e,f)\},\ \{(a,d),(e,g)\})$$
$$\mathrm{T}_{B2} = (\{a,b,c,d,e,f,g\},\ \{(a,b),(b,c),(e,f)\},\ \{(a,d),(d,e),(e,g)\})$$



- A full binary tree:

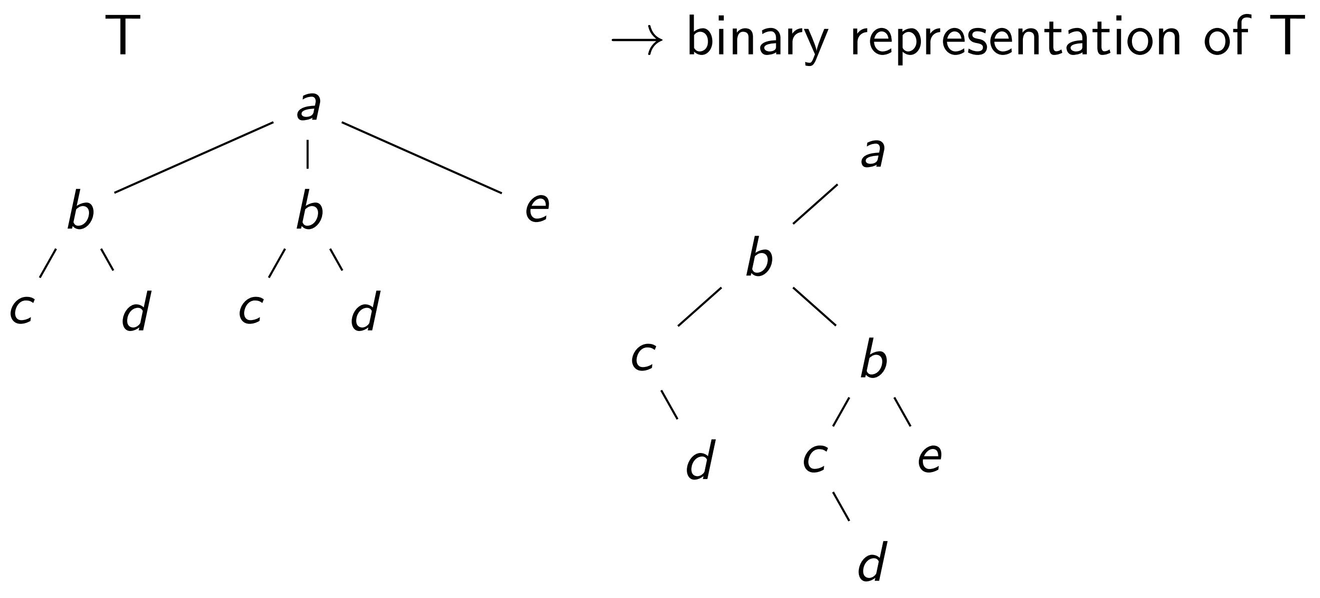


## Binary Representation of a Tree

- Binary tree transformation:
  - (i) link all neighboring siblings in a tree with edges
  - (ii) delete all parent-child edges except the edge to the first child
- Transformation maintains
  - label information
  - structure information
- Original tree can be reconstructed from the binary tree:
  - a left edge represents a parent-child relationships in the original tree
  - a right edge represents a right-sibling relationship in the original tree

## Example: Binary Tree Transformation

- Represent tree T as a binary tree:

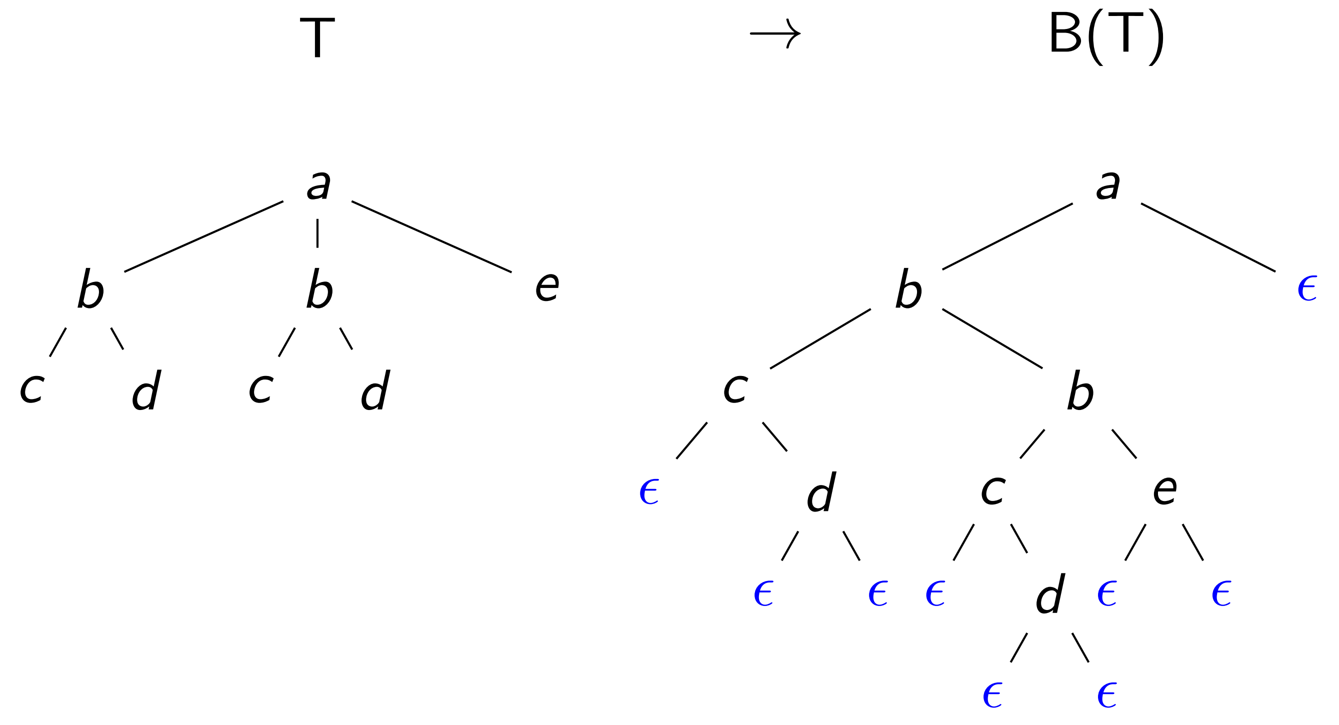


## Normalized Binary Tree Representation

- We extend the binary tree with null nodes $\epsilon$ as follows:
  - a null node for each missing left child of a non-null node
  - a null node for each missing right child of a non-null node
- Note: Leaf nodes get two null-children.
- The resulting normalized binary representation
  - is a full binary tree
  - all non-null nodes have two children
  - all leaves are null nodes (and all null nodes are leaves)

