ALGORITHMICS\$APPLIED

APPLIEDALGORITHMICS\$

CS\$APPLIEDALGORITHMI

DALGORITHMICS\$APPLIE

EDALGORITHMICS\$APPLIE

HMICS\$APPLIEDALGORITHMI

ICS\$APPLIEDALGORITHM

E DALG GA

Text Indexing – Searching whole genomes

16 March 2021

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 Linear-Time Suffix Sorting
- 6.7 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

- ▶ 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:

- 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)

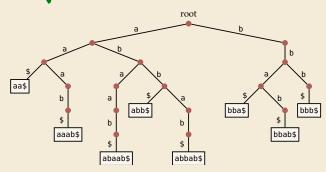
some character $\notin \Sigma$

► strings of same length

▶ strings have "end-of-string" marker \$

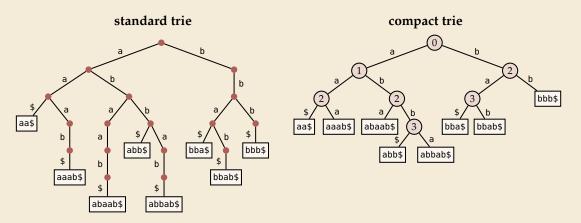
Example:

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



Compact tries

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



- → 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



fast lookup

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 = superiorcalifornialives, S_2 = 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)]

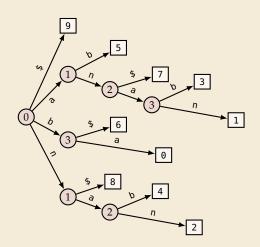
Suffix trees – Definition

- ► suffix tree \mathcal{T} for text T = T[0..n 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 $\Theta(n^2)$. \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)!

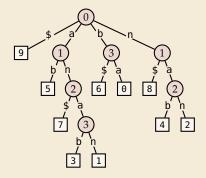
→ for now, take linear-time construction for granted. What can we do with them?

6.3 Applications

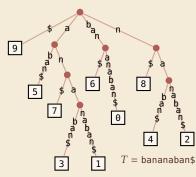
Applications of suffix trees

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

Recall: 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 \$)

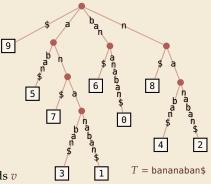
Application 1: Text Indexing / String Matching

- ightharpoonup P occurs in $T \iff P$ is a prefix of a suffix of T
- ▶ we have all suffixes in T!
- → (try to) follow path with label *P*, until
 - 1. we get stuckat internal node (no node with next character of P)or inside edge (mismatch of next characters)→ P does not occur in T
 - 2. we run out of patternreach end of *P* at internal node *v* or inside edge towards *v*→ *P* occurs at all leaves in subtree of *v*
 - 3. we run out of tree reach a leaf ℓ with part of P left \leadsto compare P to ℓ .



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

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

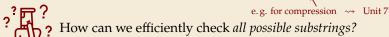


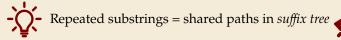
Examples:

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

Application 2: Longest repeated substring

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







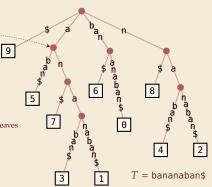
- ► T_5 = aban\$ and T_7 = an\$ have longest common prefix 'a'
- → ∃ internal node with path label 'a'

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 $T^{(1)}, ..., T^{(k)}$ 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 \Im for T
- \Rightarrow \$ $_{\rm j}$ -edges always leads to leaves \Rightarrow \exists leaf (j,i) for each suffix $T_i^{(j)} = T^{(j)}[i..n_j]$



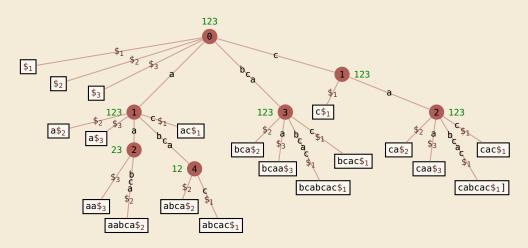
Application 3: Longest common substring

- ▶ 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.

