3. Exact Pattern Matching

String Matching

Given: pattern P, text T (P, T are strings)

Aim: find occurrences of P in T

Exmpl:

$$\begin{array}{ll} & 1\,2\,3\,4\,5\,6\,7\,8\,9\,10\,\ldots \\ T = & AATGCATGCA\,\ldots\ldots \\ P = & ATG \end{array}$$

P occurse on position 2, 6, ...

This has applications in:

- Bioinformatics (eg. sequence assembly where one may align fragments of your DNA to reference genome to get read of your DNA; also applications in finding repeated regions & many more
- general word processing
- internet search
- "fgrep" in Unix
- search for plagiarism
- subtask for eg inexact matching

Basics:

string $S = x_1 \ldots\ldots x_n$, $|S| = n$

$S[i..j] = x_i x_{i+1} \ldots x_j$

$S(i) = x_i$

$S[1..j] \hat{=}$ prefix of S ending at j

$S[j..n] \hat{=}$ suffix of S starting at j

$$\begin{array}{ll} & 1\;2\;3\;4\;5\;6\;7\;8 \\ S: & \underbrace{HONO}_{\substack{S[1..4] \\ \text{prefix}}}LU\underbrace{LU}_{\substack{S[7..8] \\ \text{suffix}}} \end{array}$$

$S(5) = L$

if $P(i) = T(k)$ for some i, k then they match

else mismatch.

Naïve Method

```
NAIVE(P, T)                                 // compare T(i ... i+|P|-1)
                                            // with P for all i = 1 ... |T|-|P|+1
    occurences = ∅
    FOR (i = 1 ... |T|-|P|+1)               // loop over "pos." in T
        FOR (j = 1 .. |P|)                  // loop over P
            match = TRUE
            IF ( P(j) ≠ T(i+j-1))           // compare characters
                match = FALSE
                break
        IF (match)
            add i to occurences             // save pos. on which
                                            // P occurs
    RETURN occurrences.
```

Q: How often can P occur in T?
A: $|T| - |P| + 1$ times

$$
\begin{array}{rcccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 \\
T = & A & A & A & A & A & A
\end{array}
$$

$P = AA$,

P occurs at pos. 1, 2, 3, 4, 5
= 5 times = $6 - 2 + 1$

Q: What is greatest Nr of character comparisons?
A: $|P| \cdot (|T| - |P| + 1)$ (worst case)

See example above: $2 \cdot 5 = 10$ comparisons

Q: What is least Nr of character comparisons?
A: $|T| - |P| + 1$ (best case)

$T = AAAAAA$
$P = BA$

⇒ RUNTIME NAIVE-alg

$|T| - |P| + 1$ 1. loop
$|P|$ 2 loop

$$\Rightarrow |T||P| - |P|^2 + 1 \underset{|T| \geq |P|}{\leq} |T||P|$$

⇒ $O(|T||P|)$ time

look now to one of many linear-time algorithms, i.e. instead of $O(|P||T|)$ we have runtime $O(|P| + |T|)$

Z-algorithm [fundamental preprocessing used in many alg]

General idea: pre-process P in $O(|P|)$ time to gain insight of internal structure of P

DEF: Let S be a string (usually $S = P$ pattern) & $i > 1$.

$Z_i := Z_i(S) =$ length of longest substring in S that starts at position i & matches prefix of S

Example:

i	1	2	3	4	5	6	7	8	9	10	11
S	a	a	b	c	a	a	b	x	a	a	z
Z_i	–	1	0	0	3	1	0	0	2	1	0

DEF (Z-Box): $\forall\, i > 1$ s.t. $Z_i > 0$, the Z-Box at i is the interval $[i, i + Z_i - 1]$

Exmple:

i	1	2	3	4	5	6	7	8	9	10	11
S	a	a	b	c	a	a	b	x	a	a	z
z_i	–	1	0	0	3	1	0	0	2	1	0

$z_i > 0$ at pos. 2, 5, 6, 9, 10

$$
\begin{aligned}
\text{z-Box at } 2 &= [2,\ 2+1-1] = [2,2] \\
\text{at } 5 &= [5,\ 5+3-1] = [5,7] \\
\text{at } 6 &= [6,\ 6+1-1] = [6,6] \\
\text{at } 9 &= [9,\ 9+2-1] = [9,10] \\
\text{at } 10 &= [10,\ 10+1-1] = [10,10]
\end{aligned}
$$

i	1	2	3	4	5	6	7	8	9	10	11
S	a	a	b	c	a	a	b	x	a	a	z

this intervals $[i,j]$ correspond to $S[i..j]$ = longest substring starting at $i > 1$ & matches prefix of S

DEF $\forall i > 1$:

(r = right) r_i denotes right-most endpoint of Z-Boxes Z_j with $Z_j > 0$ & $j \leq i$

(equ. to r_i = largest value of $j + Z_j - 1$ over all $1 < j \leq i$ st $Z_j > 0$)

"store index j": $l_i = j$ for j satisfying this

(l = left)

(equ. to l_i = position of left-end of Z-Box ending in r_i)

if MORE than one Z-Box ends in r_i then l_i can be chosen arbitrarily among those values

Formal: $r_i = \max\limits_{2 \leq j \leq i} \{ j + Z_j - 1 : Z_j > 0 \}$

i	1	2	3	4	5	6	7	8	9	10	11
S	a	a	b	c	a	a	b	x	a	a	z
r_i	–	2	2	2	7	7	7	7	10	10	10
l_i	–	2	2	2	5	5	5	5	9	9	9

right: $r_6 = \max\{ \underbrace{2+1-1}_{\text{for } j=2}, \underbrace{5+3-1}_{j=5}, \underbrace{6+1-1}_{j=6} \} = 7$

left: $l_6 = 5$

this essentially gives pos. of "large" Z-Boxes.

How to compute z_i, r_i, l_i efficiently?

main idea: iterative approach

start with z_2 (explicit comparison from left-to-right)

Assume $\forall i < k$ values z_i, r_i, l_i have been computed.

for k use: z_i, l_i, r_i $(i < k)$
WITHOUT EXPLICITE character comparisons as much as possible.

Overview of steps of Z-alg

① compute z_2 (explicit comparison of $S[1..n]$ with $S[2..n]$ until mismatch)

IF $(z_2 > 0)$ put $l_2 = 2$, $r_2 = z_2 + 1$
ELSE put $l_2 = r_2 = 0$

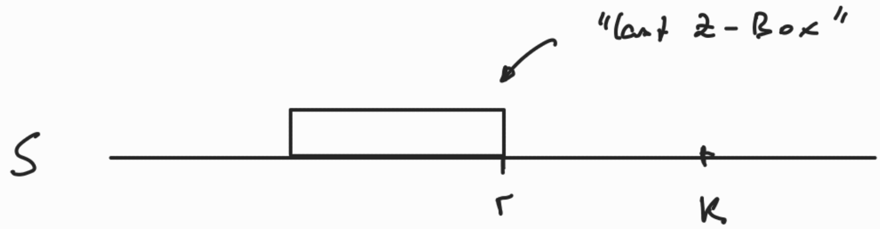
② k-th step $(k \geq 2)$.

$\Rightarrow$ all z_i, l_i, r_i computed for all $i \leq k-1$

Compute z_k, l_k, r_k based on the following cases.

$$l := l_{k-1}, \quad r := r_{k-1}$$

$\boxed{\text{Case 1: } \quad r < k}$



in this case compute z_k via explicit comparison of $S[k..n]$ & $S[1...n]$ until mismatch.

