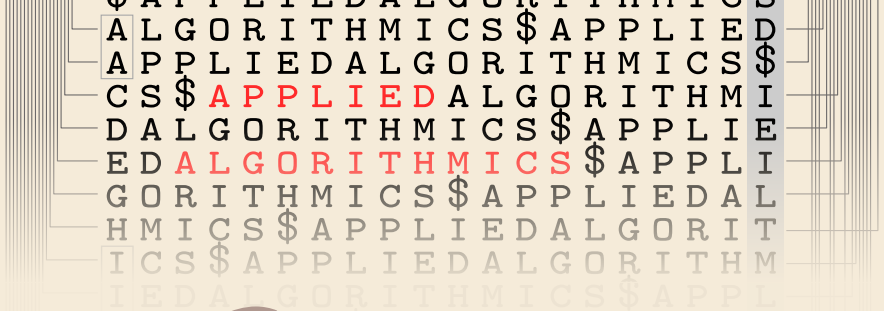

6 Text Indexing – Searching whole genomes

7 March 2022

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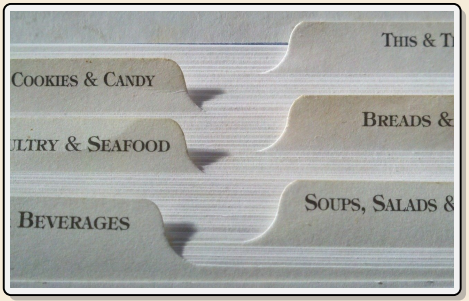
COMP526 (Spring 2022)
University of Liverpool
version **2022-03-07 21:18**

Learning Outcomes

1. Know and understand methods for text indexing: *inverted indices*, *suffix trees*, *(enhanced) suffix arrays*
2. Know and understand *generalized suffix trees*
3. Know properties, in particular *performance characteristics*, and limitations of the above data structures.
4. Design (simple) *algorithms based on suffix trees*.
5. Understand *construction algorithms* for suffix arrays and LCP arrays.

Unit 6: *Text Indexing*



Outline

6 Text Indexing

6.1 Motivation

Text indexing

- *Text indexing* (also: *offline text search*):
  - case of string matching: find $P[0..m)$ in $T[0..n)$
  - but with *fixed* text $\rightsquigarrow$ preprocess T (instead of P)
  - $\rightsquigarrow$ expect many queries P, answer them without looking at all of T
  - $\rightsquigarrow$ essentially a data structuring problem: "building an *index* of T"

Latin: "one who points out"

- application areas
  - web search engines
  - online dictionaries
  - online encyclopedia
  - DNA/RNA data bases
  - . . . searching in any collection of text documents (that grows only moderately)

Inverted indices

- original indices (same as "indexes") in books: list of (key) words $\mapsto$ page numbers where they occur
- assumption: searches are only for **whole** (key) **words**

$\rightsquigarrow$ often reasonable for natural language text

Inverted indices

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Inverted index:

- collect all words in T
  - can be as simple as splitting T at whitespace
  - actual implementations typically support *stemming* of words
    `goes` $\rightarrow$ `go`, `cats` $\rightarrow$ `cat`
- store mapping from words to a list of occurrences $\rightsquigarrow$ *how?*

could use BST ↳ $\Omega(\log n)$ too slow!

dictionary

keys = words

values = list of starting indices of occurrences

Clicker Question

Do you know what a *trie* is?

- **A** A what? No!
- **B** I have heard the term, but don't quite remember.
- **C** I remember hearing about it in a module.
- **D** Sure.