"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



6.4 Longest Common Extensions

Application 4: Longest Common Extensions

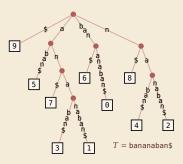
▶ We implicitly used a special case of a more general, versatile idea:

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 $(i, j) = \max\{\ell : T[i..i + \ell) = T[j..j + \ell)\}$
- \rightsquigarrow use suffix tree of T!

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

- ► In \mathfrak{I} : LCE(i,j) = LCP (T_i,T_j) \leadsto 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
- ► Could store all LCAs in big table \rightarrow $\Theta(n^2)$ 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

- Assume longest common extensions in $T \$_1 P \$_2$ can be found in O(1)
 - → generalized suffix tree T has been built
 - → string depths of all internal nodes have been computed

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

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

mismatches := mismatches + 1

if \ell = m then

return \ell = m
```

- ▶ **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
 - 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_we_will 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
- linear time and space
- suddenly many questions efficiently solvable in theory

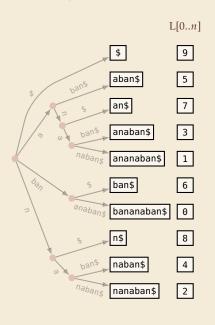


- construction of suffix trees: linear time, but significant overhead
- Construction methods fairly complicated
- many pointers in tree incur large space overhead



6.5 Suffix Arrays

Putting suffix trees on a diet



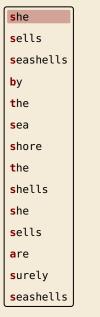
- ► **Observation:** order of leaves in suffix tree = suffixes lexicographically *sorted*
- ▶ Idea: only store list of leaves L[0..n]
- ► Enough to do efficient string matching!
 - **1.** Use binary search for pattern *P*
 - **2.** check if *P* is prefix of suffix after found position
- **Example:** P = ana
- \rightsquigarrow L[0..n] is called *suffix array*:
 - L[r] =(start index of) rth suffix in sorted order
- ▶ using L, can do string matching with $\leq (\lg n + 2) \cdot m$ character comparisons

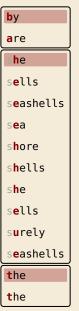
Suffix arrays – Construction

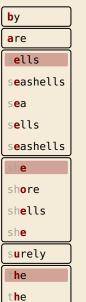
How to compute L[0..n]?

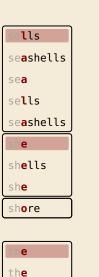
- from suffix tree
 - ▶ possible with traversal . . .
 - $\hfill \Box$ but we are trying to avoid constructing suffix trees!
- ▶ sorting the suffixes of *T* using general purpose sort
 - trivial to code!
 - **b** but: comparing two suffixes can take $\Theta(n)$ character comparisons
 - \bigcap $\Theta(n^2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

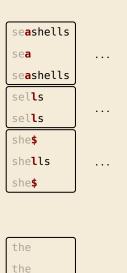
Fat-pivot radix quicksort – Example











Fat-pivot radix quicksort

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

- **partition** based on *d*th character only (initially d = 0)
- \rightarrow 3 segments: smaller, equal, or larger than dth symbol of pivot
- recurse on smaller and large with same d, on equal with d + 1
 - → never compare equal prefixes twice
- \sim can show: $\sim 2 \ln(2) \cdot n \lg n \approx 1.39 n \lg n$ character comparisons in expectation
- simple to code
- efficient for sorting many lists of strings

random pivots

• fat-pivot radix quicksort finds suffix array in $O(n \log n)$ expected time

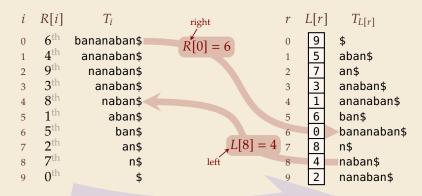
but we can do O(n) time worst case!

6.6 Linear-Time Suffix Sorting

Inverse suffix array: going left & right

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

►
$$R[i] = r$$
 \iff $L[r] = i$ $L = leaf array$ \iff there are r suffixes that come before T_i in sorted order \iff T_i has $(0\text{-based}) rank r$ \rightsquigarrow call $R[0..n]$ the $rank array$



sort suffixes

Linear-time suffix sorting

DC3 / Skew algorithm

not a multiple of 3

- **1.** Compute rank array $R_{1,2}$ for suffixes T_i starting at $i \not\equiv 0 \pmod{3}$ recursively.
- **2.** Induce rank array R_3 for suffixes T_0 , T_3 , T_6 , T_9 , ... from $R_{1,2}$.
- **3.** Merge $R_{1,2}$ and R_0 using $R_{1,2}$.
 - \rightarrow rank array R for entire input

▶ We will show that steps 2. and 3. take $\Theta(n)$ time

$$ightharpoonup$$
 Total complexity is $n + \frac{2}{3}n + \left(\frac{2}{3}\right)^2 n + \left(\frac{2}{3}\right)^3 n + \cdots \le n \cdot \sum_{i \ge 0} \left(\frac{2}{3}\right)^i = 3n = \Theta(n)$

- ▶ **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

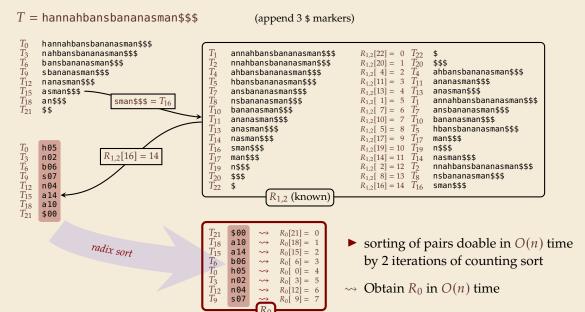
► **Assume:** rank array $R_{1,2}$ known:

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

- ▶ **Task:** sort the suffixes T_0 , T_3 , T_6 , T_9 , . . . 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 $R_{1,2}[4]!$

