

COMP526 (Fall 2022) University of Liverpool version 2022-11-08 22:19 H

Learning Outcomes

- 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
- 6.2 Suffix Trees
- 6.3 Applications
- 6.4 Longest Common Extensions
- 6.5 Suffix Arrays
- 6.6 Linear-Time Suffix Sorting: Overview
- 6.7 Linear-Time Suffix Sorting: The DC3 Algorithm
- 6.8 The LCP Array
- 6.9 LCP Array Construction

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

same as "indexes"

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

Inverted index:

- collect all words in T
 - 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?

Tries

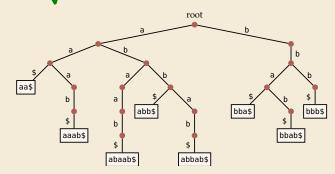
- efficient dictionary data structure for strings
- name from retrieval, but pronounced "try"
- tree based on symbol comparisons
- Assumption: stored strings are *prefix-free* (no string is a prefix of another)

some character $\notin \Sigma$

- strings of same length
- strings have "end-of-string" marker \$



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

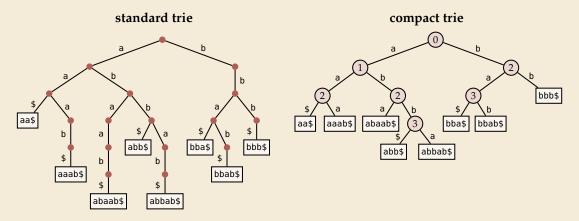


Compact tries

compress paths of unary nodes into single edge

=1 child

nodes store *index* of next character to check



→ searching slightly trickier, but same time complexity as in trie

▶ all nodes \geq 2 children \rightsquigarrow #nodes \leq #leaves = #strings \rightsquigarrow linear space

Tries as inverted index

simple

🖒 fast lookup

C cannot handle more general queries:

- 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

→ 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: $S_1 = \text{superiorcalifornialives}, S_2 = \text{sealiver}$
- ► Goal: find the longest substring that occurs in all *k* strings

→ 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 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

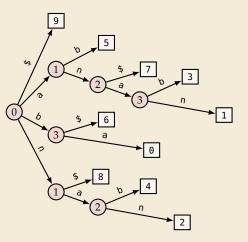
suffix tree \mathcal{T} for text T = T[0..n) = compact trie of all suffixes of T\$ (set <math>T[n] := \$)

except: in leaves, store *start index* (instead of copy of actual string)

Example:

```
T = bananaban$
suffixes: {bananaban$, ananaban$, nanaban$, anaban$, anaban$, ananaban$, anaban$, an
```

- ▶ 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. But that takes time Θ(n²). → not interesting!



same order of growth as reading the text! **Amazing result:** Can construct the suffix tree of *T* in $\Theta(n)$ time!

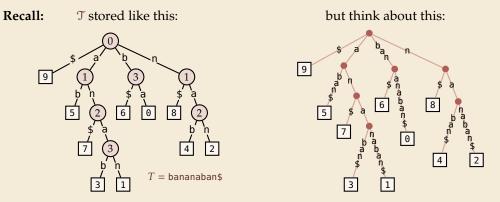
- algorithms are a bit tricky to understand
- but were a theoretical breakthrough
- and they are efficient in practice (and heavily used)!

→ 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 T for T given.



▶ Moreover: assume internal nodes store pointer to *leftmost leaf in subtree*.

• Notation: $T_i = T[i..n]$ (including \$)

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

at internal node (no node with next character of *P*) or *inside edge* (mismatch of next characters)

- \rightsquigarrow *P* does not occur in *T*
- 2. we run out of pattern

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

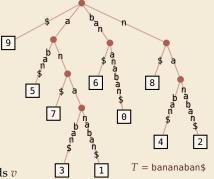
- \rightsquigarrow *P* occurs at all leaves in subtree of *v*
- 3. we run out of tree

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!