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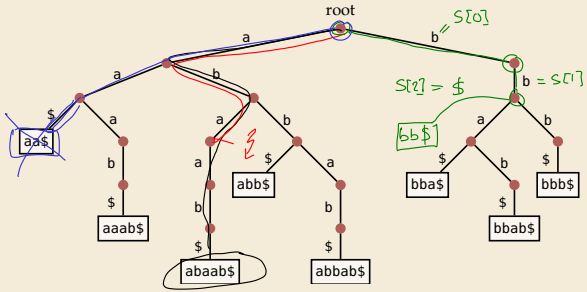
Tries

- efficient dictionary data structure for strings
- name from re**trie**val, but pronounced "try"
- tree based on symbol comparisons
- **Assumption:** stored strings are *prefix-free* (no string is a prefix of another)
  - strings of same length ✓
  - strings have "end-of-string" marker $ ✓ (some character $\notin \Sigma$)
- **Example**: $\Sigma = \{a, b\}$

  {aa$, aaab$, abaab$, abb$, abbab$, bba$, bbab$, bbb$}



insert S=bb$ aba$ ∉ ST

delete aa$

Clicker Question

does the string occur?

Suppose we have a trie that stores n strings over $\Sigma = \{\texttt{A}, \ldots, \texttt{Z}\}$. Each stored string consists of m characters.
We now search for a query string Q with $|Q| = q$ (with $q \leq m$).
How many **nodes** in the trie are **visited** during this **query**?

A	$\Theta(\log n)$	**F**	$\Theta(\log m)$
B	$\Theta(\log(nm))$	**G**	$\Theta(q)$
C	$\Theta(m \cdot \log n)$	**H**	$\Theta(\log q)$
D	$\Theta(m + \log n)$	**I**	$\Theta(q \cdot \log n)$
E	$\Theta(m)$	**J**	$\Theta(q + \log n)$

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Clicker Question

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F ~~$\Theta(\log m)$~~

G $\Theta(q)$ ✓

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I ~~$\Theta(q \cdot \log n)$~~

J ~~$\Theta(q + \log n)$~~

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Clicker Question

Suppose we have a trie that stores n strings over $\Sigma = \{\texttt{A}, \ldots, \texttt{Z}\}$. Each stored string consists of m characters.
How many **nodes** does the trie have **in total** *in the worst case*?

A $\Theta(n)$

B $\Theta(n + m)$

C $\Theta(n \cdot m)$

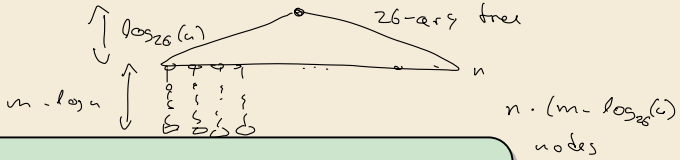
D $\Theta(n \log m)$

E $\Theta(m)$

F $\Theta(m \log n)$

sli.do/comp526

Clicker Question



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E ~~$\Theta(m)$~~

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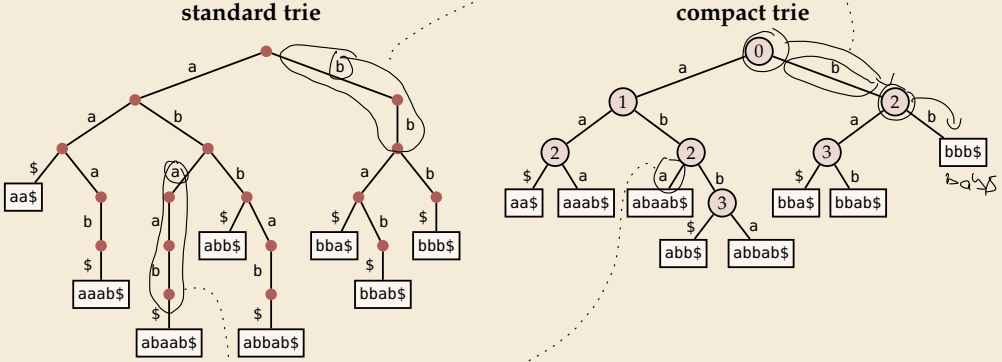
Compact tries

=1 child

- compress paths of unary nodes into single edge
- nodes store *index* of next character to check



- searching slightly trickier, but same time complexity as in trie
- all nodes ≥ 2 children ⇝ #nodes ≤ #leaves = #strings ⇝ linear space

Tries as inverted index


simple


fast lookup


cannot handle more general queries:

- search part of a word
- search phrase (sequence of words)

Tries as inverted index

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cannot handle more general queries:

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what if the 'text' does not even have words to begin with?!