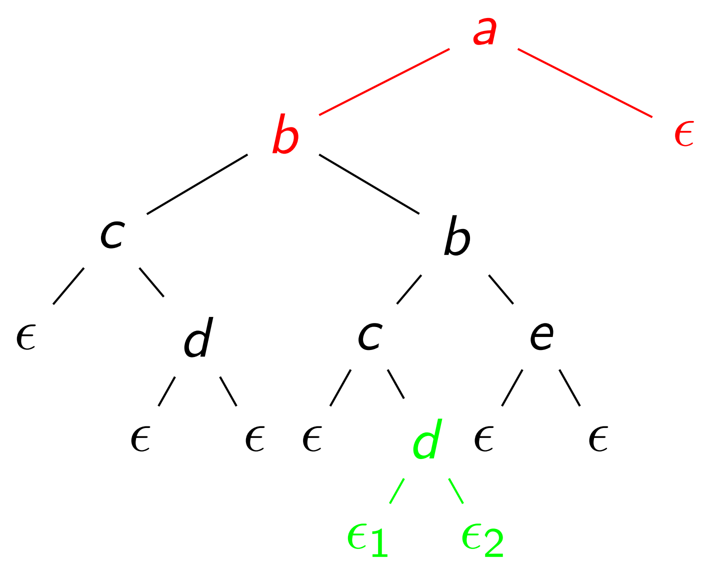
## Example: Normalized Binary Tree

- Transforming T to the normalized binary tree $B(\mathrm{T})$:



## Binary Branch

- A binary branch $BiB(\mathrm{v})$ is
  - a subtree of the normalized binary tree $B(\mathrm{T})$
  - consisting of a non-null node v and its two children
- Example:
  $BiB(a) = (\{a, b, \epsilon\}, \{(a, b)\}, \{(a, \epsilon)\})$
  $BiB(d) = (\{d, \epsilon_1, \epsilon_2\}, \{(d, \epsilon_1)\}, \{(d, \epsilon_2)\})$ [1]



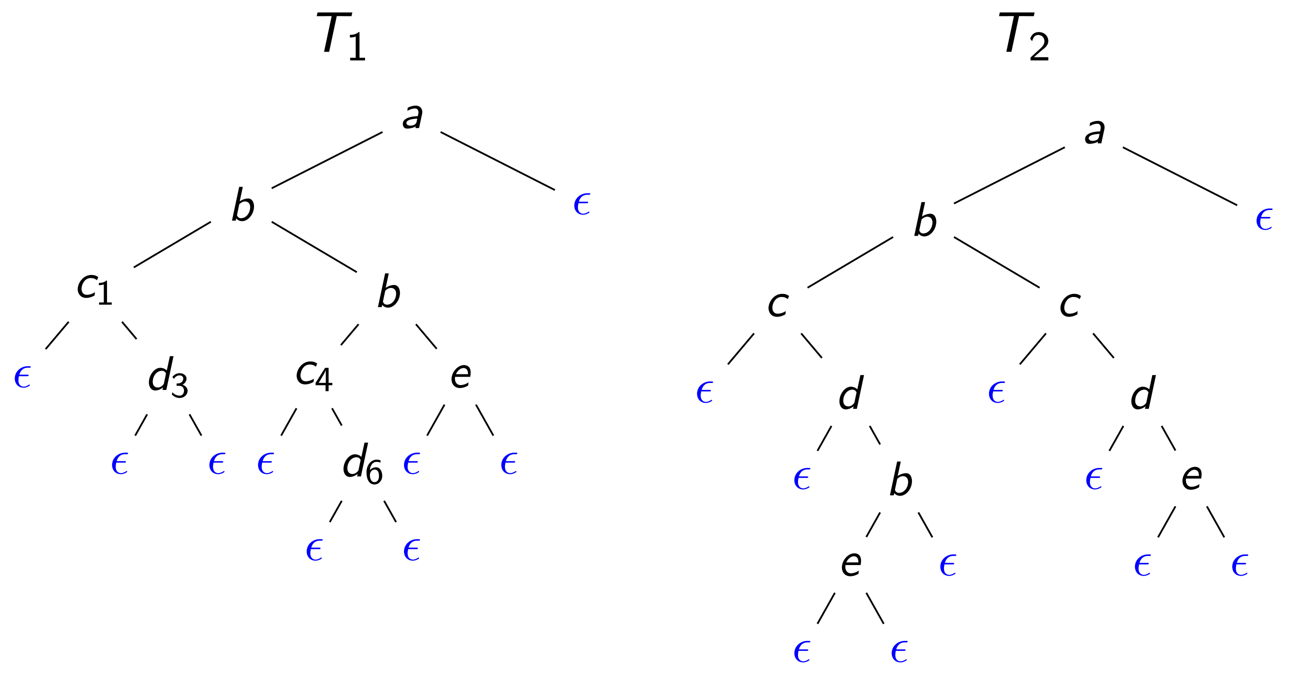
[1] Although the two null nodes have identical labels ($\epsilon$), they are different nodes. We emphasize this by showing their IDs in subscript.

## Binary Branches of Trees and Datasets

- Binary branches can be serialized as label tuples:
  - $BiB(\mathsf{v}) = (\{\mathsf{v}, \mathsf{a}, \mathsf{b}\}, \{(\mathsf{v}, \mathsf{a})\}, \{(\mathsf{v}, \mathsf{b})\}) \rightarrow \lambda(\mathsf{v}) \circ \lambda(\mathsf{a}) \circ \lambda(\mathsf{b})$
- Binary branch profile and index:
  - $P_{bb}(\mathsf{T})$ is the set of all binary branches of T
  - $\mathcal{I}_{bb}(\mathsf{T})$ is the multiset of all binary branch label tuples of T
- Note:
  - nodes are unique in the tree, thus binary branches are unique
  - labels are *not* unique, thus the label tuples are *not* unique
- Binary branch distance: The binary branch distance between two trees $\mathsf{T}_1$ and $\mathsf{T}_2$ is defined as:

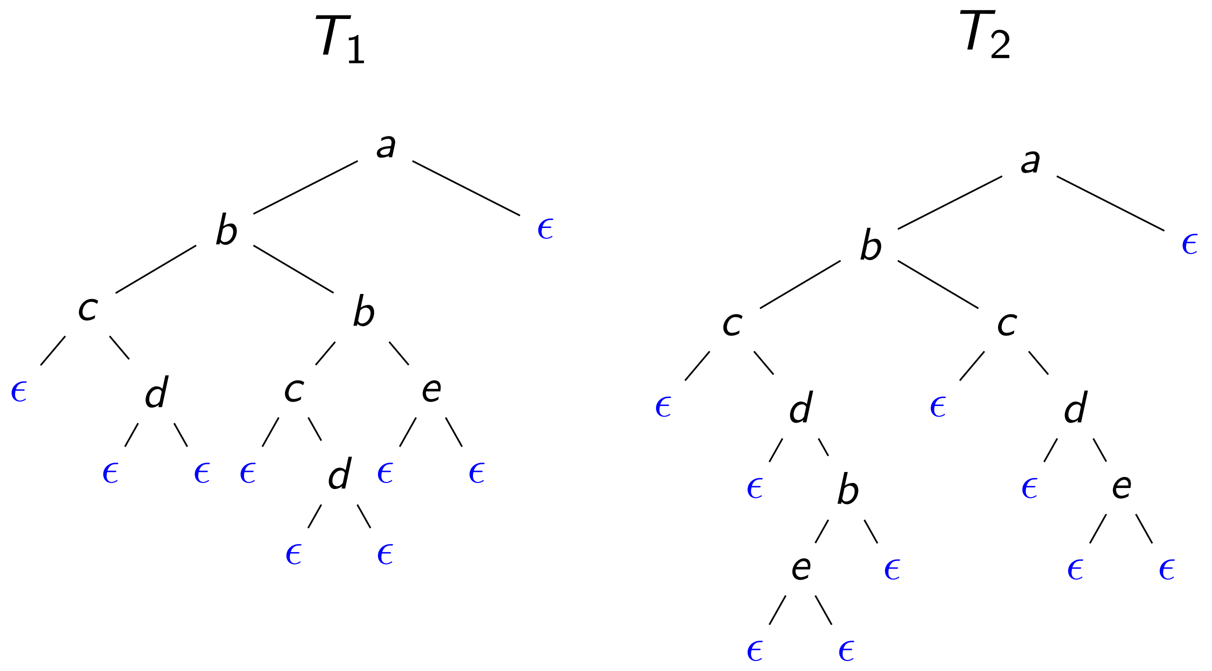
$$\delta_{bb}(\mathsf{T}_1, \mathsf{T}_2) = |\mathcal{I}_{bb}(\mathsf{T}_1) \uplus \mathcal{I}_{bb}(\mathsf{T}_2)| - 2|\mathcal{I}_{bb}(\mathsf{T}_1) \Cap \mathcal{I}_{bb}(\mathsf{T}_2)|$$

