Similarity Search

The *pq*-Gram Distance

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Outline

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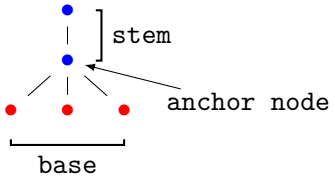
pq-Grams – Intuition

- *q*-Grams for strings:
  - split string into substrings (*q*-grams) of length *q*
  - strings with many common substrings are similar
- *pq*-Grams for trees:
  - split tree into small subtrees (*pq*-grams) of the same shape
  - trees with many common subtrees are similar

pq-Grams

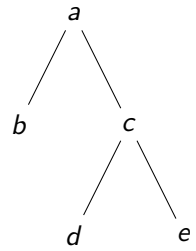
- The shape of a pq-gram ($p=2$, $q=3$):



- 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?

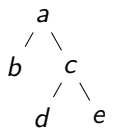


- Solution: Extend tree T with dummy nodes (•):
  - $p-1$ ancestors to the root node
  - $q-1$ children before the first and after the last child of each non-leaf
  - q children for each leaf
- The result is the pq-extened tree T^{pq}.

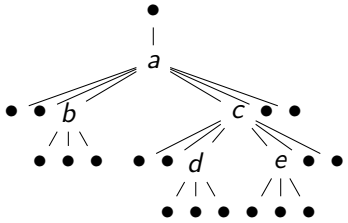
Example: Extended Tree

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

T



2, 3-extended tree $T^{2,3}$



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 $T^{p,q}$.

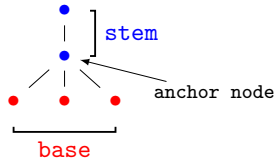
- Stem: anchor node and its ancestors in the pq-gram.
- Base: children of the anchor node in the pq-gram.

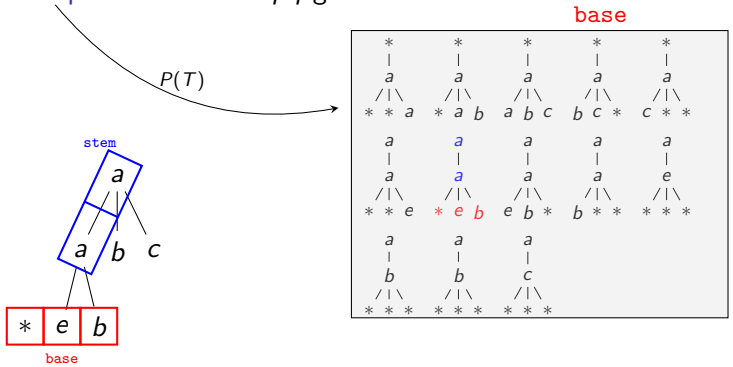
Definition (pq-Gram Profile)

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

Example: Systematically Split Tree

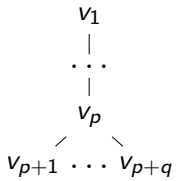
- *pq*-Gram: small subtree with stem and base
  Example: $p = 2$, $q = 3$
- Systematically split tree into *pq*-grams
- *pq*-Gram profile: set of all *pq*-grams of a tree.





Label Tuples

- Linear encoding of a *pq*-gram g with anchor node v_p:
  (traverse *pq*-gram in preorder)



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

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

$$\lambda(g) = (\lambda(v_1), \ldots, \lambda(v_{p+q}))$$

for the *pq*-gram $g = (v_1, \ldots, v_{p+q})$.

pq-Gram Index

Definition (*pq*-Gram Index)

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

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

- 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

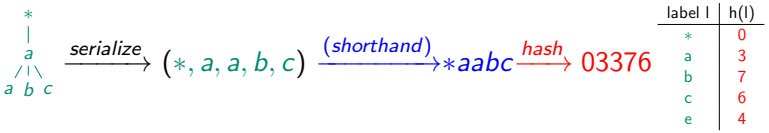
Storing the *pq*-Gram Index Efficiently

- 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: The *pq*-Gram Index

- pq-Gram profile:

- Hashing: map pq-gram to integer:



label l	h(l)
∗	0
a	3
b	7
c	6
e	4

Note: labels may be strings of arbitrary length!

- *pq*-Gram index: bag of hashed *pq*-grams

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

Intuition: similar trees have similar *pq*-gram indexes.