IF $(z_k > 0)$ put $l_k = k$, $r_k = k + z_k - 1$
ELSE $l_k = l$, $r_k = r$

Example:

i	1	2	3	4	5	6	7	8	9	10	11
S	a	a	b	c	a	a	b	x	a	a	z
r_i	–	2	2	2	7	7	7	7			
l_i	–	2	2	2	5	5	5	5			

$k = 9 \rightarrow r_8 = 8 < k = 9$ need to compare $S[9..11]$ with $S[1..n]$

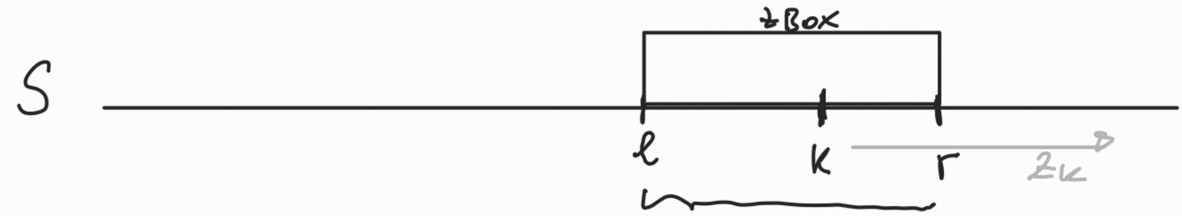
$\Rightarrow$ $S[9] = S[1]$ ✓
$S[10] = S[2]$ ✓
$S[11] \neq S[3]$ ✗

$\Rightarrow$ $z_9 = 2, \; l_9 = 9$

$r_9 = 9 + 2 - 1 = 10$

Case 2: $r \geq k$

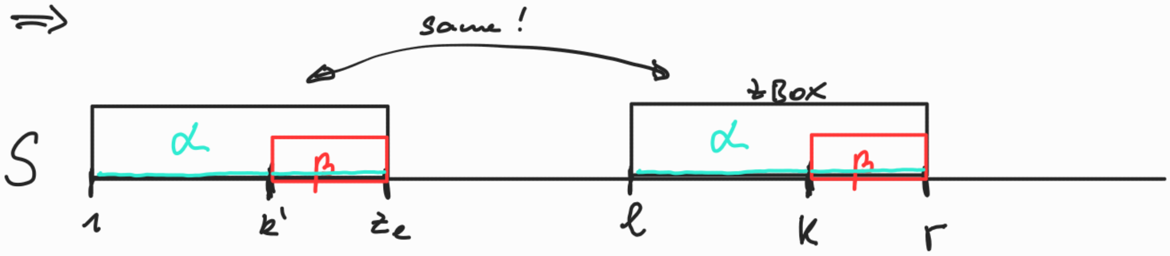
[Now we have some pre-knowledge about about z_k]



length $r - \ell + 1 = z_\ell$

z-Box $\hat{=}$ prefix of S

$\Rightarrow$



$S[1..z_\ell] \quad = \quad S[\ell..r] = \alpha$

$S[k'..z_\ell] \quad = \quad S[k..r] = \beta$

We want to know now z_k (longest string starting at k & is prefix of S)

Question: what we know about β ?

if we know β or "first part" of β is prefix of S, we don't need to compare the respective positions.

! This knowledge is already stored in $z_{k'}$

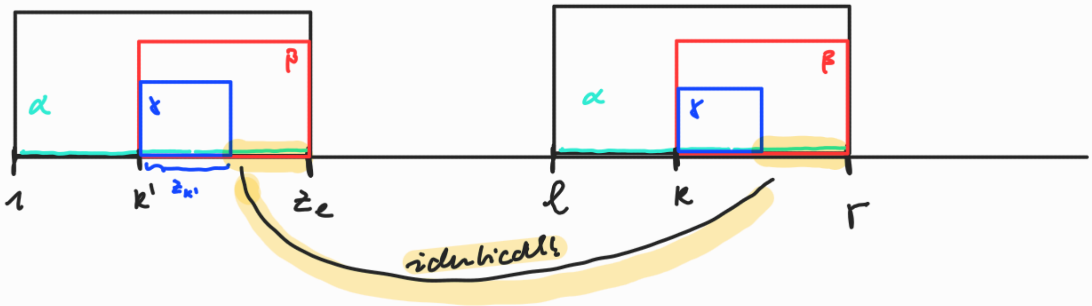
$\boxed{k' = k - \ell + 1}$

and leads to following sub cases.

2A, 2B

2A

$z_{k'} < |\beta| = r - k + 1$



$z_{k'}$ = length of γ = length of longest substring starting at k' & is prefix of S

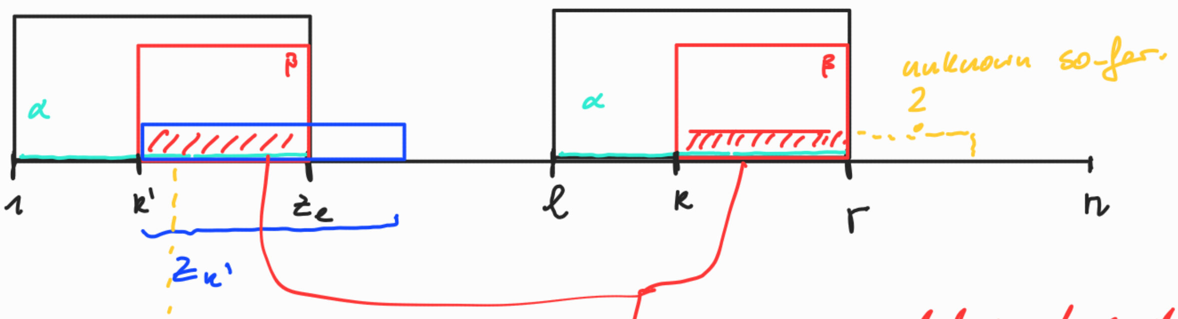
Since $\beta_{\text{left}} = \beta_{\text{right}}$ $\Rightarrow$ $\gamma_{\text{(right)}}$ is longest substring starting at k & is prefix of S.

$\Rightarrow$ $z_k = z_{k'}$

ℓ & r remain unchanged.

2B

$z_{k'} \geq |\beta| = r - k + 1$



this part matches already,

i.e. $\beta_{\text{(right)}}$ is part of longest substring starting at k & prefix of S.

β+1 pos.

$\beta = S[k..r]$ is prefix of S.

& $z_k \geq |\beta| = r - k + 1$

However $Z_k > |\beta|$ may be possible.

$\Rightarrow$ compare $S[r+1 .. n]$ [yellow part above]

with $S[\underset{\substack{/\!/ \\ r-k+1+1 \\ = r-k+2}}{|\beta|}+1, \ldots n]$ until mismatch to possibly extend Z-Box starting at k

let q be pos. in S of 1st mismatch
& if no mismatch put $q = |S| + 1$

put $Z_k = q - k$ $\quad (= k + Z_k - 1)$

$r = q - 1$

$\ell = k$

Z Algorithm

$r \leftarrow \ell \leftarrow 0$
for $k = 2$ to $|S|$ **do**
// Case 1:
    if $r < k$ **then**
        Compare characters in $S[k..n]$ with the ones in $S[1..n]$ until mismatch is found (from left-to-right).
        Set Z_k to the length of the matched characters
        if $Z_k > 0$ **then**
            Set $r \leftarrow k + Z_k - 1$, $\ell \leftarrow k$.
// Case 2:
    else
        $k' \leftarrow k - \ell + 1$
// Case 2a:
        if $Z_{k'} < r - k + 1$ **then**
            $Z_k \leftarrow Z_{k'}$
// Case 2b:
        else
            $\ell \leftarrow k$
            Compare characters in $S[r+1..n]$ with the ones in $S[r-k+2..n]$ until mismatch is found (from left-to-right).
            let $q > r$ be the position of the first mismatch or $q = |S| + 1$ if no mismatch occurs
            $Z_k \leftarrow q - k$, $r \leftarrow q - 1$

latter discussion implies:

<u>Thm:</u> Z-alg. correctly computes all Z-Box Z_i, $i > 2$

however more important:

<u>Thm:</u> All $Z_i(S)$ values are computed in $O(|S|)$ time.