- biological sequences

```
ACAAGATGCCATTGTCCCCCGGCCTCCTGCTGCTGCTGCTCTCCGGGGCCACGGCCACCGCTGCCCTGCCCCTGGAGGGTGGCCCCACCGGC
CGAGACAGCGAGCATATGCAGGAAGCGGCAGGAATAAGGAAAAGCAGCCTCCTGACTTTCCTCGCTTGGTGGTTTGAGTGGACCTCCCAGGC
CAGTGCCGGGCCCCTCATAGGAGAGGAAGCTCGGGAGGTGGCCAGGCGGCAGGAAGGCGCACCCCCCCAGCAATCCGCGCGCCGGGACAGAA
TGCCCTGCAGGAACTTCTTCTGGAAGACCTTCTCCTCCTGCAAATAAAACCTCACCCATGAATGCTCACGCAAGTTTAATTACAGACCTGAA
```

- binary streams

```
00000010101001111010111000001111100011111011111001101101000011100010011011110000010001101010
01101100001101011010000000100000000111010110000010000111101011101100100011001011011101111111
11000101000101100101000000111010101001100000000111011000011001111100000101 01010111011110000111
10101110010010101010100000011111010011000000111100110101000000010010010000010110001100011011 1
```

need new ideas

6.2 Suffix Trees

Suffix trees – A 'magic' data structure

Appetizer: Longest common substring problem

- Given: strings $S_1, \ldots, S_k$ **Example:** S_1 = superiorcalifornialives, S_2 = sealiver
- Goal: find the longest substring that occurs in all k strings

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Can we do this in time $O(|S_1| + \cdots + |S_k|)$? How??

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Can we do this in time $O(|S_1| + \cdots + |S_k|)$? How??

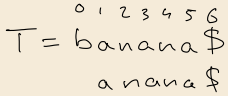
Enter: ***suffix trees***

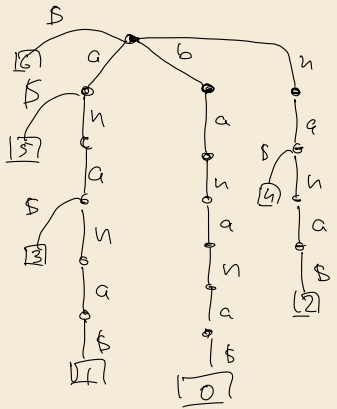
- versatile data structure for index with full-text search
- linear time (for construction) and linear space
- allows efficient solutions for many advanced string problems

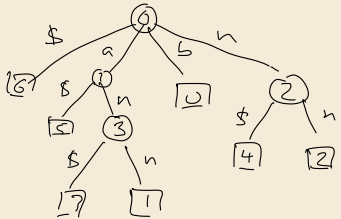
"Although the longest common substring problem looks trivial now, given our knowledge of suffix trees, it is very interesting to note that in 1970 Don Knuth conjectured that a linear-time algorithm for this problem would be impossible." *[Gusfield: Algorithms on Strings, Trees, and Sequences (1997)]*

Suffix trees – Definition

- suffix tree $\mathcal{T}$ for text $T = T[0..n)$ = compact trie of all suffixes of $T\$$ (set $T[n] := \$$)