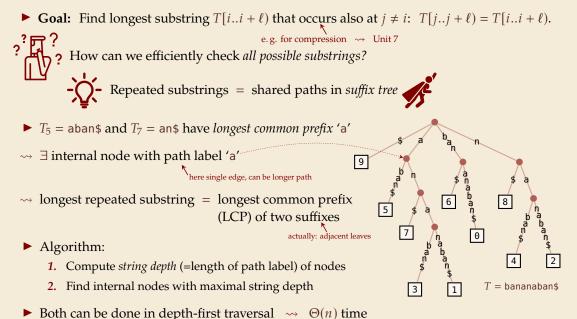


Examples:



- P = baa
- ▶ *P* = ana
- ▶ *P* = ba
- ▶ P = briar

Application 2: Longest repeated substring



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?
- 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
- Construct suffix tree T for T

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



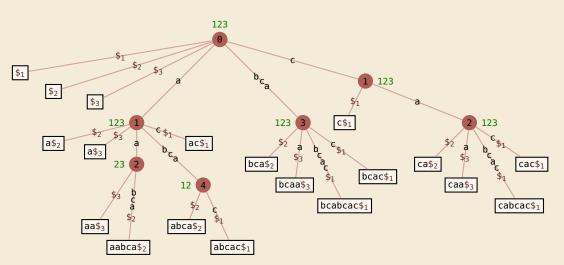
Application 3: Longest common substring

- With that new idea, we can find longest common 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 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.

"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

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



6.4 Longest Common Extensions

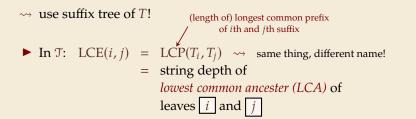
Application 4: Longest Common Extensions

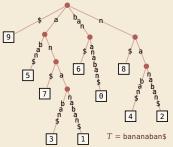
• We implicitly used a special case of a more general, versatile idea:

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

- ► **Given:** String *T*[0..*n*)
- ► 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{ $\ell : T[i..i + \ell) = T[j..j + \ell)$ }





▶ 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
- Could store all LCAs in big table $\rightsquigarrow \Theta(n^2)$ space and preprocessing \square



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

and suffix tree construction inside . .



 \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), pattern P[0..m), $k \in [0..m)$
- ▶ Output: "Hamming distance ≤ k"
 ▶ smallest i so that T[i..i + m) are P differ in at most k characters
 - or NO_MATCH if there is no such i

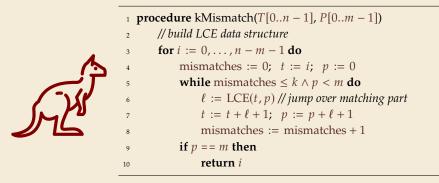
 \rightsquigarrow searching with typos

• Adapted brute-force algorithm $\rightsquigarrow O(n \cdot m)$

• Assume longest common extensions in T_{P}^{2} can be found in O(1)

- $\rightsquigarrow~$ generalized suffix tree $\mathbb T$ has been built
- $\rightsquigarrow~$ string depths of all internal nodes have been computed
- $\rightsquigarrow\ \text{constant-time LCA}$ data structure for $\mathbb T$ has been built

Kangaroo Algorithm for approximate matching



• Analysis: $\Theta(n+m)$ preprocessing + $O(n \cdot k)$ matching

 \rightsquigarrow very efficient for small k

State of the art

- $O(n\frac{k^2 \log k}{m})$ possible with complicated algorithms
- extensions for edit distance $\leq k$ possible

Application 6: Matching with wildcards

- Allow a wildcard character in pattern stands for arbitrary (single) character
- ▶ similar algorithm as for *k*-mismatch $\rightarrow O(n \cdot k + m)$ 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

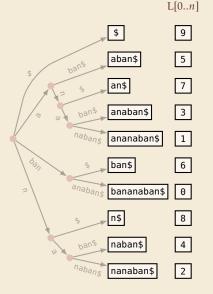
- Suffix trees were a threshold invention
- linear time and space
- suddenly many questions efficiently solvable in theory
- construction of suffix trees: linear time, but significant overhead
- \bigcirc construction methods fairly complicated
- nany pointers in tree incur large space overhead