<u>proof</u>:

FOR loop (line 2-20) runs $O(|S|)$ times.

<u>Q:</u> What happens within FOR-loop?

to answer this question let us count character-comparisons.

Each character comparison results either in match or mismatch.

$\Rightarrow$ let us count match / mismatches.

each comparison ends when 1st mismatch occurs

$\Rightarrow$ since $O(|S|)$ different comparisons

$\Rightarrow$ total $O(|S|)$ mismatches

Notation: c_k = NR of comparisons in k-th iteration
m_k = NR of matches in k-th iteration

$\boxed{\text{Claim: } r_k - r_{k-1} \geq m_k}$

proof: in Z-Alg we either use Case 1/2A/2B.

Assume CASE 1 applies:

& thus, $r_{k-1} < k$ $\xrightarrow{\text{Alg.}}$ explicit comparison of $S[k..n]$ with $S[1..n]$ until mismatch.

$\Rightarrow$ at most $n-k+1$ comparisons

in Alg we put $z_k = m_k$

in Alg case $z_k > 0$ & [$z_k = 0$ implizit by leaving "$r = r_k = r_{k-1}$" unchanged].
$\overset{\shortparallel}{m_k}$

$z_k > 0$: $r_k = k + z_k - 1 = k + m_k - 1 > k + m_k$
$> r_{k-1} + m_k$

$\Leftrightarrow r_k > r_{k-1} + m_k$
$\Leftrightarrow r_k - r_{k-1} > m_k$ ✓

$z_k = 0$: $r_k = r_{k-1} = r_{k-1} + \underset{0}{\underset{\shortparallel}{m_k}}$
(implizit in algo) $\Leftrightarrow r_k - r_{k-1} = m_k = 0$. ✓

Now Case 2A/2B.

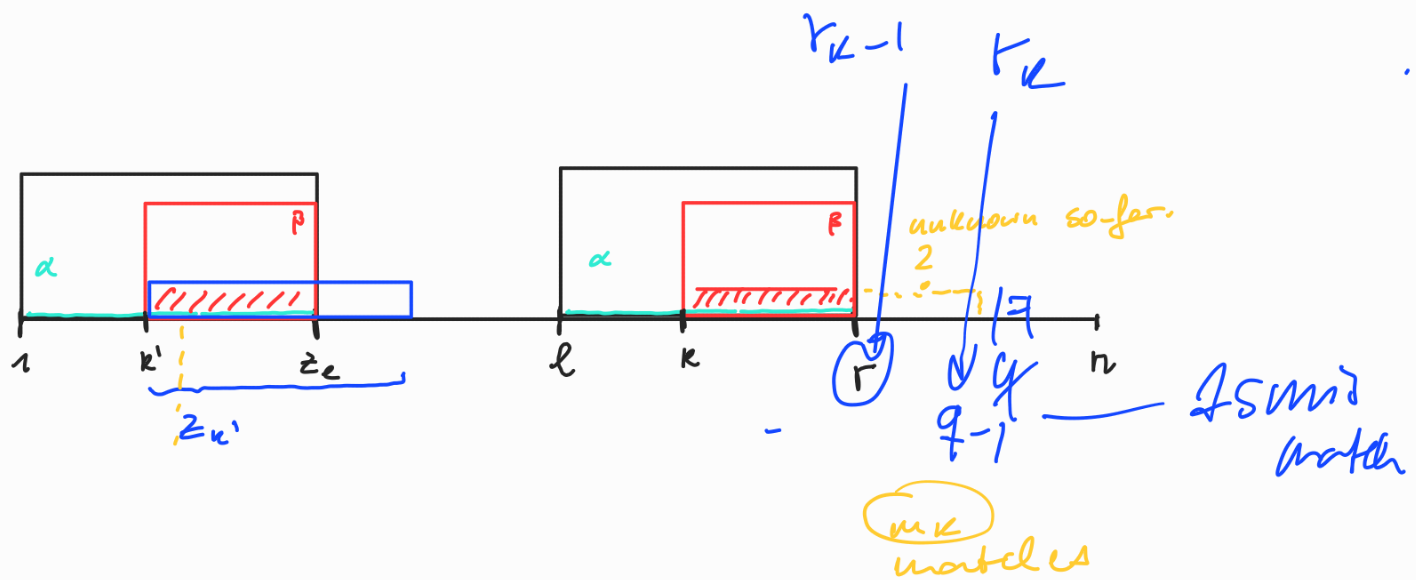
CASE 2A: in Alg "r" $= r_{k-1}$ remains unchanged,

i.e. $r_k = r_{k-1}$

moreover no comparisons are made, i.e., $m_k = 0$

$\Longleftrightarrow$ $r_k - r_{k-1} = m_k$ ✓

CASE 2B: in Alg: $q > r_{k-1}$ & $r_k = q-1$:



$\Longrightarrow$ $r_k - r_{k-1} \geq m_k$ ✓ [see picture].

$n := |S|$

$$\Longrightarrow \sum_{k=2}^{n} c_k \leq \underbrace{\sum_{k=2}^{n} 1}_{\text{(mism.)}} + \underbrace{\sum_{k=2}^{n} m_k}_{\text{(match)}} = n-1 + \sum_{k=2}^{n} m_k$$

$$\underset{\text{(claim)}}{\leq} n-1 + (r_2-r_1) + (r_3-r_2) + (r_4-r_3) \dots + (r_n - r_{n-1}) = n-1 + \underbrace{r_n}_{\leq n} - \underbrace{r_1}_{=0} \leq 2n-1 \in O(n)$$

□

in Algo $r_1 = \ell_1 = 0$

Exmpl

i	1	2	3	4	5	6	7	8	9	10
S	a	c	a	c	a	b	a	c	a	c
z_i	–									
l_i	–									
r_i	–									

Init $r = l = 0$

$k = 2$: $k = 2 > r = 0$ (Case 1)

compare $S[2 \dots n]$ with $S[1 \dots n]$

$\Rightarrow$ $S(2) \neq S(1)$ mismatch

$\Rightarrow$ $z_k = 0$, r, l unchanged.

i	1	2	3	4	5	6	7	8	9	10
S	a	c	a	c	a	b	a	c	a	c
z_i	–	0								
l_i	–	0								
r_i	–	0								

$k = 3$. , $k = 3 > r = 0$ (Case 1)

Compare $S[3 \dots n]$ with $S[1 \dots n]$

$S(3) = S(1)$
$S(4) = S(2)$
$S(5) = S(3)$
$S(6) \neq S(4)$

$\Rightarrow$ $\boxed{z_k = 3 > 0 \quad r = 3 + 3 - 1 = 5 \quad l = 3}$

i	1	2	3	4	5	6	7	8	9	10
S	a	c	a	c	a	b	a	c	a	c
z_i	–	0	3							
l_i	–	0	3							
r_i	–	0	5							

$k=4$, $\quad r=5 \geq k=4 \quad$ (case 2)

$(\alpha = aca, \; \beta = c\alpha)$

$k' = k - l + 1 = 4 - 3 + 1 = 2$

$z_{k'} = z_2 = 0 < r - k + 1 = 5 - 4 + 1 = 0$

$\Rightarrow$ case 2A: $\quad z_4 = z_{k'} = 0$, r, l unchanged.

