

# ADS: Algorithmen und Datenstrukturen 2

## Teil VII: Suffix Trees

Steve Hoffmann

Bioinformatics Group, Dept. of Computer Science & Interdisciplinary Center for  
Bioinformatics, **University of Leipzig**

21. Mai 2010

# suffix and prefix: intuition

What is a suffix?

- “*suffix?*” is a suffix of “*What is a suffix?*”
- “*a suffix?*” is a suffix of “*What is a suffix?*”
- “*What is a suffix?*” for sure is a suffix of “*What is a suffix?*”

What is a prefix?

- “*What*” is a prefix of “*What is a suffix?*”
- “*What is*” is a prefix of “*What is a suffix?*”
- “*What is a suffix?*” for sure is a prefix of “*What is a suffix?*”

# formalities: alphabet and characters

Let  $\mathcal{A}$  be a finite set, the alphabet.

- the elements of  $\mathcal{A}$  are characters.
- $\epsilon$  denotes the empty string.
- strings are written by juxtaposition of characters:

The set  $\mathcal{A}^*$  of strings over  $\mathcal{A}$  is defined by

$$\mathcal{A}^* = \bigcup_{i \geq 0} \mathcal{A}_i \tag{1}$$

where  $\mathcal{A}_0 = \{\epsilon\}$  and  $\mathcal{A}_{i+1} = \{aw \mid a \in \mathcal{A}, w \in \mathcal{A}^i\}$ .

- $\mathcal{A}^+$  denotes a non-empty string

# formalities: strings, suffixes and prefixes

Let  $s$  be a string over the alphabet  $\mathcal{A}$

- let  $|s|$  denote the length of  $s$ .

We assume a string of the form  $s = uvw$ ,  $u, v, w \in \mathcal{A}^*$ :

- $u$  is a prefix of  $s$
- $v$  is a substring of  $s$
- $w$  is a suffix of  $s$

Note, that by using  $\epsilon$  every string may be partitioned to  $uvw$ !

# Searching strings

Current genome projects and internet data bases accumulate massive amounts of sequences (texts). Searching such texts can be pretty cumbersome!

Considering a large sequence  $S$  over  $\mathcal{A} = \{A, C, T, G\}$ . We may ask:

- does ACTGCTTACGTACGGTA occur in  $S$ ?
- how often does ACTGCTTACGTACGGTA occur in  $S$ ?
- where does ACTGCTTACGTACGGTA occur in  $S$ ?

For **large sequences** that are **frequently queried** we need more sophisticated strategies to answer these questions quickly.

# Indexing

For a large string  $s$  that is frequently queried (ie. a genome) we could think about **indexing all substrings**. The following theorem shows why this is **not such a good idea**:

## Theorem

*A string  $s$  of length  $|s| = n$  has at most  $O(n^2)$  different substrings.*

## Proof.

Idea: for each  $0 \leq i \leq n - 1$ ,

$$\bigcup_{i \leq j \leq n-1} s[i..j] \quad (2)$$

is the set of substrings beginning at position  $i$ . Alphabet?

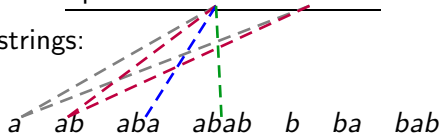
Hence, we need another way to represent this data.

# towards suffix trees: implicit representation of substrings

Consider the string  $s = abab$

string	a	b	a	b
position	0	1	2	3

we observe substrings:



- **substrings are prefixes of suffixes:**  $abab$ ,  $bab$ ,  $ab$ ,  $b$
- each substring is implicitly represented by at least one suffix
- **at most  $O(n^2)$  substrings but only  $O(n)$  suffixes!**

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# towards suffix trees: implicit representation of substrings

Consider the string  $S = abab$

we observe substrings:

$a$   $ab$   $aba$   $abab$   $b$   $ba$   $bab$

substrings are prefixes of suffixes:

$abab, bab, ab, b$



- each substring is implicitly represented by at least one suffix
- **at most  $O(n^2)$  substrings but only  $n$  suffixes!**