## Example: Binary Branches and Label Tuples



- $BiB(c_1) \neq BiB(c_4)$:
  - $BiB(c_1) = (\{c_1, \epsilon_2, d_3\}, \{(c_1, \epsilon_2)\}, \{(c_1, d_3)\})$
  - $BiB(c_4) = (\{c_4, \epsilon_5, d_6\}, \{(c_4, \epsilon_5)\}, \{(c_4, d_6)\})$
- Serialization of both, $BiB(c_1)$ and $BiB(c_2)$, is identical: '$c\epsilon d$'

## Example: Binary Branch Distance



$\mathcal{I}_{bb}(T_1) = \{ab\epsilon, bcb, c\epsilon d, d\epsilon\epsilon, bce, c\epsilon d, d\epsilon\epsilon, e\epsilon\epsilon\}$

$\mathcal{I}_{bb}(T_2) = \{ab\epsilon, bcc, c\epsilon d, d\epsilon b, be\epsilon, e\epsilon\epsilon, c\epsilon d, d\epsilon e, e\epsilon\epsilon\}$

$\delta_{bb}(T_1, T_2) = 17 - 2 \cdot 4 = 9$

## Lower Bound Theorem

**Theorem (Lower Bound)**

*Let* $\mathsf{T}_1$ *and* $\mathsf{T}_2$ *be two trees. If the tree edit distance between* $\mathsf{T}_1$ *and* $\mathsf{T}_2$ *is* $\delta_t(\mathsf{T}_1, \mathsf{T}_2)$*, then the binary branch distance between them satisfies*

$$\delta_{bb}(\mathsf{T}_1, \mathsf{T}_2) \leq 5 \times \delta_t(\mathsf{T}_1, \mathsf{T}_2).$$

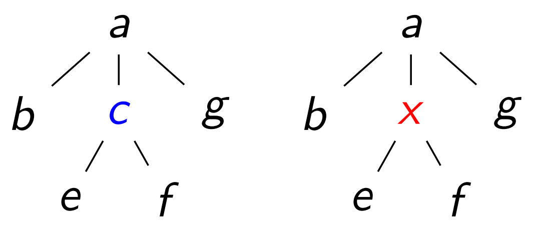
**Proof (Sketch — Full Proof in [YKT05]).**

- Each node v appears in at most two binary branches.
- *Rename*: Renaming a node causes at most two binary branches in each tree to mismatch. The sum is 4.
- Similar rational for *insert* and its complementary operation *delete* (at most 5 binary branches mismatch).

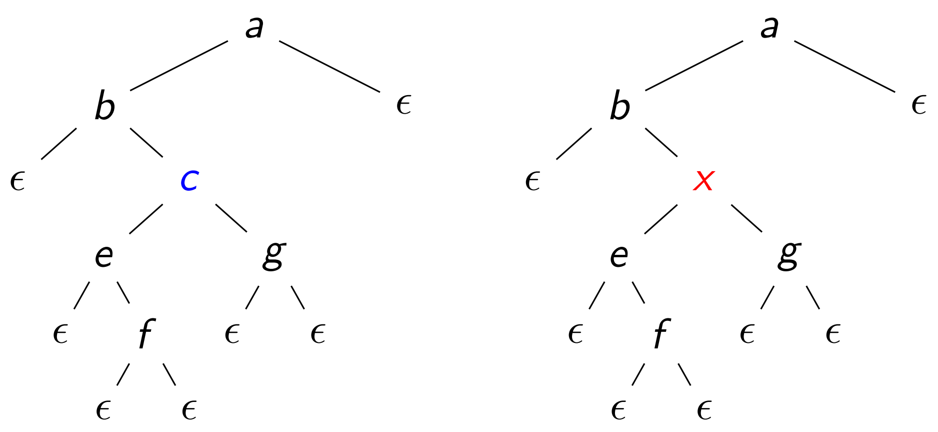
$\square$

## Proof Sketch: Illustration for Rename

- transform $T_1$ to $T_2$: $ren(c, x)$



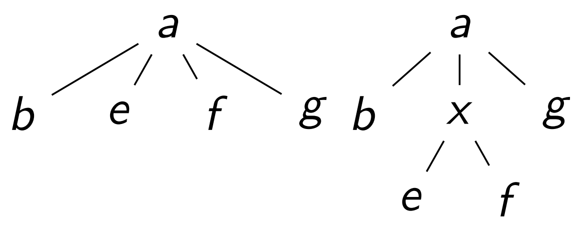
- binary trees $B(T_1)$ and $B(T_2)$



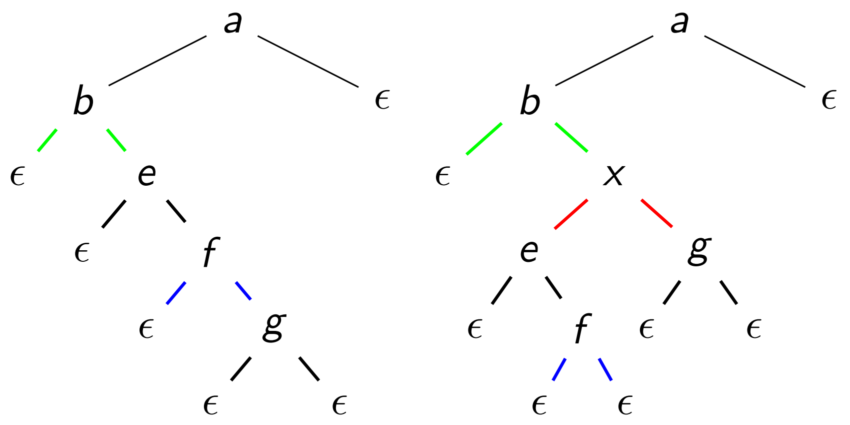
- Two binary branches ($b\epsilon c$, $ceg$) exist only in $B(T_1)$
- Two binary branches ($b\epsilon x$, $xeg$) exist only in $B(T_2)$
- $\delta_t(T_1, T_2) = 1$ (1 rename)
- $\delta_{bb}(T_1, T_2) = 4$ (4 binary branches different)

## Proof Sketch: Illustration for Insert

- transform T$_1$ to T$_2$: $ins(x, a, 2, 2)$



- binary trees $B$(T$_1$) and $B$(T$_2$)



- Two binary branches ($b\epsilon e$, $f\epsilon g$) exist only in $B$(T$_1$)
- Tree binary branches ($b\epsilon x$, $f\epsilon\epsilon$, $xeg$) exist only in $B$(T$_2$)
- $\delta_t$(T$_1$, T$_2$) $=$ 1 (1 insertion)
- $\delta_{bb}$(T$_1$, T$_2$) $=$ 5 (5 binary branches different)