i	1	2	3	4	5	6	7	8	9	10
S	a	c	a	c	a	b	a	c	a	c
z_i	–	0	3	0						
l_i	–	0	3	3						
r_i	–	0	5	5						

$k=5$, $\quad r=5 \geq k \quad$ (case 2 with $\alpha = aca$, $\beta = a$)

$k' = k - l + 1 = 5 - 3 + 1 = 3$

$z_{k'} = z_3 = 3 > r - k + 1 = 5 - 5 + 1 = 1$

$\Rightarrow$ case 2A again and so on...

i	1	2	3	4	5	6	7	8	9	10
S	a	c	a	c	a	b	a	c	a	c
z_i	–	0	3	0	1	0	4	0	2	0
l_i	–	0	3	3	5	5	7	7	9	9
r_i	–	0	5	5	5	5	10	10	10	10

Based on preprocessing with Z-alg. we can design a:

Simple linear-time exact matching Alg

```
Simple-exact-matching (P, T, $)          // $ character not in T & P
|  occurrences = ∅
|  n = |P| ,   m = |T|
|  S = P $ T
|  preprocess S with Z-Alg to compute Z_2 ... Z_|S|
|  FOR ( i = n+2, ..., |S| = m+n+1 )
|  |     IF (Z_i = n)
|  |     L   add  i-n-1  to occurrences
```

Exmpl $P = bbac$, $T = abba\ bbaca$

i	1	2	3	4	5	6	7	8	9	10	11	12	13	14
S	b	b	a	c	$	a	b	b	a	b	b	a	c	a
Z_i	(doesn't matter ..)					0	3	1	0	$\boxed{4}$	1	0	0	0

$Z_{10} = |P| = 4$ => P occurs on pos $10 - 4 - 1 = 5$ of S runtime: Line 1 constant

2 $n+m \in O(n+m)$

3 $n+m+1 \in O(m+n)$

4 $O(|S|) = O(m+n)$

5-7 $m+n-1-(n+2) = O(m)$

TOTAL: $O(m+n)$ time.

correctness:

Since \$ not in P and T

$\Rightarrow z_i \le |P| \quad \forall i$

if $|z_i| = |P| \Rightarrow \underbrace{S[1 \dots |P|]}_{P}\overset{\text{Def}}{=} \underbrace{S[i \dots i+n-1]}_{\text{substring of } T}$

$\Rightarrow$ P in S at pos i

$\equiv$ P in T at pos $n-i-1$

if P occurs in T at pos j, then P occurs in S at pos $i = j+n+1$ where $i \in [n+2, m+2]$

$\Rightarrow |z_i| \ge |P|$

Since $|z_i| \le |P| \rightarrow |z_i| = |P|$ & occurrence at pos j is reported

$\square$

Thm: Simple-exact matching correctly reports all occurrences of pattern P in text T in $O(|P| + |T|)$ time.

[Back to slides]

There is another important algorithm for pattern matching:

Boyer-Moore Algorithm is standard alg.
that is used in many applications to text search
(e.g. google..)

BM-Alg. is based on 3 essential ideas:

(1) Right-to-left scan
(2) Bad-Character Rule
(3) Good-Suffix Rule.

- T - - -
.. P - -
(move forward)

[due to limited time & since we want to cover further topics, we skip this alg.
more information about this alg in any Bioinf-textbook.]

<u>So far:</u> Z-alg used to preprocess P
& then find P.

Now: preprocess T instead!
(text of static & remains unchanged
(eg DNA))

8. Suffix Trees

classical "real world" problem:

For given Text & Pattern P
where and how often does P in Text occur?

Application:
- word processing
- internet search
- Bioinformatics (T = genom, P = gene sequ.)
- fgrep in Unix
- search for plagiarism
- ⋮

Def: • Σ = finite alphabet,
• string S (over Σ) = sequence of characters in Σ

Let $S = x_1 x_2 \dots x_l$, $x_i \in \Sigma$, $1 \le i \le l$

$|S| = l$ = length of S

$S[i..j]$ = substring $x_i x_{i+1} \dots x_j$ of S, starting at pos i ending at pos j

[if $i > j$, then $S[i..j] = \varepsilon$ empty string]

$S[1..j]$ - prefix of S
$S[i..l]$ = suffix of S
prefix/suffix proper if it is not S or ε.

$S(i)$ = i-th character of S

$x, y \in \Sigma$ match if $x = y$, else mismatch

Σ^* = set of all strings over Σ, Σ^l = set of all strings over Σ of length l

S' substring of S, if $\exists\, i, j$ st $S' = S[i..j]$

Aim: given string P check where/how often P occurs in string T

tree data structures can be seen as a collection of entities (= vertices) that are linked to simulate a hierarchy = **rooted tree**

= trees T where one vertex $\varrho \in V(T)$ is called root

Given $\varrho \in V(T)$ we obtain a **partial order** $\leq_T$ on $V(T)$ st

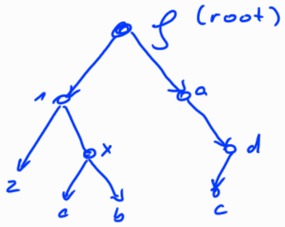
$x \leq_T y$ if y lies on simple path from ϱ to x.

in this case: x is **descendant** of y & y is **ancestor** of x

$v \in V(T)$ is **common ancestor** of vertices in $W \subseteq V(T)$, if $w \leq_T v \ \forall w \in W$

a $\leq_T$-minimal common ancestor v of vertices in W is called **least common ancestor** ($lca(W)$)

Exmpl:



the arrows indicate $\leq_T$

Note: $x \leq_T x \quad \forall x \in V(T)$

Notation: $x <_T y$ if $x \leq_T y$ & $x \neq y$

Exmpl

ϱ

1 has children 2 and x which are siblings

leaves are 2, a, b, c

root

children of x: $y \in V(T)$ st $y <_T x$ & $(xy) \in E(T)$

x is parent of its children

Siblings are vertices with the same parent

leaf: vertices with no children

Exmpl: $S =$ honolulu

$S[1..3] =$ hon , prefix & substring of S, no suffix

$S[5..8] =$ lulu , suffix & substring of S, no prefix

$S[5..7] =$ lul , substring of S, no prefix, no suffix

NOTE: empty string ε is substring, prefix, suffix of all strings.

Naive Way:

check occurence of P in T

by comparing 1 letter of P with i letter of T

$\vdots$ j letter of P with $i+j-1$ letter of T

$\vdots$ n letter of P with $i+n-1$ letter of T

$\forall\ i = 1 .. n-m+1$

$\Rightarrow$ run time $O(m\,n)$

Often, the text (= long string) is fixed & does not change

eg. • collected work of Shakespeare

• Genom

To find a pattern P (= string), we need a datastructure that represents the text so that we can find efficiently P

To this end: suffix trees

Def [suffix tree] Let S be string of length $|S| = m$

A suffix tree for S is a rooted tree T (with root s_r) that satisfies the following properties:

(X1) T has precisely m leaves that are uniquely labeled with $1, 2 \dots m$

(X2) all inner vertices, (= vertices that are not leaves) except possibly the root, have at least 2 children

(X3) every edge of T is labeled by a non-empty substring of S

(X4) For all distinct children v_1, v_2 of v we have: label of edge (v, v_1) & (v, v_2) start with different characters

(X5) if we concatenate the labels on the edges in order from s_r to leaf i, we obtain the suffix $S[i..m]$

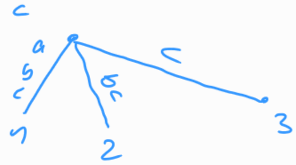
Exmpl: $S = a$, T

[this is the only case where s_r has only one child, since if $|S| > 1$ & T:

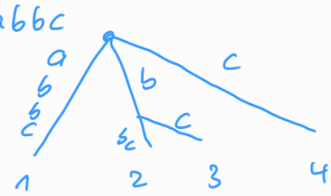
we dont get $S[m..m]$, since $|S[m..m]| = 1$ & (X3).]

