ALGORITHMICS\$APPLIED

APPLIEDALGORITHMICS\$

CS\$APPLIEDALGORITHMI

DALGORITHMICS\$APPLIE

EDALGORITHMICS\$APPLIE

GORITHMICS\$APPLIEDAL

HMICS\$APPLIEDALGORIT

ICS\$APPLIEDALGORITHM

6

Text Indexing – Searching whole genomes

9 March 2020

Sebastian Wild

Outline

6 Text Indexing

- 6.1 Motivation
- 6.2 Suffix Trees
- 6.3 Applications
- 6.4 Longest Common Extensions
- 6.5 Suffix Arrays
- 6.6 The LCP Array

6.1 Motivation

Text indexing

- ► *Text indexing* (also: *offline text search*):
 - case of string matching: find P[0..m-1] in T[0..n-1]
 - ▶ but with *fixed* text \rightarrow preprocess T (instead of P)
 - \rightarrow expect many queries P, answer them without looking at all of T
 - \leadsto 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

- same as "indexes"
- ▶ original indices in books: list of (key) words → page numbers where they occur
- ► assumption: searches are only for **whole** (key) **words**
- \leadsto often reasonable for natural language text

Inverted indices

- ▶ original indices in books: list of (key) words → page numbers where they occur
- ▶ assumption: searches are only for whole (key) words
- → often reasonable for natural language text

Inverted index:

- ightharpoonup collect all words in T
 - ightharpoonup can be as simple as splitting T at whitespace
 - actual implementations typically support stemming of words goes → go, cats → cat
- ► store mapping from words to a list of occurrences ~ (how? ______ 857

Clicker Question

Do you know what a *trie* is?



- 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.

Tries

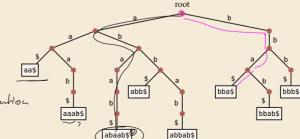
(aa,a)

- efficient dictionary data structure for strings
- ▶ name from retrieval, 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 some character $\notin \Sigma$
 - strings have "end-of-string" marker \$
- ► Example:

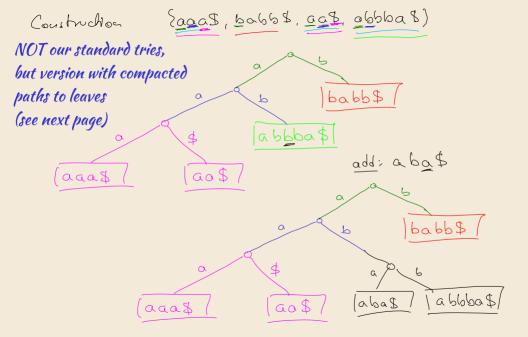
{aa\$, aaab\$, abaab\$, abb\$,
abbab\$, bba\$, bbab\$, bbb\$}

o construction: lop-down

independent of order of intertions of query: (get)ex: lobas







Trie construction (correct version)

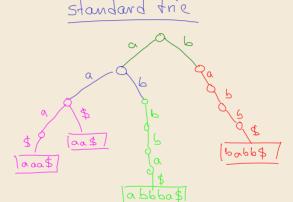
(aaa\$

{aaa\$, ba66\$, aa\$, a666a8)

tric with composted porths to leaves



(ao\$ 7



Clicker Question

Suppose we have a trie that stores n strings over $\Sigma = \{A, ..., Z\}$. Each stored string consists of m characters.

We now search for a query string Q with |Q| = q.

How many **nodes** in the trie are **visited** during this **query**?