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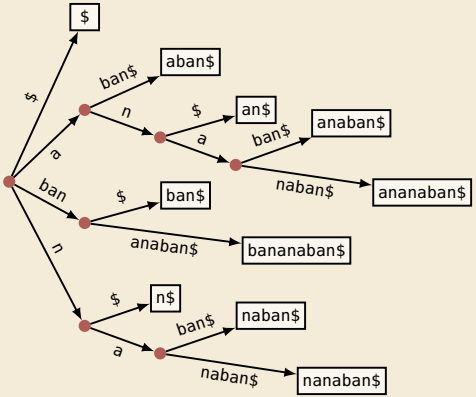
Example:

T = bananaban$

suffixes: {bananaban$, ananaban$, nanaban$, anaban$, naban$, aban$, ban$, an$, n$, $}

	0	1	2	3	4	5	6	7	8	9
T =	b	a	n	a	n	a	b	a	n	$



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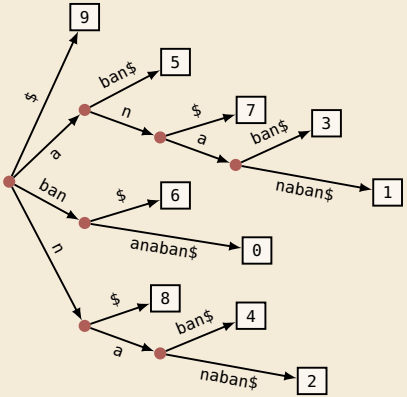

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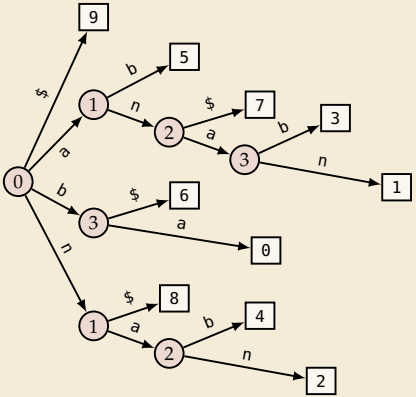
- also: edge labels like in compact trie
- (more readable form on slides to explain algorithms)



Suffix trees – Construction

- $T[0..n]$ has $n+1$ suffixes (starting at character $i \in [0..n]$)
- We can build the suffix tree by inserting each suffix of T into a compressed trie.
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same order of growth as reading the text!

Amazing result: Can construct the suffix tree of T in $\Theta(n)$ time!

- algorithms are a bit tricky to understand
- but were a theoretical breakthrough
- and they are efficient in practice (and heavily used)!

$\rightsquigarrow$ for now, take linear-time construction for granted. What can we do with them?

Clicker Question

Recap: Check all correct statements about suffix tree $\mathcal{T}$ of $T[0..n)$.

- **A** We require T to end with \$.
- **B** The size of $\mathcal{T}$ can be $\Omega(n^2)$ in the worst case.
- **C** $\mathcal{T}$ is a standard trie of all suffixes of $T\$$.
- **D** $\mathcal{T}$ is a compact trie of all suffixes of $T\$$.
- **E** The leaves of $\mathcal{T}$ store (a copy of) a suffix of $T\$$.
- **F** Naive construction of $\mathcal{T}$ takes $\Omega(n^2)$ (worst case).
- **G** $\mathcal{T}$ can be computed in $O(n)$ time (worst case).
- **H** $\mathcal{T}$ has n leaves.

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- **H** ~~$\mathcal{T}$ has n leaves.~~

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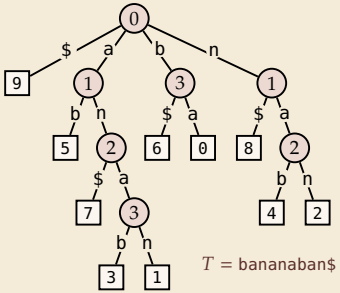
6.3 Applications

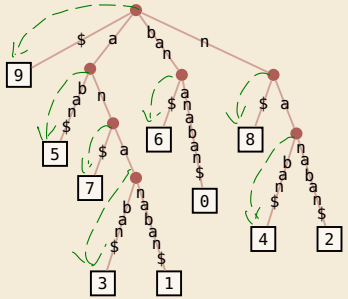
Applications of suffix trees

- In this section, always assume suffix tree $\mathcal{T}$ for T given.