$S = abc$

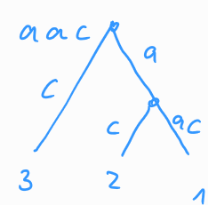
T



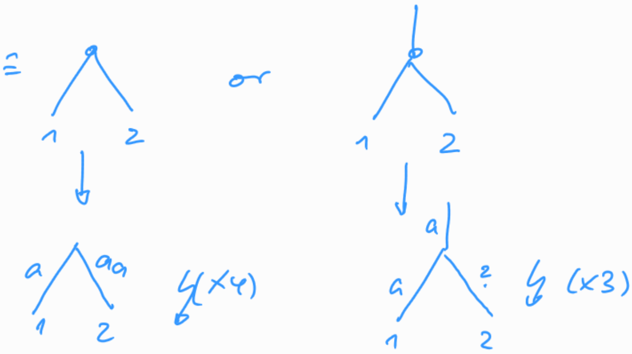
$S = abbc$



$S = aac$



What is with $S = aa$? $T \stackrel{?}{=}$



Observation: not for all strings a suffix tree exists!

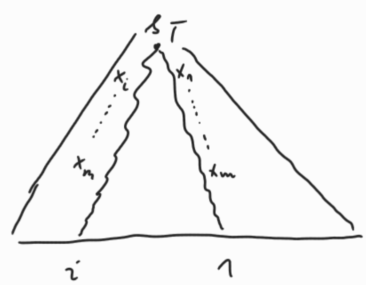
Lemma 8.1 If $S = \underbrace{x_1 \cdots x_k}_{\text{prefix}} \cdots \underbrace{x_i \cdots x_m}_{\text{suffix}}$ st $x_1 \cdots x_k = x_i \cdots x_m$

that is S contains prefix that is also a suffix of S.

Then, no suffix tree for S exists

proof: Wlog, we assume that such suffix/prefix are chosen in S to be maximal (there is no longer prefix that is also suffix)

T:



or

lowest common ancestor of 1 & i is ρ_T

Since $x_i = x_1$, this does not work due to (X4)

lowest common ancestor of 1 & i is $v <_T \rho_T$

$$\begin{array}{ccccccc} x_1 & x_2 & x_3 & \cdots & x_k & \cdots\cdots & x_m \\ \shortparallel & \shortparallel & \shortparallel & & \shortparallel & & \\ x_i & x_{i+1} & x_{i+2} & \cdots & x_m & & \end{array}$$

, $\ell < m$

↯(X4) since $x_{i+\ell} = x_{\ell+1}$

⇒ only possibility:

↯(X3)

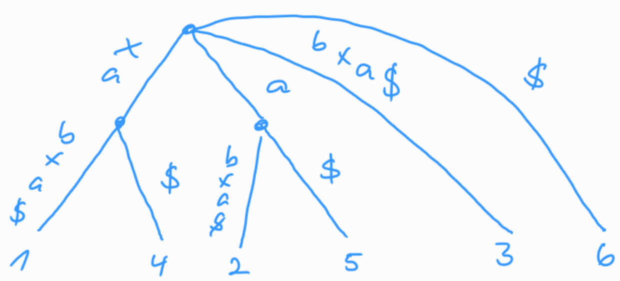
∎

$\Rightarrow$ if suffix of S is also prefix of S no suffix tree exists!

<u>IDEA:</u> simply add special symbol $\$$ at end of S, where $\$$ does not occur in S.

<u>From here on:</u> $S = x_1 \dots x_m$ with $x_m = \$$

<u>Example:</u> $S = \underset{1\,2\,3\,4\,5\,6}{xabxa\$}$ (for "xabxa" no suffix tree)

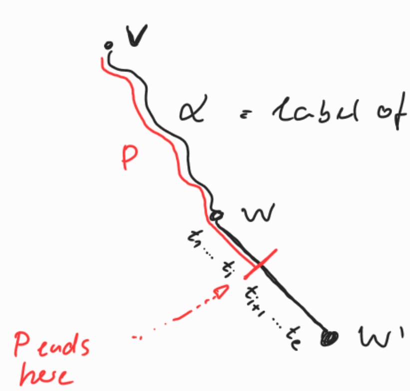


<u>Def.</u>

Let $v \le_T w$ & P be the unique simple path from v to w

label of P = concatenation of labels of edges in order from v to w.

! By slight abuse of notation, we also consider simple paths in suffix tree that may end on edge (and not on vertex)



α = label of path from v to w

$(w\,w') \in E(T)$ with label $t_1 \dots t_\ell$

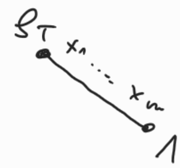
label of $P = \alpha\, t_1 \dots t_i$

How to construct suffixtree & how does this help?

<u>Alg. SUFFIXTREE (idea)</u>

// iteratively build suffixtrees $T_1 \dots T_m$ by adding $S[1 \dots m], \dots S[m \dots m]$ in previously constructed T_i

Input: $S = x_1 \dots x_m$

1) construct $T_1 =$ 

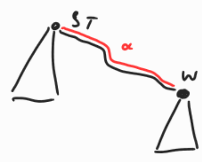
2) Assume T_i is constructed, then construct T_{i+1} $(i<m)$ as follows:

(a) Find path P in T_i that starts in ρ_{T_i} with <u>longest</u> label that is a prefix of $S[i+1..m]$ [path could end in ρ]

(i) By similar arguments as in proof of L. 8.1 <u>this path is uniquely determined</u> since no two edges $(v,v_1), (v,v_2)$, v_1, v_2 children of v have labels starting with same symbol (X4).

(ii) <u>this path will never end in leaf of T_i</u> since P starts at root & concatenation of edge labels to leaf i yields $S[i..m]$ where $|S[i...m]| > |S[i+1..m]|$ [by induction – Exerc]

(b) This path P either ends in edge or non-leaf vertex of T_i

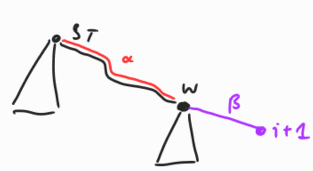
P ends in vertex: 

w no leaf $\Rightarrow$ w has children.

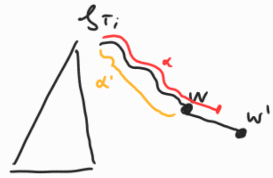
α prefix of $S[i+1 \dots m]$, $m = \$$
But $\alpha \neq S[i+1 \dots m]$
otherwise $S[i+1 \dots m] = S[\ell..m]$ for some ℓ but $\ell < i+1$ ↯

$\Rightarrow \alpha = S[i+1..m-j]$, $j \geq 1$

$\Rightarrow$ add edge $(w, i+1)$ with label $\beta = S[m-j+1..m]$



P ends in edge:



$\alpha = S[i+1 \dots m-j]$

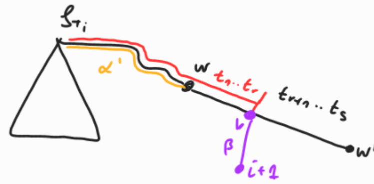
label edge $(w,w') = t_1 \dots t_r t_{r+1} \dots t_s$