 $\mathbf{B} \quad \Theta(\log(nm))$

 $\mathbf{G} \ \Theta(q)$

 \bigcirc $\Theta(m \cdot \log n)$

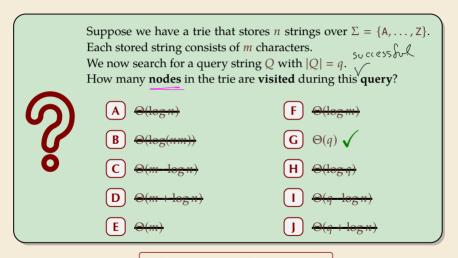
 $\Theta(\log q)$

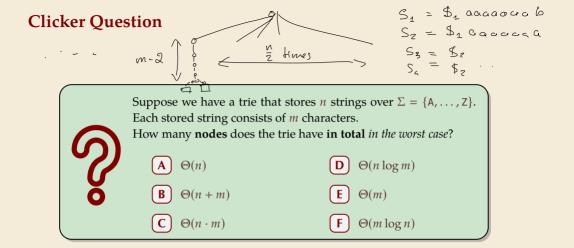
 $\mathbf{D} \quad \Theta(m + \log n)$

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

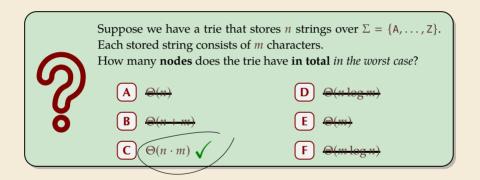
 $[\mathbf{E}] \Theta(m)$

Clicker Question



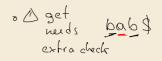


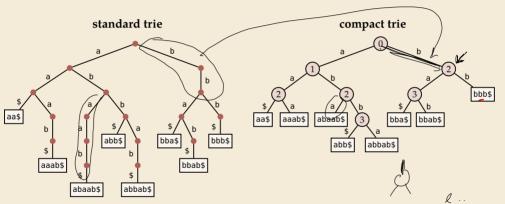
Clicker Question



Compact tries

- =1 child
- compress paths of unary nodes into single edge
- nodes store index of next character





- $\rightsquigarrow\,$ searching slightly trickier, but same time complexity as in trie
- ▶ all $nodes \ge 2$ children \rightsquigarrow $\#nodes \le \#leaves = \#strings <math>\rightsquigarrow$ linear space

O(n) O(nm)

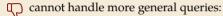
Tries as inverted index

- simple
- fast lookup
- cannot handle more general queries:
 - search part of a word
 - ► search phrase (sequence of words)

Tries as inverted index



fast lookup



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

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

biological sequences

binary streams

6.2 Suffix Trees

Suffix trees – A 'magic' data structure

Appetizer: Longest common substring problem

► Given: strings $S_1, ..., S_k$ Example: S_1 = superiorcalifornialives, S_2 = sealiver

▶ Goal: find the longest substring that occurs in all *k* strings

Suffix trees – A 'magic' data structure

Appetizer: Longest common substring problem

- ▶ Given: strings $S_1, ..., S_k$ Example: S_1 = superiorcalifornialives, S_2 = sealiver
- ► Goal: find the longest substring that occurs in all *k* strings → alive



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

Suffix trees – A 'magic' data structure

Appetizer: Longest common substring problem

- ► Given: strings $S_1, ..., S_k$ Example: S_1 = superiorcalifornializes, S_2 = sealizer
- ▶ Goal: find the longest substring that occurs in all k strings \rightarrow alive



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



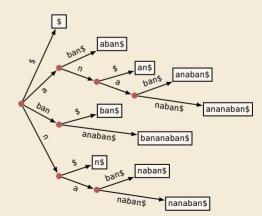
"Although the longest common substring problem looks trivial now, given our knowledge of suffix trees, it is very interesting to note that in 1970 <u>Don Knuth</u> conjectured that a linear-time algorithm for this problem would be impossible." [Gusfield: Algorithms on Strings, Trees, and Sequences (1997)]

suffix tree \mathcal{T} for text $T = T[0..n-1] = \text{compact trie of all suffixes of } \underline{T} \text{ (set } T[n] := \$)$

► suffix tree \Im for text T = T[0..n - 1] = compact trie of all suffixes of T\$ (set <math>T[n] := \$)

Example:

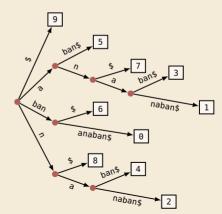
 $T = \mbox{bananaban\$} \\ suffixes: \{ \mbox{bananaban\$}, \mbox{nanaban\$}, \mbox{nanaban$Anaban$}, \mbox{nanaban$Anaban$}, \mbox{nanaban$Anaban$}, \mbox{nanaban$Anaban$}, \mbox{nanaban$}, \mbox{nanaban$}, \mbox{nanaban$}, \mbox{$