## Proof Sketch

- In general it can be shown that
  - Rename changes *at most* 4 binary branches
  - Insert changes *at most* 5 binary branches
  - Delete changes *at most* 5 binary branches
- Each edit operation changes at most 5 binary branches, thus

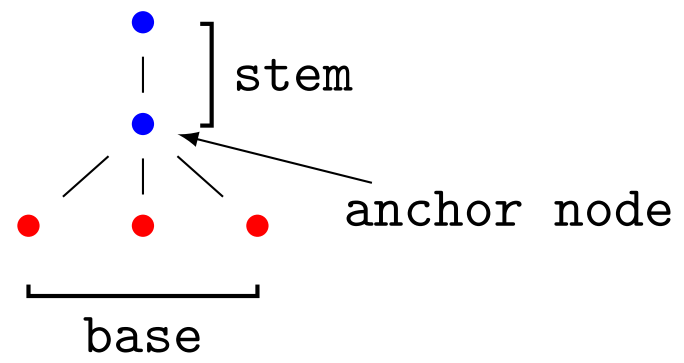
$$\delta_{bb}(\mathsf{T}_1, \mathsf{T}_2) \leq 5 \times \delta_t(\mathsf{T}_1, \mathsf{T}_2).$$

## Complexity: Binary Branch Distance

- Generating the binary branches: $O(n)$ time and space ($n = \max\{|T_1|, |T_2|\}$)
  - the binary branches are formed in a single traversal of the tree
  - for each node of a tree a single binary branch is formed
- Computing the distance: $O(n \log n)$ time and $O(n)$ space
  - sort binary branch indexes to compute intersection: $O(n \log n)$
  - alternative: average case $O(n)$ runtime complexity
    1. build hash map for index $\mathcal{I}_{bb}(T_2)$
    2. probe label tuples of $\mathcal{I}_{bb}(T_1)$ to compute size of intersection

## *pq*-Grams

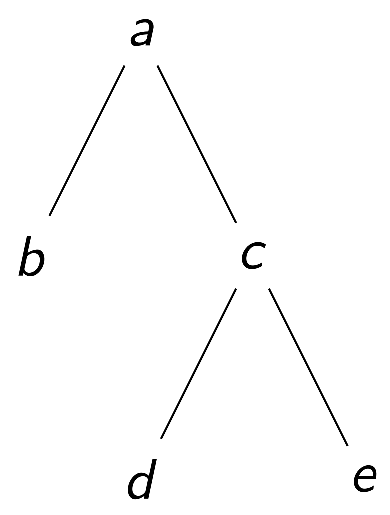
- The shape of a *pq*-gram ($p=2$, $q=3$):



- $p$ nodes (anchor node and $p-1$ ancestors) form the stem
- $q$ nodes ($q$ consecutive children of the anchor node) form the base

## *pq*-Extended Tree

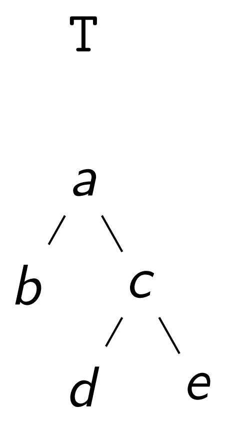
- Problem: How can we split the following tree T into 2, 3-grams?

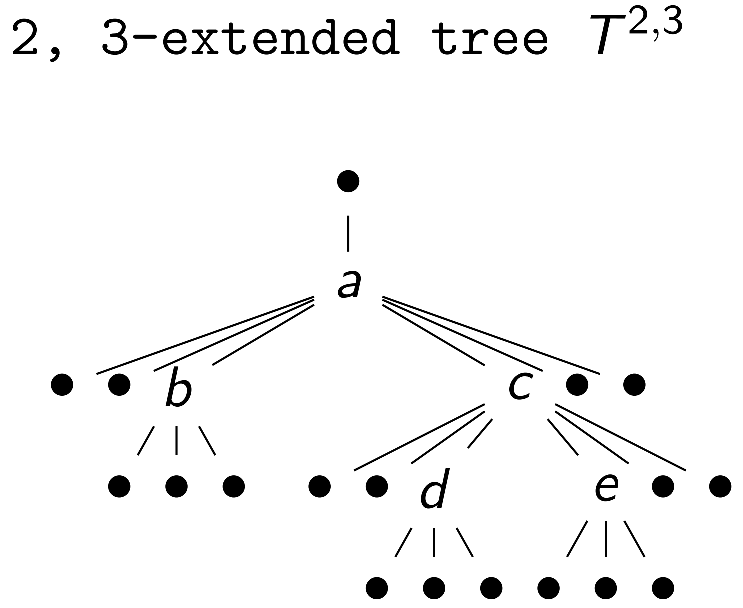


- Solution: Extend tree T with dummy nodes (•):
  - $p-1$ ancestors to the root node
  - $q-1$ children before the first and after the last child of each non-leaf
  - $q$ children for each leaf
- The result is the *pq*-extened tree $T^{pq}$.

## Example: Extended Tree

- An example tree T and its extended tree T$^{pq}$ ($p=2$, $q=3$):





## Definition: *pq*-Gram [ABG05]

**Definition (*pq*-Gram)**

Let T be a tree, $T^{p,q}$ the respective extended tree, $p > 0$, $q > 0$. A subtree of $T^{p,q}$ is a *pq-gram* $g$ of T iff

(a) $g$ has $q$ leaf nodes and $p$ non-leaf nodes,

(b) all leaf nodes of $g$ are children of a single node $a \in N(g)$ with fanout $q$, called the anchor node,

(c) the leaf nodes of $g$ are consecutive siblings in $T^{p,q}$.

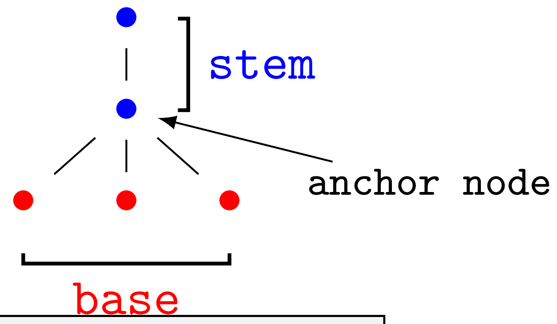
- Stem: anchor node and its ancestors in the *pq*-gram.
- Base: children of the anchor node in the *pq*-gram.