$\Rightarrow \alpha = \alpha' t_1 \dots t_r$ for some $1 \le r < s$

add new vertex v on edge (w,w') & put label$(wv) = t_1 \dots t_r$

label$(vw') = t_{r+1} \dots t_s$

+ add new edge $(v, i+1)$ with label$(v, i+1) = S[m-j+1 \dots m] = \beta$

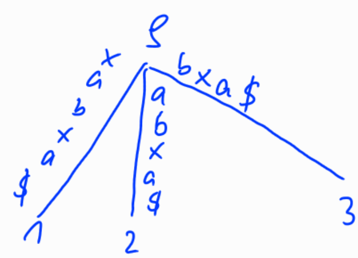


For both cases, T_{i+1} contains now path from $\varrho_{T_{i+1}}$ to $i+1$ with label $S[i+1 \dots m]$

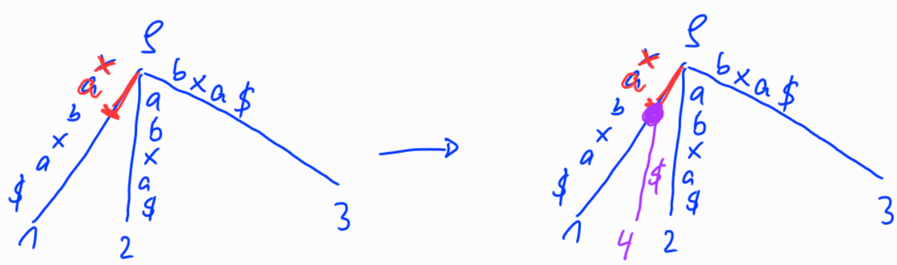
Exmpl: $S = xabxa\$$

T_1:

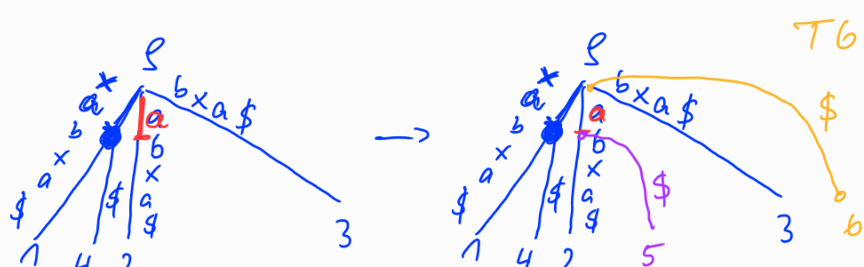
T_2 / T_3 (longest path ends in ϱ)



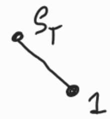
T_4: $S[4..m] = xa\$$ longest path P



T_5: $S[5..m] = a\$$



SUFFIX-TREE(S)

init T as  and label$(\rho_T, 1) = S[1..m]$

FOR($i = 2..m$) DO

- $(end, i', \ell') = $ FIND_LONGEST_PATH $(T, S[i..m])$ // returns end of path, that is, either end = v or end = e & index i' & ℓ'
- IF(end = edge e) // $e = (uw)$ with label γ
  - remove $e = (uw)$ // 
  - add new vertex v
  - add new edges $e_1 = (u,v)$, $e_2 = (v,w)$
  - & label $e_1 = \gamma[1..\ell']$
  - label $e_2 = \gamma[\ell'+1..|\gamma|]$
- add edge (v,i) to T with label $S[i+i'..m]$

FIND_LONGEST_PATH(T, S')

[sketch → more details in Appendix]

"Follow path from ρ_T to v/e as long as possible, i.e., as long as letter on this path match with letters $S' = x_i \cdots x_m$" & return corresponding positions i', ℓ' + if end is edge or vertex".

Theorem [Ukkonen]: for S of length m the suffix tree can be constructed in $O(m)$ time

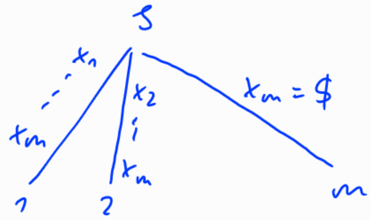
[without proof]

[quite sophisticated pointer-adjustments].

Space complexity

Suffix tree without labels $O(m)$
but we need to store labels!

worst case:



each edge label of (S, i) is of size i

$\Rightarrow \sum_{i=1}^{m} i = O(m^2)$ space

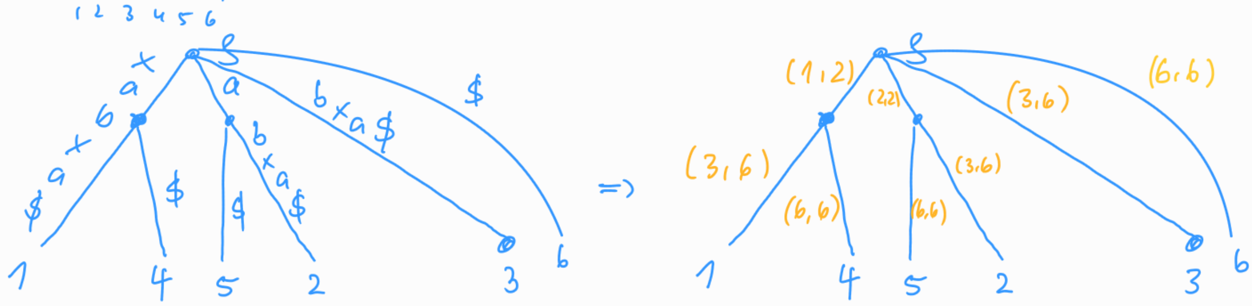
$O(m^2)$ space is bad (e.g. genome of small bacteria has 10^6 characters ~ 1 TB storage

IDEA:

instead of saving label $S[i..j]$ for e
we only save pair (i, j)
= compressed suffix tree

$\Rightarrow O(m)$ space (same space as text S)

Exampl: $S = xabxa\$$
1 2 3 4 5 6



Why suffix trees?

A: Examples!

! In what follows, we assume to have Ukkonen's version: $O(m)$ time

Exmpl 1 "exact text-search"

Given (long) text S & patter P (= string)
Does P in S occur?
Let T be suffix tree of S.

Call FLP (T, P) once O(|P|) time
return value is (end, index i', ..)
st P[1..i'] corresponds to label of path in T that starts in ϱ_T

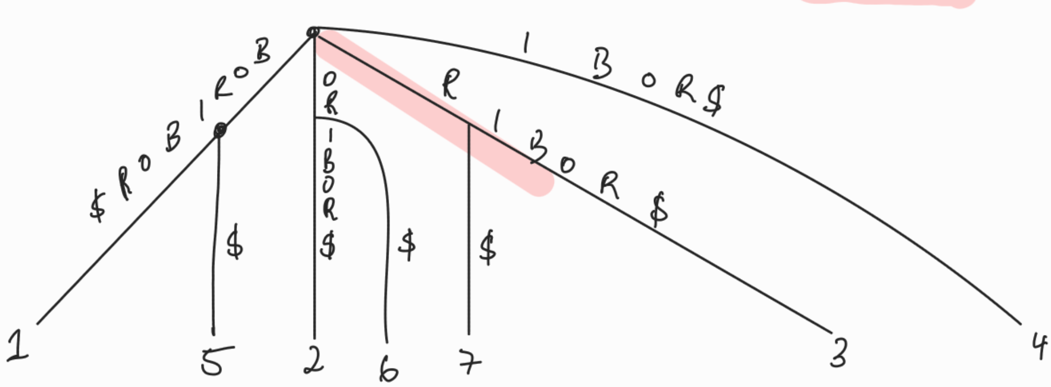
Observe, any path in T von ϱ to leaf i corresponds to S[i..m]
& P[1..i'] corresponds therefore to a prefix of some suffix of S, that is, a substring of S.