# towards suffix trees: implicit representation of substrings

Consider the string  $S = abab$

- we observe substrings  $a$ ,  $ab$ ,  $aba$ ,  $abab$ ,  $b$ ,  $ba$  and  $bab$
- **substrings are prefixes of suffixes**:  $abab$ ,  $bab$ ,  $ab$ ,  $b$
- each substring is implicitly represented by at least one suffix
- **at most  $O(n^2)$  substrings but only  $n$  suffixes!**

We append a unique character (sentinel)  $\$$  to the end of  $s$ :

$$S\$ = abab\$$$

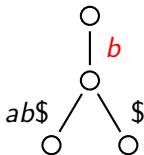
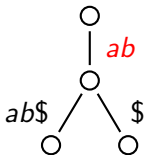
Reason?

## towards suffix trees: common prefixes

Given all suffixes  $abab\$, bab\$, ab\$, b\$, \$$  we observe

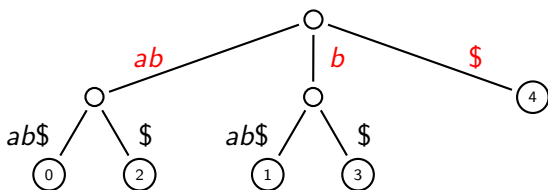
- $ab$  is longest common prefix for  $abab\$$  and  $ab\$$
- $b$  is longest common prefix for  $bab\$$  and  $b\$$
- $\$$  is longest prefix of  $\$$

This gives us three partial trees:



# a suffix tree

Combining the three partial trees leads to a complete suffix tree:



string	a	b	a	b	\$
position	0	1	2	3	4

More on suffix tree construction later ...

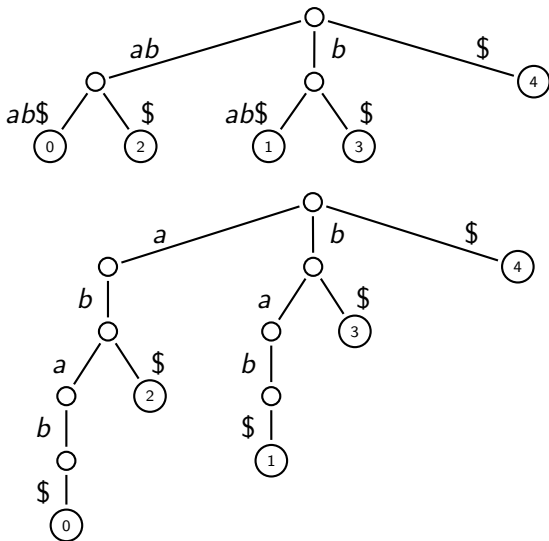
# formalities: suffix tree

## Definition (suffix tree)

A suffix tree  $ST(S\$)$  for a sequence  $S \in \mathcal{A}^+$

- 1 edges labeled by non-empty strings over  $\mathcal{A}$
- 2 for every node only one edge begins with same  $a \in \mathcal{A}$
- 3 compact, ie. has no internal nodes with less than two successors (in contrast to suffix trie)
- 4 represents all substrings of  $S$

a suffix tree is compact, a suffix trie is not

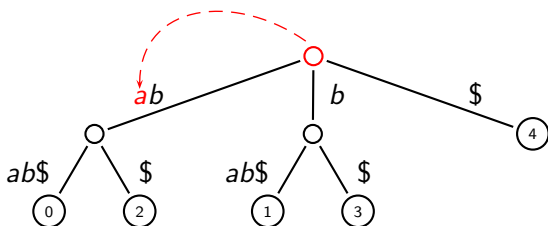


# searching in a suffix tree

Searching a query sequence  $q$  in a suffix tree is easy. At internal nodes we look for a branch that starts with next character in  $q$ , on edges we simply continue to match the labels.

Lets search the query  $q = ab$ .