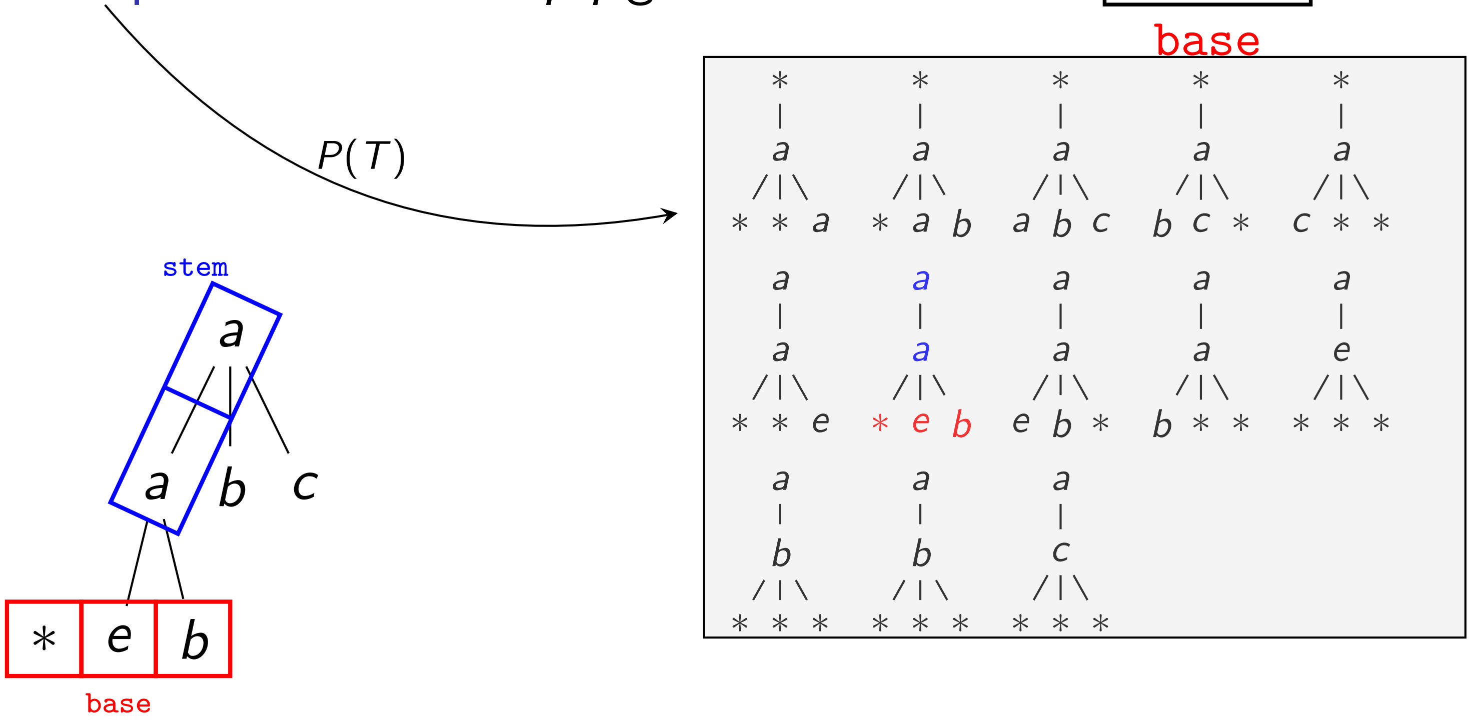
**Definition (*pq*-Gram Profile)**

The *pq*-gram profile, $P_T$, of a tree T is the set of all its *pq*-grams.

## Example: Systematically Split Tree

- *pq*-Gram: small subtree with stem and base
  Example: $p = 2$, $q = 3$
- Systematically split tree into *pq*-grams
- *pq*-Gram profile: set of all *pq*-grams of a tree.





## Label Tuples

- Linear encoding of a *pq*-gram *g* with anchor node $\mathrm{v}_p$: (traverse *pq*-gram in preorder)

$$\begin{tikzcd}
 & v_1 \arrow[d, dash] & \\
 & \cdots \arrow[d, dash] & \\
 & v_p \arrow[dl, dash] \arrow[dr, dash] & \\
v_{p+1} & \cdots & v_{p+q}
\end{tikzcd}
= (v_1, \ldots, v_p, v_{p+1}, \ldots, v_{p+q})$$

- Label tuple: tuple of the *pq*-gram's node labels

$$\lambda(g) = (\lambda(\mathrm{v}_1), \ldots, \lambda(\mathrm{v}_{p+q}))$$

for the *pq*-gram $g = (\mathrm{v}_1, \ldots, \mathrm{v}_{p+q})$.

## *pq*-Gram Index

**Definition (*pq*-Gram Index)**

Let T be a tree with profile $\mathsf{P}_\mathsf{T}$, $p > 0$, $q > 0$. The *pq*-gram index, $\mathcal{I}$, of tree T is the **bag of all label tuples** of T,

$$\mathcal{I}(\mathsf{T}) = \biguplus_{g \in \mathsf{P}_\mathsf{T}} \lambda(g)$$

- Note:
  - *pq*-grams are unique within a tree
  - but: different *pq*-grams may yield identical label tuples
  - thus the *pq*-gram index may contain duplicates

## Size of the *pq*-Gram Index

**Theorem (Size of the *pq*-Gram Index)**

*Let* T *be a tree of size $n = l + i$ with $l$ leaves and $i$ non-leaves. The size of the pq-gram index of* T *is linear in the tree size:*

$$|\mathcal{I}^{pq}(\mathrm{T})| = 2l + qi - 1 = O(n)$$

**Proof.**

1. We count all *pq*-grams whose leftmost leaf is a dummy node: Each leaf is the anchor node of exactly one *pq*-gram whose leftmost leaf is a dummy node, giving $l$ *pq*-grams. Each non-leaf is the anchor of $q - 1$ *pq*-grams whose leftmost leaf is a dummy, giving $i(q-1)$ *pq*-grams.
2. We count all *pq*-grams whose leftmost leaf is not a dummy node: Each node of the tree except the root is the leftmost leaf of exactly one *pq*-gram, giving $l + i - 1$ *pq*-grams.

Overall number of *pq*-grams: $l + i(q-1) + (l + i - 1) = 2l + qi - 1$. □

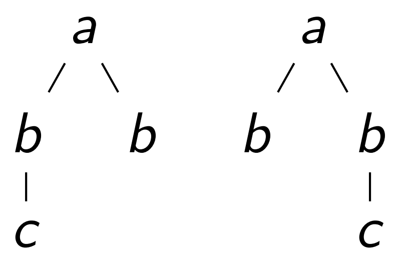
## The *pq*-Gram Distance

**Definition (*pq*-Gram Distance)**

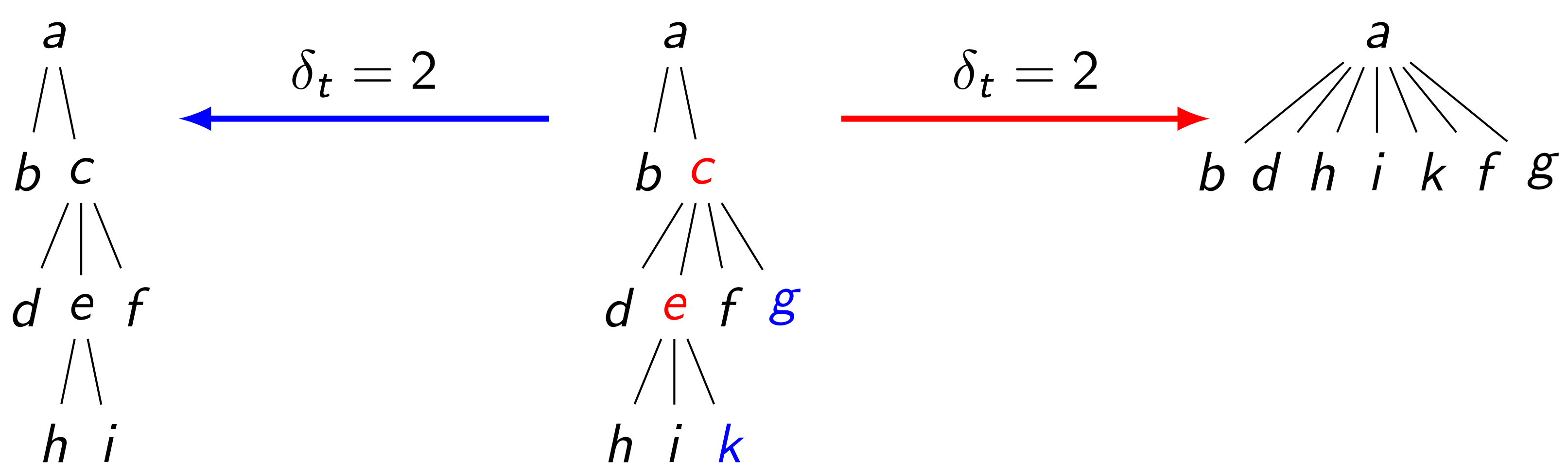
The *pq*-gram distance between two trees, T and T′, is defined as

$$\delta_g(\mathsf{T},\mathsf{T}') = |\mathcal{I}(\mathsf{T}) \uplus \mathcal{I}(\mathsf{T}')| - 2|\mathcal{I}(\mathsf{T}) \mathbin{⩀} \mathcal{I}(\mathsf{T}')|$$