⇒ if i' = |P| ⇒ P occurs in T
else, not.

⇒ runtime O(|P|)

Exmpl: T = BORIBOR$. P = RIB

[every exist letter appears once at first letter of edge (ϱ v) for some v.]



Exmpl 2 "substring - database - search"

Given strings $S_1 \dots S_\ell$ (Database of Texts)
Does P occur in (at least) one of the S_i?

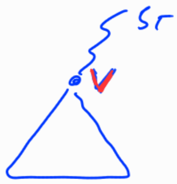
$\Rightarrow$ let $\$_1 \dots \$_\ell$ pairw. distinct symbols that do not occure in any S_i & P

put $S = S_1 \$_1 S_2 \$_2 \dots S_\ell \$_\ell$
Construct suffixtree T for S $\quad (O(|S_1| + |S_2| + \dots |S_\ell|)$ time$)$
use IDEA of Exmpl 1

Exmpl 3 Find all occurences of P

given S with suffixtree T & pattern P with $|P| = n$
Find all occurrences of P in T, that is,
all indices i st $P = S[i \dots i+n-1]$

Call $FLP(T, P)$
$\longrightarrow$ this gives $end = v$ or $end = edge(uv)$

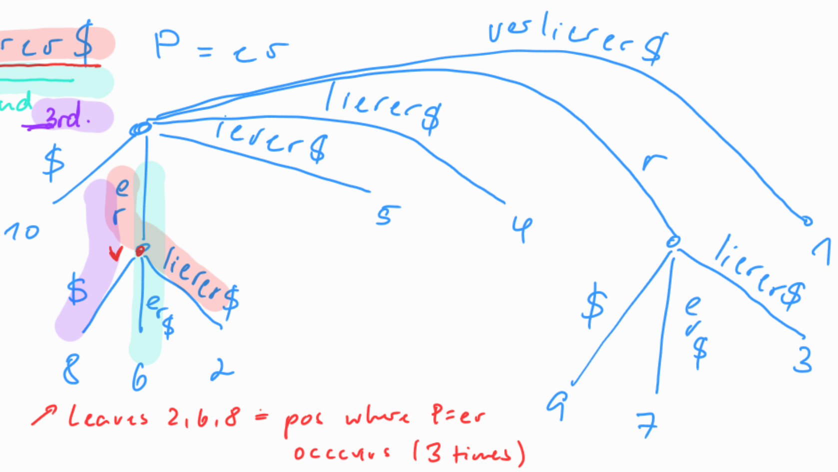


$\#$ leaves $i \leq_T v$ = $\#$ occurrences of P in S

& P occurs in pos i $\forall$ all leaves $i \leq_T v$.

[Exercise: works in $O(|P| + k)$ time]
k = nr of occurrences of P

$S =$ verlierer$ $\quad P = er$
1st occ, 2nd, 3rd.



Leaves 2, 6, 8 = pos where P=er occurs (3 times)

Exampl 4

Find longest substring in S that occurs at least 2 times

[Application: Find repeated regions in genom]

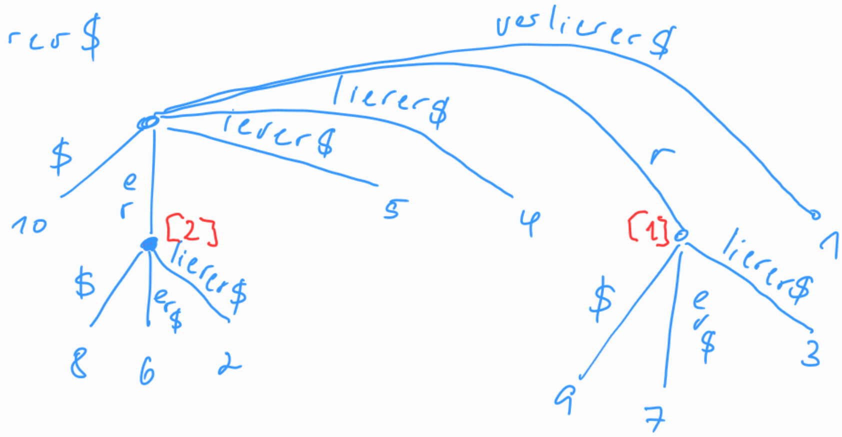
MISSISSIPPI   issi

string depth of v in T is $|\alpha|$

α = path label of path from r_T to v

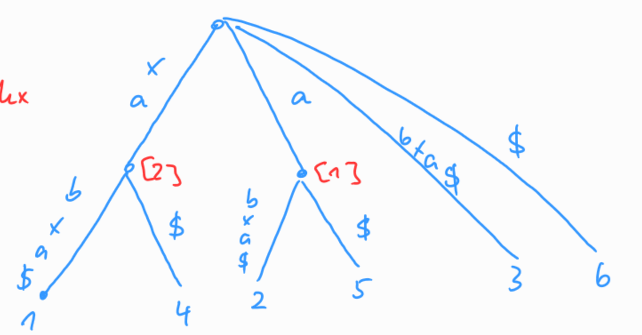
$S =$ verlierer\$

string depth of inner vertex



$S =$ xabxa\$

string depth of inner vertex



xa occurs 2 times.

- every inner vertex has 2 children (at least) & first symbol on edges with same parent have distinct symbols

$\Rightarrow$ length of longest substring that occurs at least 2 times

= maximum string-depth of inner vertices.

[Exus.: works in $O(|S|)$ time.]

Exampl 5 efficient detection of pairwise overlaps

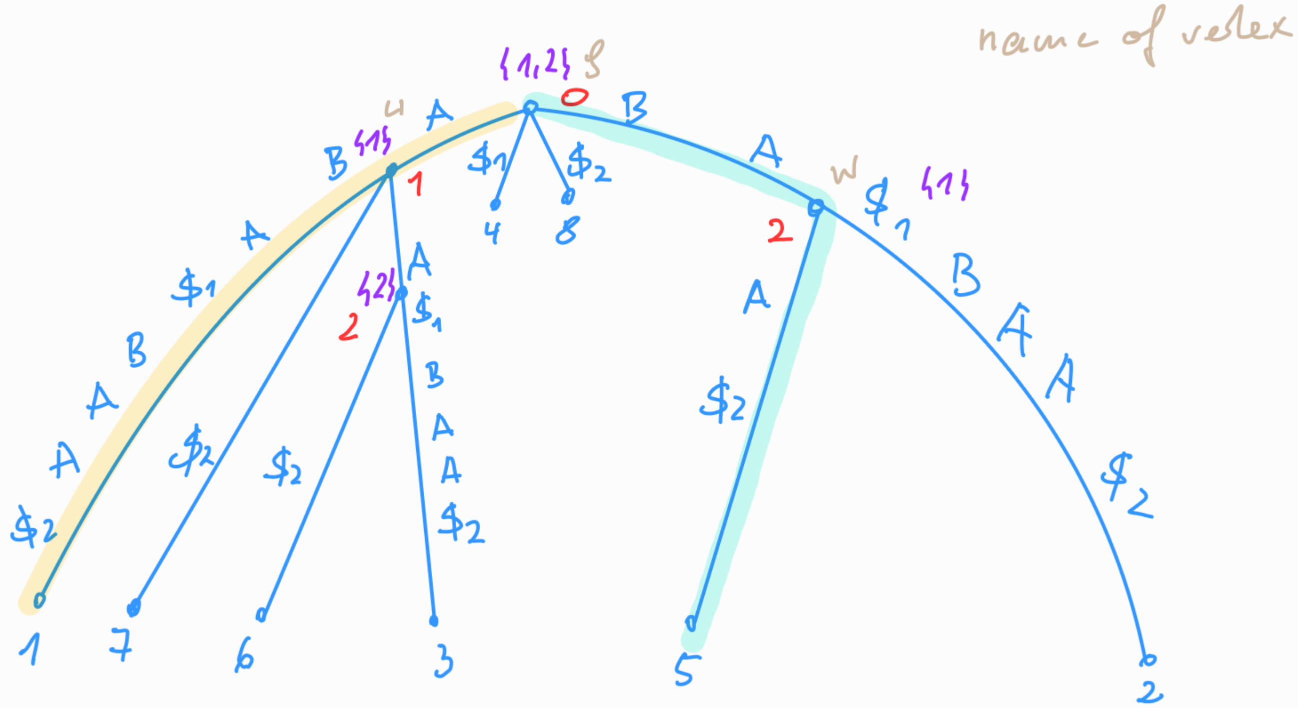
given $J = \{S_1 \dots S_N\}$ set of strings (e.g. sequenced DNA fragments)