6.5 Suffix Arrays

Putting suffix trees on a diet



- Observation: order of leaves in suffix tree
 = suffixes lexicographically sorted
 - ▶ 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 position found
 - Example: P = ana
- \rightsquigarrow *L*[0..*n*] is called *suffix array*:

L[r] = (start index of) r th suffix in sorted order

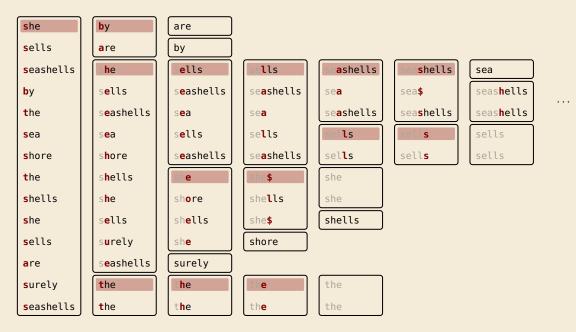
• using *L*, can do string matching with $\leq (\lg n + 2) \cdot m$ character comparisons

Suffix arrays – Construction

How to compute L[0..n]?

- from suffix tree
 - possible with traversal . . .
 - D but we are trying to avoid constructing suffix trees!
- sorting the suffixes of *T* using general purpose sorting method
 trivial to code!
 - ▶ but: comparing two suffixes can take $\Theta(n)$ character comparisons $\bigcirc \Theta(n^2 \log n)$ time in worst case
- We can do better!

Fat-pivot radix quicksort – Example



Fat-pivot radix quicksort

details in §5.1 of Sedgewick, Wayne Algorithms 4th ed. (2011), Pearson

random string

- ▶ **partition** based on *d***th** character only (initially *d* = 0)
- \rightsquigarrow 3 segments: smaller, equal, or larger than *d*th symbol of pivot
- recurse on smaller and large with same *d*, on equal with *d* + 1
 never compare equal prefixes twice

for random strings \rightarrow can show: $\sim 2 \ln(2) \cdot n \lg n \approx 1.39n \lg n$ character comparisons on average

- simple to code
- efficient for sorting many lists of strings
 - 1
 - ▶ fat-pivot radix quicksort finds suffix array in *O*(*n* log *n*) expected time

but we can do O(n) time worst case!

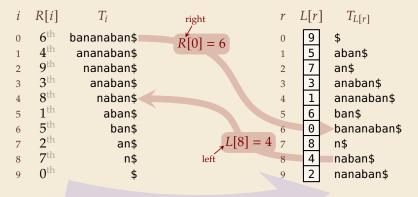
6.6 Linear-Time Suffix Sorting: Overview

Inverse suffix array: going left & right

• to understand the fastest algorithm, it is helpful to define the *inverse suffix array*:

- $\blacktriangleright R[i] = r \iff L[r] = i \qquad L = leaf array$
 - \iff there are *r* suffixes that come before T_i in sorted order

 \iff T_i has (0-based) *rank* $r \rightsquigarrow$ call R[0..n] the *rank array*



sort suffixes

Linear-time suffix sorting

DC3 / Skew algorithm

1. Compute rank array $R_{1,2}$ for suffixes T_i starting at $i \neq 0 \pmod{3}$ recursively.

not a multiple of 3

- **2.** Induce rank array R_3 for suffixes $T_0, T_3, T_6, T_9, \ldots$ from $R_{1,2}$.
- **3.** Merge $R_{1,2}$ and R_0 using $R_{1,2}$. \rightsquigarrow rank array *R* for entire input

- We will show that steps 2. and 3. take $\Theta(n)$ time
- \sim Total complexity is $n + \frac{2}{3}n + \left(\frac{2}{3}\right)^2 n + \left(\frac{2}{3}\right)^3 n + \cdots \leq n \cdot \sum_{i \ge 0} \left(\frac{2}{3}\right)^i = 3n = \Theta(n)$
- Note: L can easily be computed from R in one pass, and vice versa.
 ~> Can use whichever is more convenient.