- Metric normalization to [0..1]: $\delta'_g(\mathsf{T},\mathsf{T}') = \frac{\delta_g(\mathsf{T},\mathsf{T}')}{|\mathcal{I}(\mathsf{T}) \uplus \mathcal{I}(\mathsf{T}')| - |\mathcal{I}(\mathsf{T}) \mathbin{⩀} \mathcal{I}(\mathsf{T}')|}$
- Pseudo-metric properties hold for normalization [ABG10]:
  - ✓ self-identity: $x = y \not\Leftarrow \Rightarrow \delta_g(x,y) = 0$
  - ✓ symmetry: $\delta_g(x,y) = \delta_g(y,x)$
  - ✓ triangle inequality: $\delta_g(x,z) \leq \delta_g(x,y) + \delta_g(y,z)$
- Different trees may have identical indexes:



## Motivation: Unit Cost Model Not Always Intuitive



- Unit cost edit distance:
  - no difference between leaves and non-leaves
  - may lead to non-intuitive results
- Conclusion: Non-leaves should have more weight than leaves.

## Fanout Weighted Tree Edit Distance

**Definition (Fanout Weighted Tree Edit Distance)**

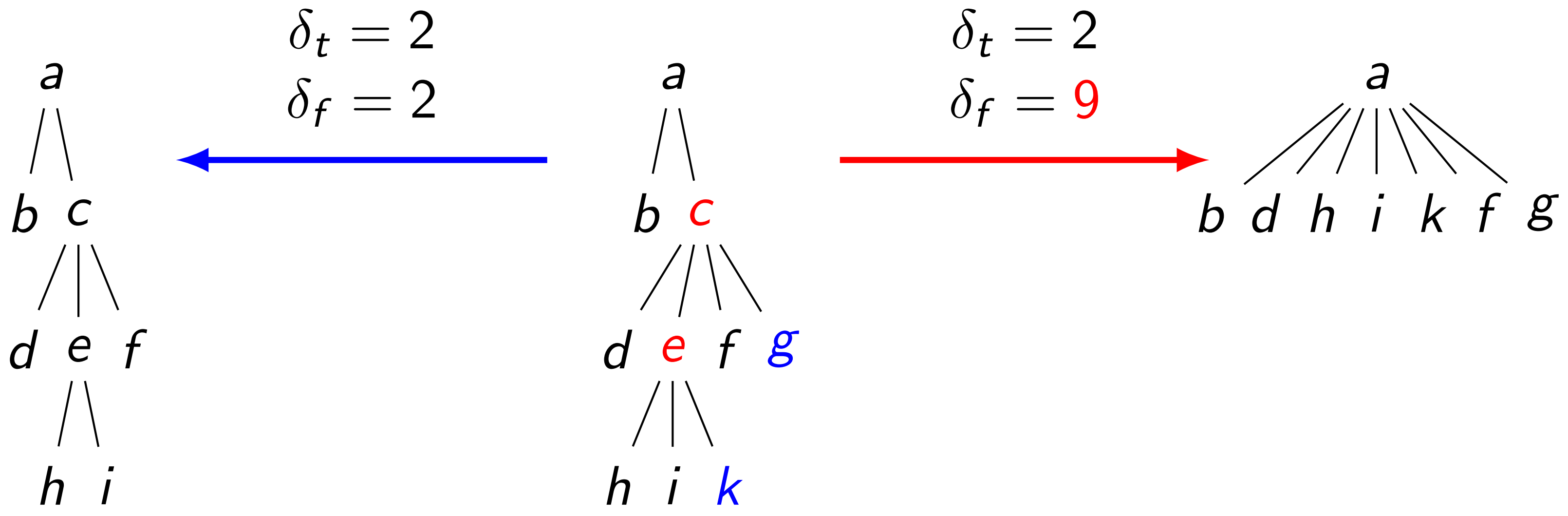
Let T and $\mathrm{T}'$ be two trees, $\mathrm{w} \in N(\mathrm{T})$ a node with fanout $f$, $\mathrm{w}' \in N(\mathrm{T}')$ a node with fanout $f'$, $c > 0$ a constant. The fanout weighted tree edit distance, $\delta_f = (\mathrm{T}, \mathrm{T}')$, between T and $\mathrm{T}'$ is defined as the tree edit distance with the following costs for the edit operations:

- Delete: $\alpha(\mathrm{w} \rightarrow \epsilon) = f + c$
- Insert: $\alpha(\epsilon \rightarrow \mathrm{w}') = f' + c$
- Rename: $\alpha(\mathrm{w} \rightarrow \mathrm{w}') = (f + f')/2 + c$

- Cost of changing a non-leaf node: proportional to its fanout.
- Cost of changing a leaf node: constant $c$.

## Example: Fanout-Weighted Tree Edit Distance

- Fanout-Weighted Tree Edit Distance:
  - leaf changes have small cost ($c = 1$ in the example)
  - non-leaf changes cost proportional to the node fanout



## pq-Gram Distance Lower Bound

**Theorem**

*Let $p = 1$ and $c \geq \max(2q-1, 2)$ be the cost of changing a leaf node. The pq-gram distance provides a lower bound for the fanout weighted tree edit distance, i.e., for any two trees,* $\mathrm{T}$ *and* $\mathrm{T}'$,

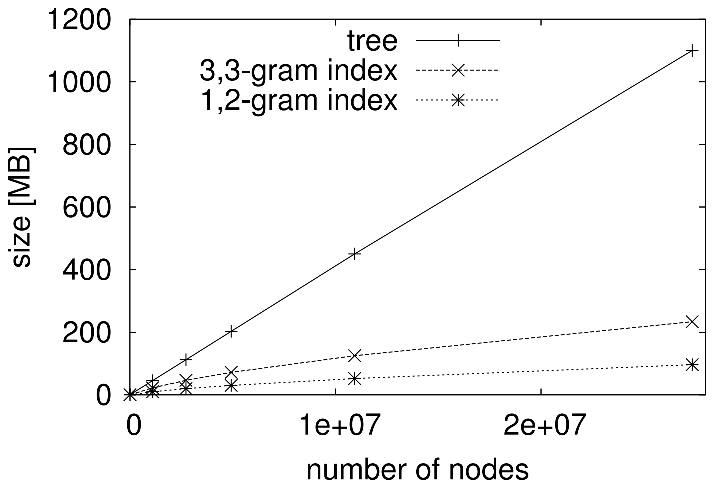
$$\frac{\delta_g(\mathrm{T}, \mathrm{T}')}{2} \leq \delta_f(\mathrm{T}, \mathrm{T}').$$

**Proof.**

See [ABG10] (ACM Transactions on Database Systems). □

## Size of the *pq*-Gram Index

- *pq*-Gram index size: linear in the tree size
- Experiment:
  - compute *pq*-gram index for trees with different number of nodes
  - compare tree and index size



[Trees created with `xmlgen`.]