- ▶ suffix tree \Im for text T = T[0..n 1] = compact trie of all suffixes of T\$ (set <math>T[n] := \$)
- except: in leaves, store start index (instead of actual string)

Example:

 $T = \mbox{bananaban\$} \\ suffixes: \{ \mbox{bananaban\$}, \mbox{ananaban\$}, \mbox{nanaban\$}, \mbox{nanaban$Anaban$}, \mbox{nanaban$Anaban$}, \mbox{nanaban$Anaban$}, \mbox{nanaban$Anaban$}, \mbox$

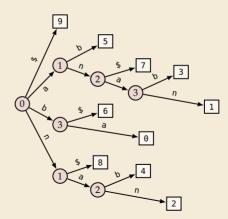


- ► suffix tree \mathcal{T} for text T = T[0..n 1] = compact trie of all suffixes of T\$ (set <math>T[n] := \$)
- except: in leaves, store *start index* (instead of actual string)

Example:

T = bananaban\$

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



Suffix trees – Construction

- ► T[0..n-1] 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. But that takes time $\Theta(n^2)$. \longrightarrow not interesting!



Suffix trees – Construction

- ► T[0..n-1] 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. But that takes time $\Theta(n^2)$. \leadsto not interesting!



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)!

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

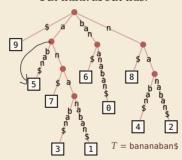
6.3 Applications

Applications of suffix trees

▶ In this section, always assume suffix tree \Im for T given.

Recall: T stored like this:

9 1 3 1 5 2 6 0 8 2 7 3 4 2 but think about this:



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

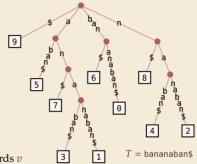
Application 1: Text Indexing / String Matching

- \blacktriangleright we have all suffixes in T!

Application 1: Text Indexing / String Matching

- ▶ P occurs in $T \iff P$ is a prefix of a suffix of T
- \blacktriangleright we have all suffixes in $\Im!$
- \rightsquigarrow (try to) follow path with label P, until
 - we get stuck

 at internal node (no node with next character of P)
 or inside edge (mismatch of next characters)
 P does not occur in T
 - we run out of pattern
 reach end of P at internal node v or inside edge towards v
 P occurs at all leaves in subtree of v
 - we run out of tree
 we reach a leaf ℓ with part of P left → P does not occur.
- ▶ Finding first match (or NO MATCH) takes O(|P|) time!



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 T!
- \rightsquigarrow (try to) follow path with label P, until
 - 1. we get stuck
- \sim *at internal node* (no node with next character of *P*)
- bb or *inside edge* (mismatch of next characters)
 - \rightarrow P does not occur in T
- \rightarrow 2. we run out of pattern

reach end of P at internal node v or inside edge towards v

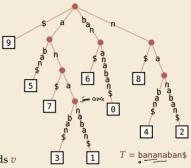
- \rightarrow *P* occurs at all leaves in subtree of v
- 3. we run out of tree

we reach a leaf ℓ with part of P left \longrightarrow P does not occur.



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

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



Examples:

- ightharpoonup P = ann
- ightharpoonup P = ana
- ightharpoonup P = briar

▶ **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?
```

▶ **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 \rightsquigarrow Unit 7



How can we efficiently check all possible substrings?

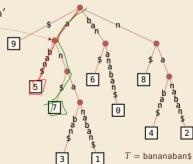


Repeated substrings = shared paths in *suffix tree*

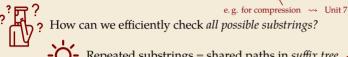


- ▶ T_5 = aban\$ and T_7 = an\$ have longest common prefix 'a'
- → ∃ internal node with path label 'a'

here single edge, can be longer path



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



Repeated substrings = shared paths in *suffix tree*



- $ightharpoonup T_5$ = aban\$ and T_7 = an\$ have longest common prefix 'a'
- → ∃ internal node with path label 'a'

here single edge, can be longer path

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

actually: adjacent leaves





▶ **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 \rightsquigarrow Unit 7

9



How can we efficiently check all possible substrings?



Repeated substrings = shared paths in *suffix tree*

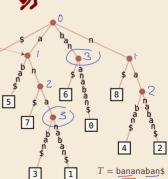


- ► T_5 = aban\$ and T_7 = an\$ have longest common prefix 'a'
- → ∃ internal node with path label 'a'

here single edge, can be longer path

- → longest repeated substring = longest common prefix (LCP) of two suffixes
 - actually: adjacent leaves

- ► 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 \rightsquigarrow $\Theta(n)$ 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 $T^{(j)} \in \Sigma^{n_j}$
- ► can we solve that in the same way?
- ightharpoonup could build the suffix tree for each $T^{(j)}$... but doesn't seem to help

Generalized suffix trees

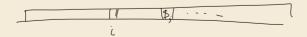
- ▶ longest *repeated* substring (of one string) feels very similar to longest *common* substring of several strings $T^{(1)}, \ldots, T^{(k)}$ with $T^{(j)} \in \Sigma^{n_j}$
- can we solve that in the same way?
- ightharpoonup could build the suffix tree for each $T^{(j)}$... but doesn't seem to help
- → need a single/joint suffix tree for several texts

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 $T^{(j)} \in \Sigma^{n_j}$
- can we solve that in the same way?
- ightharpoonup could build the suffix tree for each $T^{(j)}$... but doesn't seem to help
- → need a single/joint suffix tree for several texts

Enter: generalized suffix tree

- ▶ Define $T := T^{(1)} \$_1 T^{(2)} \$_2 \cdots T^{(k)} \$_k$ for k new end-of-word symbols
- ightharpoonup Construct suffix tree \mathfrak{T} for T
- \Rightarrow \$j-edges always leads to leaves \Rightarrow \exists leaf (j,i) for each suffix $T_i^{(j)} = T^{(j)}[i..n_j]$





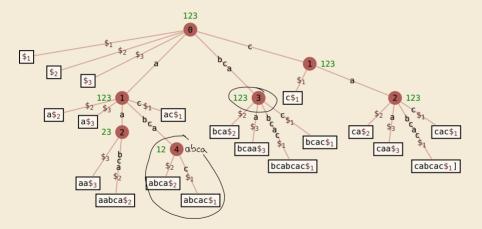
Application 3: Longest common substring

- ▶ With that new idea, we can find longest common superstrings:
 - **1.** Compute generalized suffix tree \mathcal{T} .
 - **2.** Store with each node the *subset of strings* that contain its path label:
 - 2.1. Traverse 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 $\{1, \ldots, k\}$.
- ▶ Each step takes time $\Theta(n)$ for $n = n_1 + \cdots + n_k$ the total length of all texts.

[&]quot;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

$$T^{(1)} = bcabcac$$
, $T^{(2)} = aabca$, $T^{(3)} = bcaa$ $T = bcabcac $_1 aabca $_2 bcaa $_3$



6.4 Longest Common Extensions

Application 4: Longest Common Extensions

▶ We implicitly used a special case of a more general, versatile idea:

The *longest common extension (LCE)* data structure:

```
► Given: String T[0..n-1]
```

► Goal: Answer LCE queries, i. e., given positions i, j in T, how far can we read the same text from there? formally: LCE(i, j) = max{\(\ell : T[i..i + \ell) = T[i..i + \ell)\)}

Application 4: Longest Common Extensions

▶ We implicitly used a special case of a more general, versatile idea:

The *longest common extension (LCE)* data structure:

- ▶ **Given:** String T[0..n-1]
- ► **Goal:** Answer LCE queries, i. e., given positions *i*, *j* in *T*,

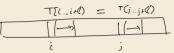
how far can we read the same text from there?

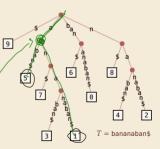
formally: LCE
$$(i, j) = \max\{\ell : T[i..i + \ell) = T[j..j + \ell)\}$$

 \rightsquigarrow use suffix tree of T!

longest common prefix of *i*th and *j*th suffix

- ► In \mathfrak{T} : LCE $(i, j) = \text{LCP}(T_i, T_j) \rightsquigarrow \text{same thing, different name!}$ = string depth of lowest common ancester (LCA) of leaves i and j
- ▶ in short: $LCE(i, j) = LCP(T_i, T_j) = stringDepth(LCA(i, j))$







Efficient LCA

How to find lowest common ancestors?

- ► Could walk up the tree to find LCA \rightsquigarrow $\Theta(n)$ worst case \bigcirc
- ► Could store all LCAs in big table \rightarrow $\Theta(n^2)$ space and preprocessing ∇

Efficient LCA

How to find lowest common ancestors?

- ► Could walk up the tree to find LCA \rightsquigarrow $\Theta(n)$ worst case
- ► Could store all LCAs in big table \rightsquigarrow $\Theta(n^2)$ space and preprocessing



Amazing result: Can compute data structure in $\Theta(n)$ time and space that finds any LCA is **constant(!)** time.

- ▶ a bit tricky to understand
- but a theoretical breakthrough
- and useful in practice



 \rightsquigarrow for now, use O(1) LCA as black box.



 \rightarrow After linear preprocessing (time & space), we can find LCEs in O(1) time.

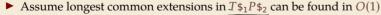
Application 5: Approximate matching

k-mismatch matching:

- ▶ **Input:** text T[0..n-1], pattern P[0..m-1], $k \in [0..m)$
- ► Output:

"Hamming distance $\leq k$ "

- \blacktriangleright smallest *i* so that T[i..i + m) are *P* differ in at most *k* characters
- ightharpoonup or NO_MATCH if there is no such i
- → searching with typos



- → generalized suffix tree T has been built
- → string depths of all internal nodes have been computed



Clicker Question



What is the Hamming distance between heart and beard?

pingo.upb.de/622222

Kangaroo Algorithm for approximate matching



```
procedure kMismatch(T[0..n-1], P[0..m-1])

// build LCE data structure

for i := 0, ..., n-m-1 do

mismatches := 0; t := i; p := 0

while mismatches \le k \land p < m do

\ell := LCE(t, p) // jump \ over \ matching \ part

t := t + \ell + 1; \ p := p + \ell + 1

mismatches := mismatches + 1

if p == m then

return i
```

brute forc O(n.m)

- ▶ **Analysis:** $\Theta(n+m)$ preprocessing + $O(n \cdot k)$ matching
- \rightsquigarrow very efficient for small k
- ► State of the art
 - $ightharpoonup O(n^{\frac{k^2 \log k}{m}})$ possible with complicated algorithms
 - ightharpoonup extensions for edit distance $\leq k$ possible

Application 6: Matching with wildcards

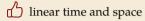
- ► Allow a wildcard character in pattern stands for arbitrary (single) character unit* P
 in_unit5_uwe_uwill T
- ▶ similar algorithm as for *k*-mismatch \rightsquigarrow $O(n \cdot k + m)$ when *P* has *k* wildcards

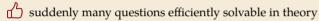
Many more applications, in particular for problems on biological sequences

20+ described in Gusfield, Algorithms on strings, trees, and sequences (1999)

Suffix trees – Discussion

► Suffix trees were a threshold invention







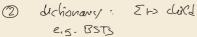
Suffix trees – Discussion

- ► Suffix trees were a threshold invention
- linear time and space
- suddenly many questions efficiently solvable in theory



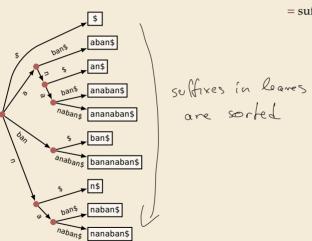
- construction of suffix trees: linear time, but significant overhead
- construction methods fairly complicated
- many pointers in tree incur large space overhead





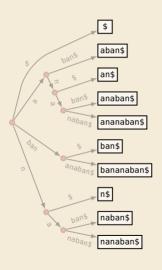
6.5 Suffix Arrays

Putting suffix trees on a diet



Observation: order of leaves in suffix tree= suffixes lexicographically sorted

Putting suffix trees on a diet



- ➤ **Observation:** order of leaves in suffix tree = suffixes lexicographically *sorted*
- ▶ Idea: only store list of leaves L[0..n]
- ► Enough to do efficient string matching!
 - **1.** Use binary search for pattern *P*
 - **2.** check if *P* is prefix of suffix after found position
- **Example:** P =ana

Putting suffix trees on a diet