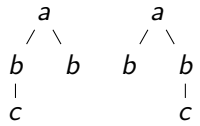
The *pq*-Gram Distance

Definition (*pq*-Gram Distance)

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

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

- Metric normalization to [0..1]: $\delta'_g(\mathsf{T}, \mathsf{T}') = \frac{\delta_g(\mathsf{T},\mathsf{T}')}{|\mathcal{I}(\mathsf{T}) \uplus \mathcal{I}(\mathsf{T}')| - |\mathcal{I}(\mathsf{T}) \intercal \mathcal{I}(\mathsf{T}')|}$
- 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:



Outline

Main Memory Algorithm (I)

CREATEINDEX(T, r, $\mathcal{I}$, *stem*, *p*, *q*)

stem := shift(*stem*, λ(r))
base: shift register of size q (filled with ∗)

if r is a leaf **then**
  $\mathcal{I} := \mathcal{I} \cup \{stem \circ base\}$
else
  for each child c (from left to right) of r **do**
    base := shift(*base*, λ(c))
    $\mathcal{I} := \mathcal{I} \cup \{stem \circ base\}$
    $\mathcal{I}$:= CREATEINDEX(T, c, $\mathcal{I}$, *stem*, *p*, *q*)
  for *k* := 1 **to** *q* − 1
    base := shift(*base*, ∗)
    $\mathcal{I} := \mathcal{I} \cup \{stem \circ base\}$

return $\mathcal{I}$

Main Memory Algorithm (II)

- Input of CREATEINDEX(T, r, $\mathcal{I}$, *stem*, p, q):
  - a subtree of T rooted in r
  - the *pq*-gram index $\mathcal{I}$ computed so far
  - the stem *stem* of r's parent
  - the parameters p and q
- Output of CREATEINDEX(T, r, $\mathcal{I}$, *stem*, p, q):
  pq-gram index including
  - the input index $\mathcal{I}$
  - the *pq*-gram index of r and all its descendants
    i.e., the *pq*-grams (label tuples) with anchor node r or a descendant of r

Main Memory Algorithm (III)

- *pq*-GRAM-INDEX(T, p, q) computes the *pq*-gram index for a complete tree T:

pq-GRAM-INDEX(T, p, q)

stem: shift register of size p (filled with $*$)
$\mathcal{I}$: empty index
$\mathcal{I}$ = CREATEINDEX(T, root(T), $\mathcal{I}$, *stem*, p, q)
return $\mathcal{I}$

Complexity of the *pq*-Gram Index Algorithm

Theorem (*pq*-Gram Index Complexity)

The pq-gram index of a tree T *with size* |T| *can be computed in* $O(|T|)$ *time.*

Proof.

Each recursive call of *createIndex*() processes one node in constant time, and each node is processed exactly once. □

Size of the *pq*-Gram Index

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

Let T *be a tree with* l *leaves and* i *non-leaves. The size of the pq-gram index of* T *is*

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

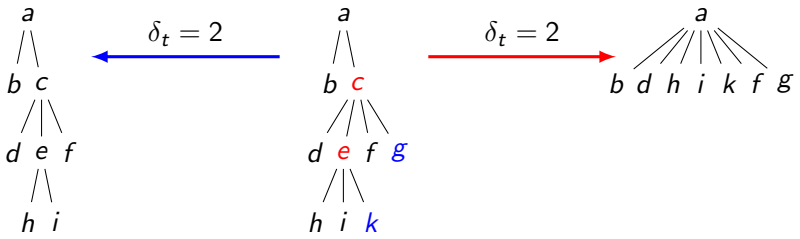
Proof.

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: $l + i(q-1) + (l + i - 1) = 2l + qi - 1$. □

Outline

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-leafs should have more weight than leafs.

Fanout Weighted Tree Edit Distance

Definition (Fanout Weighted Tree Edit Distance)

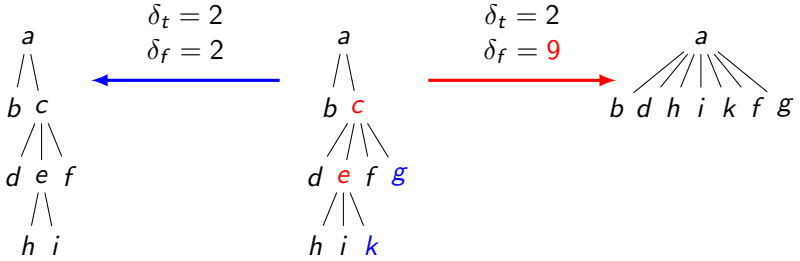
Let T and T′ be two trees, w ∈ N(T′) a node with fanout f, w′ ∈ N(T′) a node with fanout f', $c > 0$ a constant. The fanout weighted tree edit distance, $\delta_f = (\mathsf{T}, \mathsf{T}')$, between T and T′ is defined as the tree edit distance with the following costs for the edit operations:

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

- 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, T and T′,

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

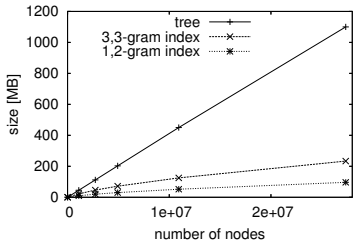
Proof.