DC3 / Skew algorithm – Step 2: Inducing ranks

▶ **Assume:** rank array *R*_{1,2} known:

 $R_{1,2}[i] = \begin{cases} \text{rank of } T_i \text{ among } T_1, T_2, T_4, T_5, T_7, T_8, \dots & \text{for } i = 1, 2, 4, 5, 7, 8, \dots \\ \text{undefined} & \text{for } i = 0, 3, 6, 9, \dots \end{cases}$

Task: sort the suffixes $T_0, T_3, T_6, T_9, \ldots$ in linear time (!)

Suppose we want to compare T_0 and T_3 .

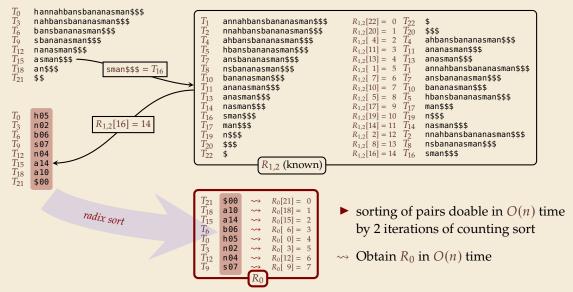
- Characterwise comparisons too expensive
- **b** but: after removing first character, we obtain T_1 and T_4
- these two can be compared in *constant time* by comparing $R_{1,2}[1]$ and $R_{1,2}[4]!$

 $\sim \begin{cases} T_0 \text{ comes before } T_3 \text{ in lexicographic order} \\ \text{iff pair } (T[0], R_{1,2}[1]) \text{ comes before pair } (T[3], R_{1,2}[4]) \text{ in lexicographic order} \end{cases}$

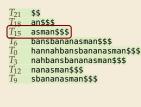
DC3 / Skew algorithm – Inducing ranks example

T = hannahbansbananasman

(append 3 \$ markers)



DC3 / Skew algorithm – Step 3: Merging



► Have:

- sorted 1,2-list: *T*₁, *T*₂, *T*₄, *T*₅, *T*₇, *T*₈, *T*₁₀, *T*₁₁, ...
- sorted 0-list: $T_0, T_3, T_6, T_9, \dots$
- ► Task: Merge them!
 - use standard merging method from Mergesort
 - ▶ but speed up comparisons using *R*_{1,2}
 - $\rightsquigarrow O(n)$ time for merge

 T_{22} \$\$\$ ahbansbananasman\$\$\$ ananasman\$\$\$ anasman\$\$\$ annahbansbananasman\$\$\$ ansbananasman\$\$\$ T_{10} bananasman\$\$\$ hbansbananasman\$\$\$ T_{17} man\$\$\$ n\$\$\$ T_{14} nasman\$\$\$ T_2 T_8 nnahbansbananasman\$\$\$ nsbananasman\$\$\$ T_{16} sman\$\$\$

Compare T_{15} to T_{11} Idea: try same trick as before $T_{15} = asman$ \$\$ = asman\$\$\$ can't compare T_{16} $= aT_{16}$ and T_{12} either! $T_{11} = ananasman$ \$\$\$ = ananasman\$\$\$ $= aT_{12}$ \rightarrow Compare T_{16} to T_{12} $T_{16} = sman$ \$\$ always at most 2 steps = sman\$\$\$ then can use $R_{1,2}!$ $= sT_{17}$ $T_{12} = nanasman$ \$\$\$ = aanasman\$\$\$

 $= aT_{13}$

6.7 Linear-Time Suffix Sorting: The DC3 Algorithm

DC3 / Skew algorithm – Fix recursive call

- ▶ both step 2. and 3. doable in *O*(*n*) time!
- ▶ But: we cheated in 1. step! *"compute rank array* R_{1,2} *recursively"*
 - Taking a *subset* of suffixes is *not* an instance of the same problem!
 - \rightsquigarrow Need a single *string* T' to recurse on, from which we can deduce $R_{1,2}$.
 - How can we make T' "skip" some suffixes?