Aim: define $ov(S_i, S_j)$ $\forall i,j$
= size of largest overlap

$S = S_1 \$_1 S_2 \$_2 \dots S_N \$_N$

$S_1 = ABA$
$S_2 = BAA$ $\longrightarrow$ $ov(S_1 S_2) = 2$
$ov(S_2 S_1) = 1$

$S = \overset{1}{A}\overset{2}{B}\overset{3}{A}\overset{4}{\$_1}\overset{5}{B}\overset{6}{A}\overset{7}{A}\overset{8}{\$_2}$



P_1 = path starting with label $S_1 \$_1$
P_2 = path starting with label $S_2 \$_2$

for non-leaf x: $L(x) = \{ i \mid \exists$ leaf v s.t. (x,v) edge in suffix tree & label (x,v) starts with $\$_i \}$.

string depth of x = # characters on path ξ to x.

For ($j = 1 .. N$)
  $x = g$ (root)
  WHILE (x not leaf)
    FOR (all $i \in L(x)$, $i \neq j$)
      IF ($depth(x) < \min(|S_i|, |S_j|)$
        or $(S_i, S_j) = depth(x)$
  $x \leftarrow$ child of x on $\#_j$

$j = 1$, $x = g$

FOR ($i \in L(g) = \{1, 2\}$, $i \neq 1$)

$\Rightarrow i = 2$

$depth(v) = 0 < \min(|S_1|, |S_2|)$

$\Rightarrow ov(S_2 S_1) = 0$

$x \leftarrow u$

FOR ($i \in L(u) = \{1\}$, $i \neq 1$)
nothing

$x \leftarrow$ leaf stop.

$j = 2$, $x = g$

For ($i \in L(g) = \{1, 2\}$, $i \neq 2$)

$\Rightarrow i = 1$

$dept(g) = 0 < \min(|S_1|, |S_2|)$

$or(S_1, S_2) = 0$

$x \leftarrow w$

For ($i \in L(w) = \{1\}$, $i \neq 2$)

$\Rightarrow i = 1$

$depth(w) = 2 < \min(S_1, S_2)$

$\Rightarrow or(S_1, S_2) = 2$

$x \leftarrow$ leaf stop.

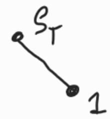
[without proof of correctness or runtime analysis]
$O(N \, \|S\|)$

Exercise ↗ Book "Alg. Aspects of Bioinf.")

Appendix

Details of $O(n^2)$ Algorithm

SUFFIX-TREE (S)

init $\mathcal{T}$ as  and label $(\varrho_\mathcal{T}, 1) = S[1..m]$

FOR ($i = 2..m$) DO

  (end, i', ℓ') = FIND_LONGEST_PATH ($\mathcal{T}$, $S[i..m]$) // returns end of path, that is, either end = v or end = e & index i' & ℓ'

  IF (end = edge e) // $e = (uw)$ with label γ

    remove $e = (uw)$ 
    add new vertex v
    add new edges $e_1 = (uv)$, $e_2 = (v, w)$
      & label $e_1 = \gamma[1..\ell']$
      label $e_2 = \gamma[\ell'+1..|\gamma|]$

  add edge (v, i) to $\mathcal{T}$ with label $S[i+i'..m]$

FIND_LONGEST_PATH ($\mathcal{T}$, S')

$j = 1$, $v = \varrho_\mathcal{T}$

WHILE ($j \le |S'|$) DO

  Find edge $e = (vw)$ in $\mathcal{T}$, $w \le_\mathcal{T} v$, whose label starts with $S'(j)$

  IF (such edge does not exist)
      RETURN (v, $j-1$, $\emptyset$) // path ends in v

  Let γ be label of e

  $\ell = 1$

  WHILE ($j \le |S'|$ & $\ell \le |\gamma|$ & $S'(j) = \gamma(\ell)$) DO
      $j = j+1$
      $\ell = \ell + 1$

  IF ($\ell \le |\gamma|$) // while loop ended at some point before "$S'(j) = \gamma(\ell)$ $\forall \ell = 1..|\gamma|$" ie, $S(j) \ne S(\ell)$
      RETURN (e, $j-1$, $\ell - 1$)

  $v = w$ // go to consider edges starting at w

RETURN (v, $|S'|$, $\emptyset$)

Prop. 8.2 Alg. SUFFIXTREE correctly computes suffixtree for $S = x_1 \dots x_m$, $x_m = \$$.

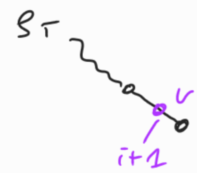
proof: (X1): T_1 has 1 leaf, T_2 has 2 leaves $\overset{\text{Ind}}{\dots}$ T_m has m leaves ✓

(sketch) (X2): T_1: 

✓

Assume, for T_i, each inner vertex (except possibly ϱ) has at least 2 children

reconstr. T_{i+1}: 



✓

(X3) by construction & induction each edge has non-empty string as label

(X4) T_1 ✓ Assume for T_i $\forall v$: label (vv_1), (vv_2) starts with different symbol, where v_1, v_2 are children of v.

T_{i+1}: 

Since α is longest substring that is prefix of

$S[i+1..m] = \underbrace{x_{i+1} \dots x_r}_{\alpha} \underbrace{\dots x_m}_{\beta}$

$\beta(1) \neq x_{r+1}$ as otherwise α not longest prefix! ✓

(X5) by constr. & induct. concatenating edge-labels from ϱ to i yields $S[i \dots m]$.

$\square$

Runtime:

[suffix-tree has $O(m)$ edges & vertices]

SUFFIXTREE(S), $S = x_1 \dots x_m$

add/remove etc in $O(1)$ time

→ m times FIND_LONGEST_PATH (FLP) is called.

FPL: • in each of the $|S'|$-steps in 1st while-loop

Find-edge → for v all neighbors w are considered

$\Rightarrow$ $\deg_T(v)$ many vertices

over all calls of 1st-while loop, "FIND_edge" is called,

$\leq \sum_{v \in V} \deg(v) = 2|E| = O(|E|)$ times $= O(m)$

• 1st + 2nd while loop:

```
WHILE (j ≤ |S'|) DO
  :
  WHILE (j ≤ |S'| & l ≤ |γ| & S'(j) = γ(l)) DO
  |  j = j + 1
  |  :
```

$\Rightarrow$ $j \leq m$ $\Rightarrow$ $O(m)$ time

• Remaining operation in 1st-while loop: $O(1)$

$\Rightarrow$ FLP runs in $O(m)$ time

$\Rightarrow$ SUFFIX-TREE(S) runs in $O(m^2)$ time.

Theorem [UKKONEN]: for S of length m the suffix tree can be constructed in $O(m)$ time

[without proof]