```
T_0 comes before T_3 in lexicographic order iff pair (T[0], R_{1,2}[1]) comes before pair (T[3], R_{1,2}[4]) in lexicographic order
```

DC3 / Skew algorithm – Inducing ranks example



DC3 / Skew algorithm – Step 3: Merging

T_2	\$\$
T_1	an\$\$\$
T_1	asman\$\$\$
I_6	bansbananasman\$\$\$
T_0	hannahbansbananasman\$\$
T_3	nahbansbananasman\$\$\$
T_1	
T_9	sbananasman\$\$\$

```
ahbansbananasman$$$
 ananasman$$$
 anasman$$$
 ansbananasman$$$
bananasman$$$
 hbansbananasman$$$
 man$$$
 n$$$
 nasman$$$
 nnahbansbananasman$$$
 nsbananasman$$$
 sman$$$
```

► Have:

sorted 1,2-list: $T_1, T_2, T_4, T_5, T_7, T_8, T_{10}, T_{11}, \dots$

sorted 0-list: $T_0, T_3, T_6, T_9, \dots$

- ► Task: Merge them!
 - use standard merging method from Mergesort
 - \triangleright but speed up comparisons using $R_{1,2}$
 - \rightarrow O(n) time for merge

```
ahbansbananasman$$$
annahbansbananasman$$$
                                            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}
```

DC3 / Skew algorithm – Fix recursive call

- **b** 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!
 - \rightarrow 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 abo

$$\rightsquigarrow$$
 suffixes of $T^{\square} \iff T_0, T_3, T_6, T_9, \dots$

$$\rightarrow$$
 T^{\square} = ban ana ban \$\$\$

ana ban \$\$\$

ban \$\$\$

T = bananaban\$\$

ana ban \$\$\$

(ban) \$\$\$ \$\$\$

 $ightharpoonup T' = T[1..n)^{\square}$ \$\$\$ $T[2..n)^{\square}$ \$\$\$ \longleftrightarrow T_i with $i \not\equiv 0 \pmod{3}$.

 \sim 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'!
- → Before recursion:
 - **1.** Sort all occurring triples. (using counting sort in O(n))
 - **2.** Replace them by their *rank* (in Σ).
- \rightsquigarrow Maintains $\sigma \leq n$ without affecting order of suffixes.

DC3 / Skew algorithm – Step 3. Example

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

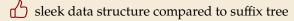
- T = hannahbansbananasman $T_2 = nnahbansbananasman$ T' = annahbansbananasman S = nnahbansbananasman
- ► Occurring triples:

```
ann ahbans ban ana sma n$$ $$$ nna hba nsb nas man
```

► Sorted triples with ranks:

T' = annahbansbananasman \$\$ \$ mnahbansbananasman\$\$\$ T'' = 03 01 04 05 02 12 08 00 10 06 11 02 09 07 00

Suffix array – Discussion



- \bigcap simple and fast $O(n \log n)$ construction
- more involved but fast O(n) construction
- supports efficient string matching
- \bigcap string matching takes $O(m \log n)$, not optimal O(m)
- Cannot use more advanced suffix tree features e.g., for longest repeated substrings



6.7 The LCP Array

String depths of internal nodes

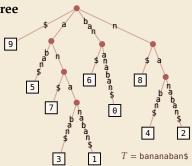
- ▶ Recall algorithm for longest repeated substring in **suffix tree**
 - 1. Compute string depth of nodes
 - 2. Find path label to node with maximal string depth
- Can we do this using suffix arrays?

Yes, by **enhancing** the suffix array with the **LCP** array!

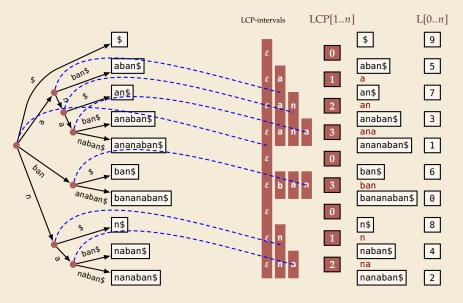
$$LCP[1..n]$$

$$LCP[r] = LCP(T_{L[r]}, T_{L[r-1]})$$
longest common prefix of suffixes of rank r and $r-1$

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



LCP array and internal nodes



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

LCP array construction

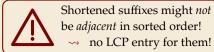
- ightharpoonup computing LCP[1..n] naively too expensive
 - ▶ each value could take $\Theta(n)$ time

$$\bigcirc \Theta(n^2)$$
 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{split} T_{L[0]} &= \$ \\ T_{L[1]} &= \texttt{alo}_{\texttt{u}} \texttt{buffalo} \$ \\ T_{L[2]} &= \texttt{alo}_{\texttt{u}} \texttt{buffalo}_{\texttt{u}} \texttt{buffalo} & \leadsto & \texttt{LCP[3]} = \texttt{19} \\ T_{L[3]} &= \texttt{alo}_{\texttt{u}} \texttt{buffalo}_{\texttt{u}} \texttt{buffalo}_{\texttt{u}} \texttt{buffalo} \$ \end{split}
```

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



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 th	naban\$	4	1	ananaban\$	3
5	$1^{ ext{th}}$	aban\$	5	6	ban\$	0
6	$5^{\rm th}$	ban\$	6	0	bananaban\$	3
7	2 th	an\$	7	8	n\$	0
8	$7^{ m th}$	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
       \ell := 0
       for i := 0, ..., n-1
           r := R[i]
           // compute LCP[r]; note that r > 0 since R[n] = 0
           i_{-1} := L[r-1]
           while T[i + \ell] == T[i_{-1} + \ell] do
                \ell := \ell + 1
            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:

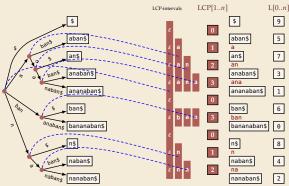
- dominant operation: character comparisons
- Separately count those with outcomes "=" resp. "≠"
- each ≠ ends iteration of for-loop ≤ n cmps
- ▶ each = implies increment of ℓ , but $\ell \le n$ and decremented $\le n$ times $\Rightarrow \le 2n$ cmps
- \rightarrow $\Theta(n)$ overall time

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
- can be harder to reason about
- can support same algorithms as suffix trees
- but use much less space
- simpler linear-time construction