→ redefine alphabet to be *triples of characters* abc

$$\rightarrow$$
 suffixes of $T^{\Box} \leftrightarrow T_0, T_3, T_6, T_9, \dots$

- $\blacktriangleright T' = T[1..n)^{\square} \text{ sss} T[2..n)^{\square} \text{ sss} \iff T_i \text{ with } i \neq 0 \pmod{3}.$
- \rightsquigarrow Can call suffix sorting recursively on T' and map result to $R_{1,2}$



DC3 / Skew algorithm – Fix alphabet explosion

Still does not quite work!

- Each recursive step *cubes* σ by using triples!
- → (Eventually) cannot use linear-time sorting anymore!
- But: Have at most $\frac{2}{3}n$ different triples **abc** in T'!
- \rightsquigarrow Before recursion:
 - **1.** Sort all occurring triples. (using counting sort in O(n))
 - **2.** Replace them by their *rank* (in Σ).
- → Maintains $\sigma \leq n$ without affecting order of suffixes.

DC3 / Skew algorithm – Step 3. Example

 $T' = T[1..n)^{\Box}$ (\$\$\$) $T[2..n)^{\Box}$ (\$\$\$)

- ▶ T = hannahbansbananasman\$ $T_2 = nnahbansbananasman$ \$
 - T' = annahbansbananasman\$\$ \$\$\$ nnahbansbananasman\$\$\$
- Occurring triples:

annahbansbananasman\$\$ \$\$\$ nnahbansb nasman

Sorted triples with ranks:

Rank	00	01	02	03	04	05	06	07	08	09	10	11	12
Triple	\$\$\$	ahb	ana	ann	ans	ban	hba	man	n\$\$	nas	nna	nsb	sma

T' = annahbans/banana/sman\$\$ \$\$\$ nnahbansbana/nas/man\$\$\$
 T'' = 03 01 04 05 02 12 08 00 10 06 11 02 09 07 00

Suffix array – Discussion

sleek data structure compared to suffix tree

 \square simple and fast $O(n \log n)$ construction

more involved but optimal O(n) construction

- supports efficient string matching
- \bigcirc string matching takes $O(m \log n)$, not optimal O(m)
- Cannot use more advanced suffix tree features e.g., for longest repeated substrings



6.8 The LCP Array

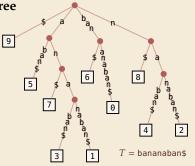
String depths of internal nodes

- Recall algorithm for longest repeated substring in suffix tree
 - 1. Compute *string depth* of nodes
 - 2. Find *path label to node* with maximal string depth
- Can we do this using **suffix** *arrays*?

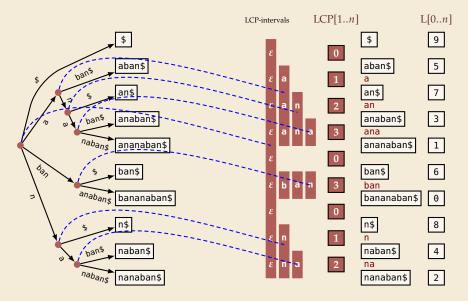
• Yes, by **enhancing** the suffix array with the *LCP array*! LCP[1..n] $LCP[r] = LCP(T_{L[r]}, T_{L[r-1]})$

length of longest common prefix of suffixes of rank r and r-1

 \rightarrow longest repeated substring = find maximum in LCP[1..*n*]



LCP array and internal nodes



 \rightarrow Leaf array L[0..n] plus LCP array LCP[1..n] encode full tree!

6.9 LCP Array Construction

LCP array construction

computing LCP[1..n] naively too expensive

• each value could take $\Theta(n)$ time

 $\Theta(n^2)$ in total

▶ but: seeing one large (=costly) LCP value → can find another large one!