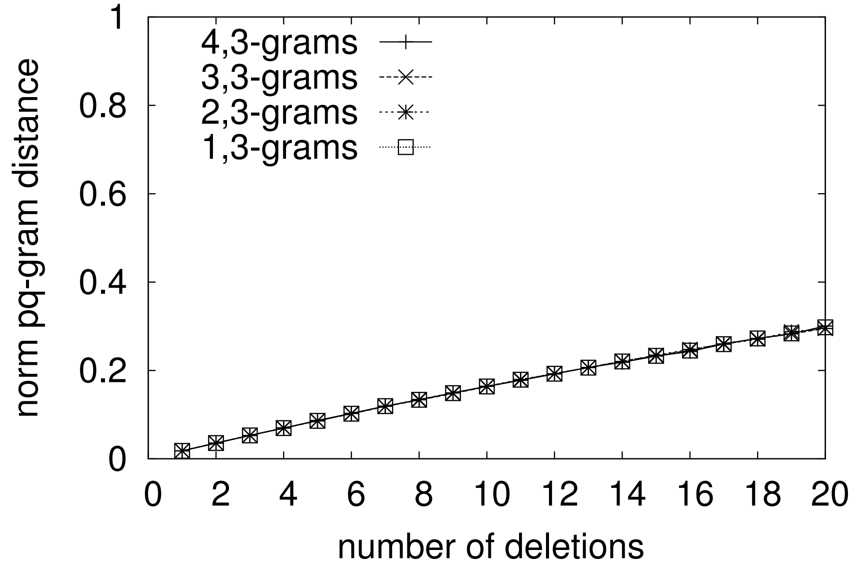
Why is the *pq*-gram index smaller than the tree?

- hash values are smaller than labels
- duplicate *pq*-grams of a tree are stored only once

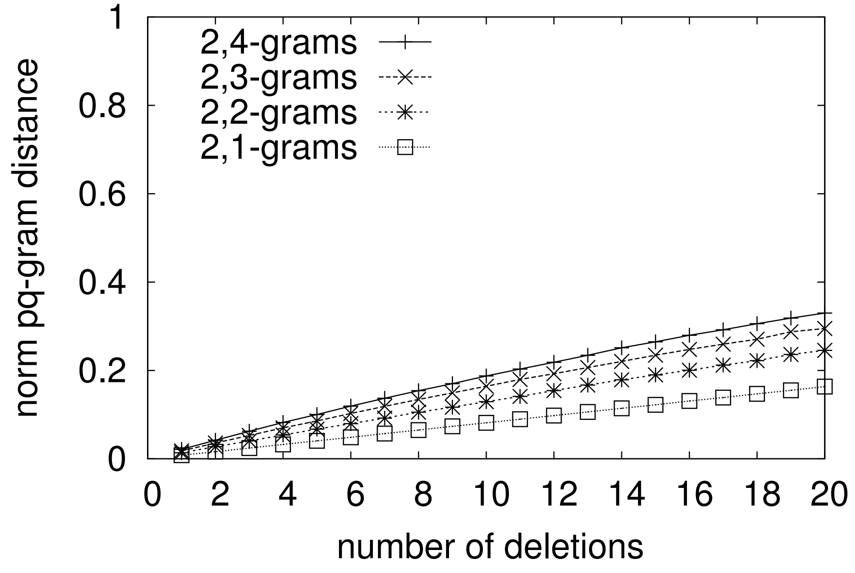
## Sensitivity to Structure Change — Leaf

- Cost of leaf change $\rightarrow$ depends only on $q$
- Experiment:
  - delete leaf nodes
  - measure normalized $pq$-gram distance

vary $p$



vary $q$

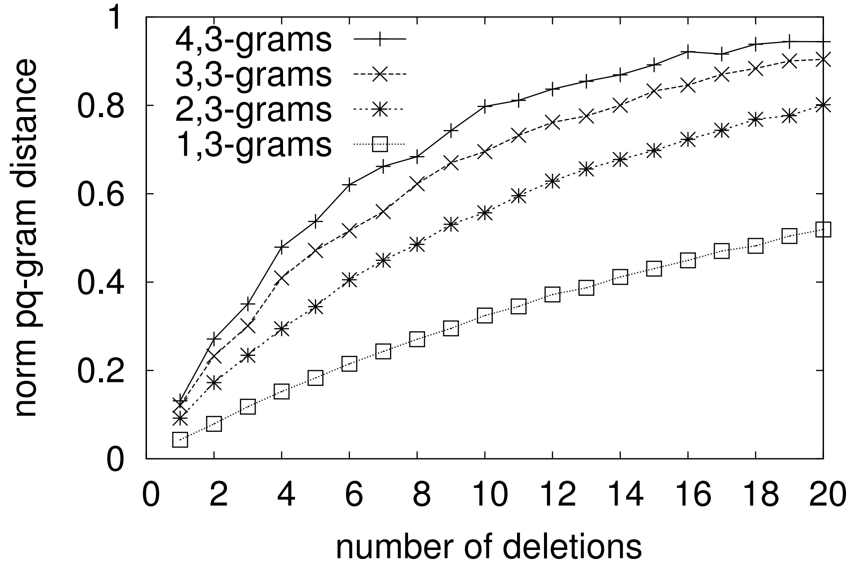


(Artificial tree with 144 nodes, 102 leaves, fanout 2–6 and depth 6. Average over 100 runs.)

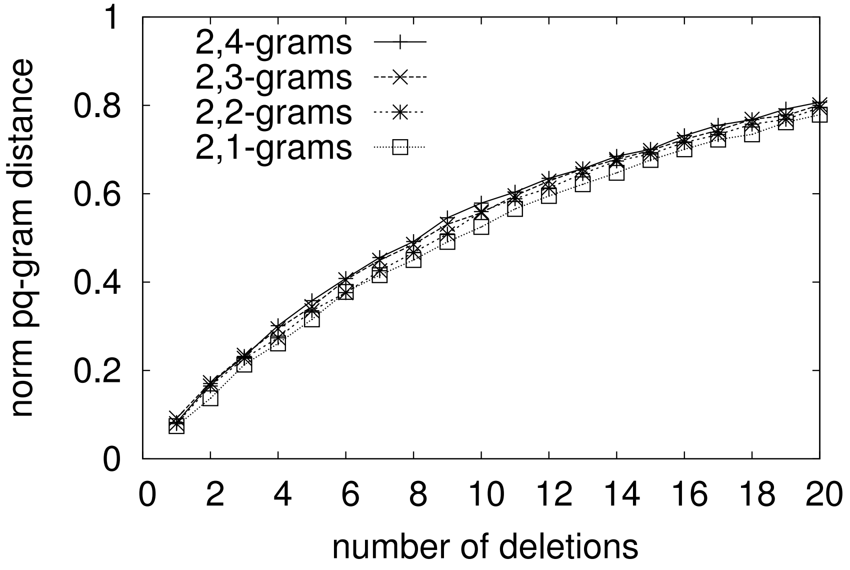
## Sensitivity to Structure Change — Non-Leaf