Recall: $\mathcal{T}$ stored like this:

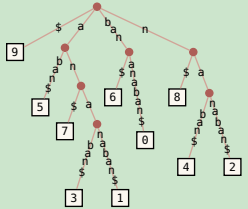


but think about this:



- Moreover: assume internal nodes store pointer to *leftmost leaf in subtree*.
- Notation: $T_i = T[i..n]$ (including \$)

Clicker Question



What does T's suffix tree (on the left) tell you about the question whether T contains the pattern $P = \texttt{ana}$?

Check all that apply to this example.

A Nothing.

B P occurs in T.

C P does not occur in T.

D P occurs once in T.

E P occurs twice in T.

F P starts at index 0.

G P starts at index 1.

H P starts at index 2.

I P starts at index 3.

J P starts at index 4.

K P starts at index 7.

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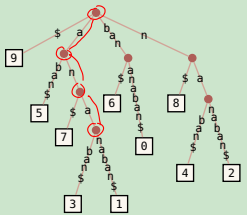
Clicker Question



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Application 1: Text Indexing / String Matching

- P occurs in $T \iff P$ is a prefix of a suffix of T
- we have all suffixes in $\mathcal{T}$!

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$\rightsquigarrow$ (try to) follow path with label P, until

1. **we get stuck**
   at internal node (no node with next character of P)
   or *inside edge* (mismatch of next characters)
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2. **we run out of pattern**
   reach end of P at internal node v or inside edge towards v
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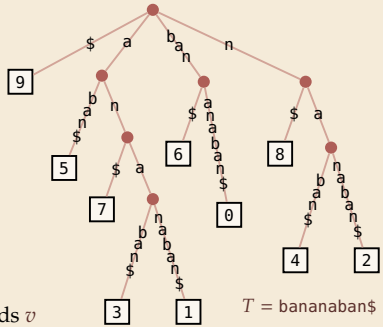
   reach a leaf ℓ with part of P left $\rightsquigarrow$ compare P to ℓ.



⚠ This cannot happen when testing edge labels since $\$ \notin \Sigma$, but needs check(s) in compact trie implementation!

- Finding first match (or `NO_MATCH`) takes $O(|P|)$ time!

follow leftmost_leaf pointer

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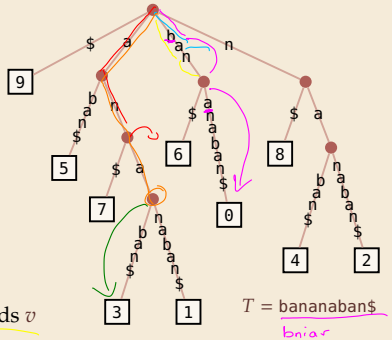


Examples:

- P = ann
- P = baa
- P = ana
- P = ba
- P = briar

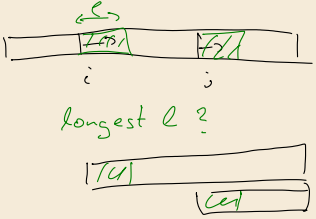
notice mismatch only in leaf

Application 2: Longest repeated substring

- **Goal:** Find longest substring $T[i..i+\ell)$ that occurs also at $j \neq i$: $T[j..j+\ell) = T[i..i+\ell)$.

e. g. for compression ⇝ Unit 7

How can we efficiently check *all possible substrings?*



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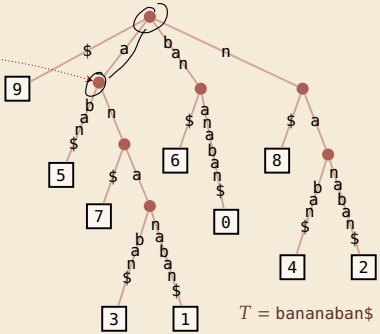
Repeated substrings = shared paths in *suffix tree*