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

Outline

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`.]

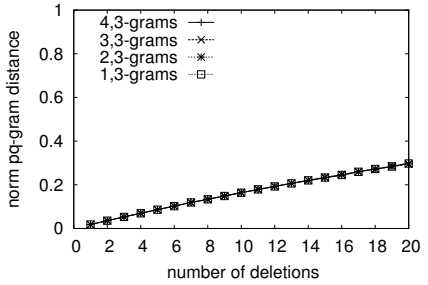
Why is the *pq*-gram index smaller than the tree?

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

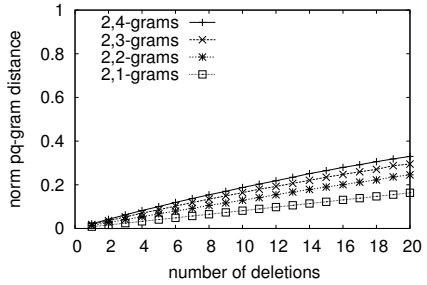
Sensitivity to Structure Change — Leaf

- Cost of leaf change → depends only on *q*
- Experiment:
  - delete leaf nodes
  - measure normalized *pq*-gram distance

vary *p*



vary *q*

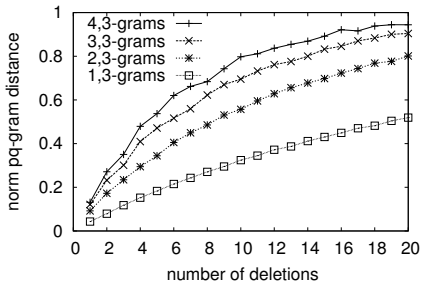


(Artificial tree with 144 nodes, 102 leaves, fanout 2–6 and depth 6. Average over 100 runs.)

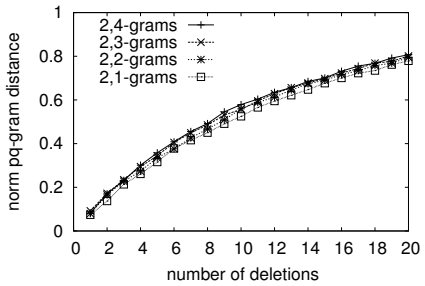
Sensitivity to Structure Change — Non-Leaf

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

vary p



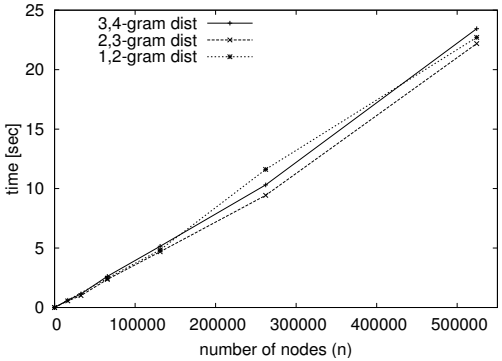
vary q



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

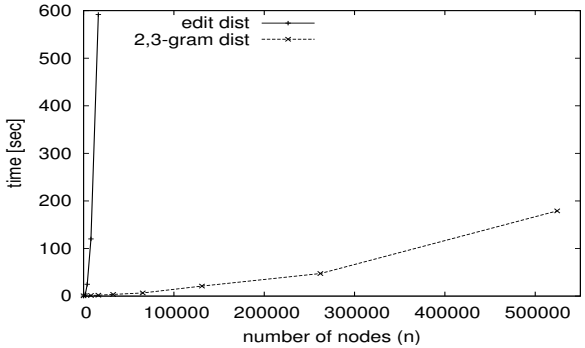
Influence of p and q on Scalability

- 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 5×10^5 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


Nikolaus Augsten, Michael Böhlen, and Johann Gamper.
Approximate matching of hierarchical data using *pq*-grams.
In *Proceedings of the International Conference on Very Large Databases (VLDB)*, pages 301–312, Trondheim, Norway, September 2005. ACM Press.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