- Cost for non-leaf change → controlled by *p*
- Experiment:
  - delete non-leaf nodes
  - measure normalized *pq*-gram distance

vary *p*



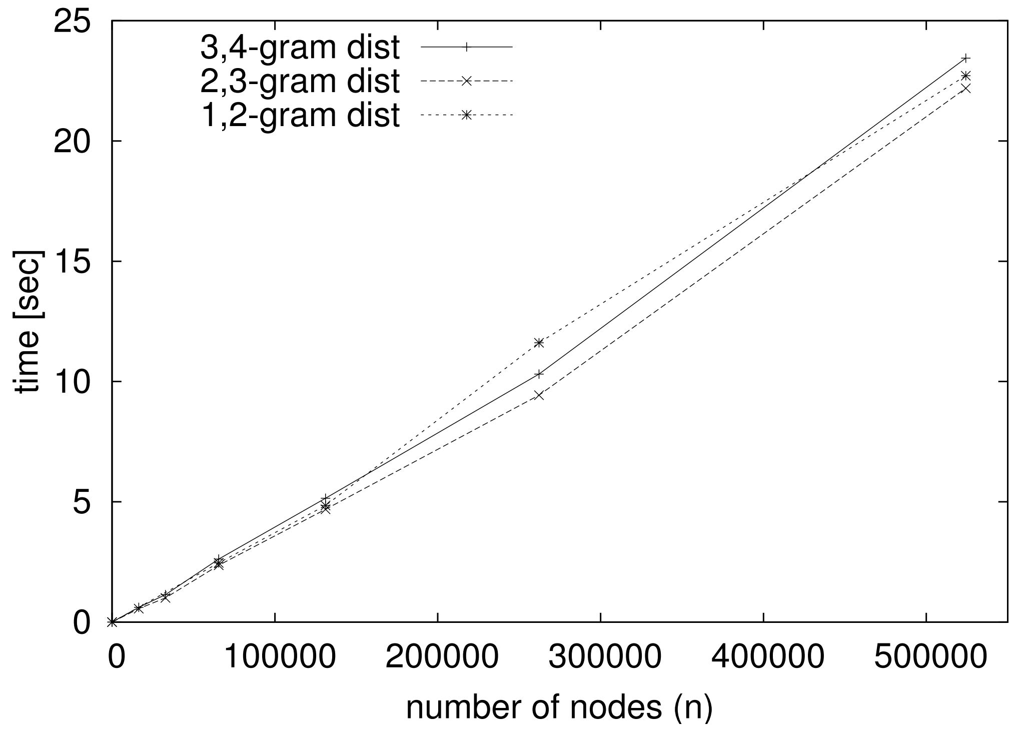
vary *q*



(Artificial tree with 144 nodes, 102 leaves, fanout 2–6 and depth 6. Average over 100 runs.)

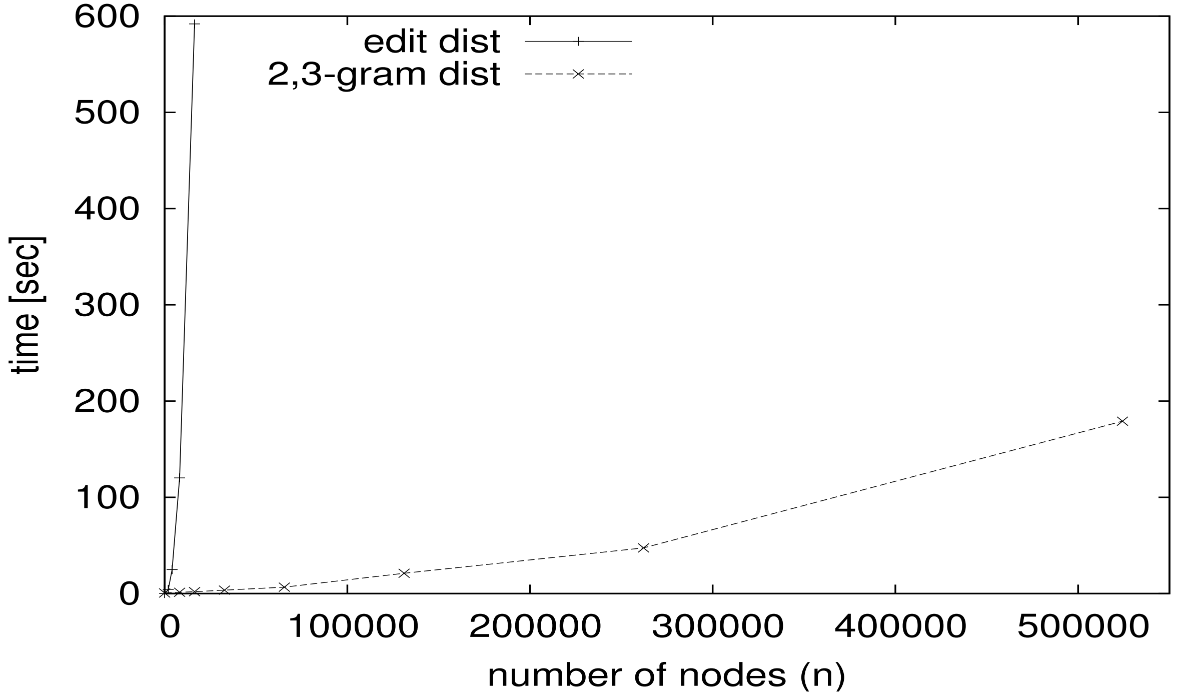
## Influence of *p* and *q* on Scalability

- Scalability (almost) independent of *p* and *q*.
- Experiment: For pair of trees
    - compute *pq*-gram distance for varying *p* and *q*
    - vary tree size: up $10^6$ nodes
    - measure wall clock time



## Scalability to Large Trees

- *pq*-gram distance → scalable to large trees
- compare with edit distance
- Experiment: For pair of trees
    - compute tree edit distance and *pq*-gram distance
    - vary tree size: up $5 \times 10^5$ nodes
    - measure wall clock time



## *pq*-Grams vs. other Edit Distance Approximations

**Effectiveness: *pq*-grams outperform all other approximations**

Experiment: two sets of address trees (299 and 302 trees)

- compute distances between all tree pairs
- find matches (symmetric nearest neighbor)

| Distance | Correct | Recall | Precision | f-Measure | Runtime |
|---|---|---|---|---|---|
| fanout edit dist | 259 | 86.6% | 98.5% | 0.922 | 19 min |
| unit edit dist | 247 | 82.6% | 96.5% | 0.890 | 14 min |
| node intersection | 197 | 65.9% | 93.8% | 0.774 | 4.3s |
| p,q-grams | 236 | 78.9% | 98.7% | 0.877 | 8.1s |
| tree-embedding | 206 | 68.9% | 96.3% | 0.803 | 7.1s |
| binary branch | 193 | 64.5% | 93.2% | 0.763 | 7.4s |
| bottom-up | 148 | 49.6% | 92.5% | 0.645 | 67.0s |

## Summary

- Binary Branch Distance
  - lower bound of the unit cost tree edit distance
  - trees are split into binary branches (small subgraphs)
  - similar trees have many common binary branches
  - complexity $O(n \log n)$ time and $(n)$ space
- *pq*-Gram Distance
  - lower bound for the fanout weighted tree edit distance
  - trees are split into *pq*-grams (small subtrees)
  - similar trees have many common *pq*-grams
  - complexity $O(n \log n)$ time and $O(n)$ space

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