- T_5 = aban$ and T_7 = an$ have *longest common prefix* 'a'

⇝ ∃ internal node with path label 'a'

here single edge, can be longer path



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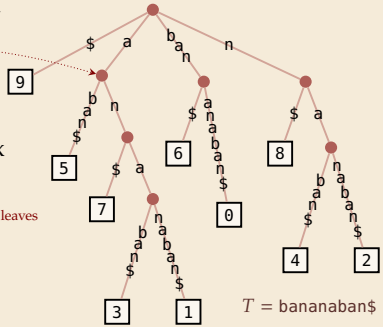
⇝ longest repeated substring = longest common prefix (LCP) of two suffixes

actually: adjacent leaves



Application 2: Longest repeated substring

- **Goal:** Find longest substring $T[i..i+\ell)$ that occurs also at $j \neq i$: $T[j..j+\ell) = T[i..i+\ell)$.

e. g. for compression ⇝ Unit 7

How can we efficiently check *all possible substrings?*

Repeated substrings = shared paths in *suffix tree*

- T_5 = aban$ and T_7 = an$ have *longest common prefix* 'a'

⇝ ∃ internal node with path label 'a'

here single edge, can be longer path

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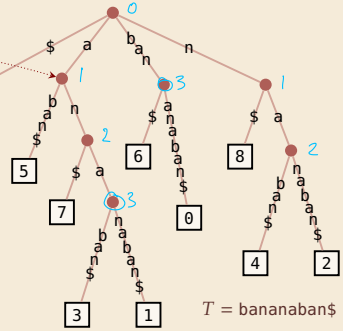

- Algorithm:
  1. Compute *string depth* (=length of path label) of nodes
  2. Find internal nodes with maximal string depth
- Both can be done in depth-first traversal ⇝ $\Theta(n)$ time

Generalized suffix trees

- longest *repeated* substring (of one string) feels very similar to
  longest *common* substring of several strings $T^{(1)}, \ldots, T^{(k)}$ with $T^{(j)} \in \Sigma^{n_j}$
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Enter: ***generalized suffix tree***

- Define $T := T^{(1)}\$_1 T^{(2)}\$_2 \cdots T^{(k)}\$_k$ for k new end-of-word symbols
- Construct suffix tree $\mathcal{T}$ for T

$\rightsquigarrow$ $\$_j$-edges always leads to leaves $\rightsquigarrow$ $\exists$ leaf (j, i) for each suffix $T_i^{(j)} = T^{(j)}[i..n_j]$

Clicker Question

What is the longest common substring of the strings `bcabcac`, `aabcca` and `bcaa`?

sli.do/comp526

Application 3: Longest common substring

- With that new idea, we can find longest common substrings:
  1. Compute generalized suffix tree $\mathcal{T}$.
  2. Store with each node the *subset of strings* that contain its path label:
     - 2.1. Traverse $\mathcal{T}$ bottom-up.
     - 2.2. For a leaf (j, i), the subset is $\{j\}$.
     - 2.3. For an internal node, the subset is the union of its children.
  3. In top-down traversal, compute *string depths* of nodes. (as above)
  4. Report deepest node (by string depth) whose subset is $\{1, \ldots, k\}$.

$O(n)$ time

- Each step takes time $\Theta(n)$ for $n = n_1 + \cdots + n_k$ the total length of all texts.

"Although the longest common substring problem looks trivial now, given our knowledge of suffix trees, it is very interesting to note that in 1970 Don Knuth conjectured that a linear-time algorithm for this problem would be impossible." *[Gusfield: Algorithms on Strings, Trees, and Sequences (1997)]*

Longest common substring – Example

$T^{(1)}$ = bcabcac, $T^{(2)}$ = aabca, $T^{(3)}$ = bcaa