- Example: T = Buffalo_buffalo_buffalo\$
 - first few suffixes in sorted order:

```
\begin{array}{l} T_{L[0]} = \$ \\ T_{L[1]} = alo_{\tt u} buffalo \$ \\ T_{L[2]} = alo_{\tt u} buffalo_{\tt u} buffalo \$ \\ & alo_{\tt u} buffalo_{\tt u} buffalo & \rightsquigarrow \ LCP[3] = 19 \\ T_{L[3]} = alo_{\tt u} buffalo_{\tt u} buffalo_{\tt u} buffalo \$ \end{array}
```

→ **Removing first character** from $T_{L[2]}$ and $T_{L[3]}$ gives two new suffixes:

$$\begin{split} T_{L[?]} &= \text{lo_ubuffalo_ubuffalos} \\ & \text{lo_ubuffalo_ubuffalo} & \rightsquigarrow & \text{LCP[?]} = 18 \\ T_{L[?]} &= \text{lo_ubuffalo_ubuffalos} & & & & \\ & & \text{unclear where...} \end{split}$$



Shortened suffixes might *not* be *adjacent* in sorted order! \rightsquigarrow no LCP entry for them!

Kasai's algorithm – Example

- Kasai et al. used above observation systematically
- ► Key idea: *compute* LCP values in *text order*
- Dropping first character of adjacent suffixes might not lead to *adjacent* shorter suffixes, but LCP entry can only be *longer*.

i	R[i]	T_i	r	L[r]	$T_{L[r]}$	LCP[r]
0	6^{th}	bananaban\$	0	9	\$	-
1	$4^{ ext{th}}$	ananaban\$	1	5	aban\$	0
2	9^{th}	nanaban\$	2	7	an\$	1
3	3^{th}	anaban\$	3	3	anaban\$	2
4	$8^{ ext{th}}$	naban\$	4	1	ananaban\$	3
5	1^{th}	aban\$	5	6	ban\$	0
6	5^{th}	ban\$	6	0	bananaban\$	3
7	2^{th}	an\$	7	8	n\$	0
8	$7^{ ext{th}}$	n\$	8	4	naban\$	1
9	0^{th}	\$	9	2	nanaban\$	2

Kasai's algorithm – Code

¹ **procedure** computeLCP(T[0..n], L[0..n], R[0..n]) *// Assume* T[n] =\$, *L* and *R* are suffix array and inverse 2 $\ell := 0$ 3 **for** $i := 0, ..., n - 1 // Consider T_i$ now 4 r := R[i]5 *// compute* LCP[r]; note that r > 0 since R[n] = 06 $i_{-1} := L[r-1]$ 7 while $T[i + \ell] = T[i_{-1} + \ell]$ do 8 l := l + 19 $LCP[r] := \ell$ 10 $\ell := \max\{\ell - 1, 0\}$ 11 return LCP[1..n] 12

• remember length ℓ of induced common prefix

use L to get start index of suffixes

Analysis:

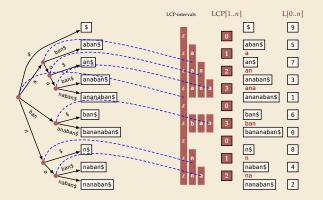
- dominant operation: character comparisons
- Separately count those with outcomes "=" resp. "≠"
- each ≠ ends iteration of for-loop
 → ≤ n cmps
- each = implies increment of ℓ, but ℓ ≤ n and decremented ≤ n times
 → ≤ 2n cmps
- $\rightsquigarrow \Theta(n)$ overall time

Back to suffix trees

We can finally look into the black box of linear-time suffix-array construction!



- **1.** Compute suffix array for *T*.
- **2.** Compute LCP array for *T*.
- **3.** Construct T from suffix array and LCP array.



Conclusion

▶ (Enhanced) Suffix Arrays are the modern version of suffix trees

 \bigcirc can be harder to reason about

can support same algorithms as suffix trees

but use much less space

simpler linear-time construction