- the search starts with the first character of  $q$ ,  $q[0] = a$



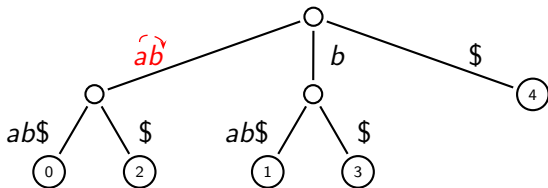


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- the search starts with the first character of  $q$ ,  $q[0] = a$
- and continues with the next character  $q[1] = b$

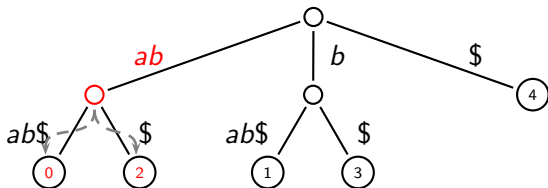


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Lets search the query  $q = ab$ .

- the search starts with the first character of  $q$ ,  $q[0] = a$
- and continues with the next character  $q[1] = b$
- we immediately see:  $q$  occurs twice in  $S\$$  at positions 0 and 2.



# complexity considerations

The suffix tree  $ST(S)$  for the sequence  $S\$$  with  $|S| = n$

- has at most  $n - 1$  internal nodes and  $n$  leaves  $\Rightarrow O_{space}(n)$

Due to their compactness suffix trees require much less space in practice compared to suffix tries.

- for a query of length  $m$ , searches in the suffix tree take at most  $m$  character comparisons  $\Rightarrow O_{search}(m)$

# naive construction: top-down

In order to devise an algorithm to construct suffix trees, we will make use of the following observations:

- a node  $\alpha$  represents all suffixes of  $S\$$  that start with the same prefix  $u$
- only one outgoing edge from  $\alpha$  begins with same  $a \in \mathcal{A}$
- we can restrict our evaluation to at most  $|\mathcal{A}|$  subsets of suffixes with  $uav$ , where  $a \in \mathcal{A}$  and  $v \in \mathcal{A}^*$

## naive construction: simplifications

We will now devise the algorithm **topdown**. For reasons of simplicity we assume

- To construct the suffix tree we call **topdown**  $(U, 0)$ , where  $U$  is a set of pairs that initially(!) holds all suffixes and their positions in  $S$ , ie.  
$$U = \{(s, i) \mid S[i..n-1] = s, 0 \leq i \leq n-1\}$$
- let **getlcp** $(U)$  be a function evaluates the longest common prefix for all strings  $s$  in  $(s, i) \in U$
- let **insertEdge** $(\alpha, u, \beta)$  be a function that inserts an edge with label  $u$  between the nodes  $\alpha$  and  $\beta$ .
- let **insertLeaf** $(\alpha, u, i)$  be a function that attaches a leaf  $i$  with edge label  $u$  to  $\alpha$ .

# naive construction: pseudo-code

algorithm: topdown

**Require:** set of pairs  $U$ , length of lcp  $\ell$

$\forall a \in \mathcal{A} : P_a = \emptyset$ , node  $\alpha$

**for all**  $(s, i) \in U$  **do**

$a := s[\ell]$

$P_a := P_a \cup (s[\ell + 1..n - 1], i)$

**end for**

**for all**  $a \in \mathcal{A}$  **do**

**if**  $|P_a| > 1$  **then**

$v := \text{getlcp}(P_a)$

$\beta := \text{topdown}(P_a, |v|)$

$\text{insertEdge}(\alpha, av, \beta)$

**else if**  $|P_a| = 1$  **then**

$(s, i) := P_a$

$\text{attachLeaf}(\alpha, as, i)$

**end if**

**end for**

**return**  $\alpha$

# naive construction: example

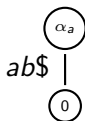
For  $s = abab\$$ :  $U = \{(abab\$, 0), (bab\$, 1), (ab\$, 2), (b\$, 3), (\$, 4)\}$

- $P_a = \{(bab\$, 0), (b\$, 2)\}$ ,  $\text{getlcp}(P_a) = 1$

# naive construction: example

For  $s = abab\$$ :  $U = \{(abab\$, 0), (bab\$, 1), (ab\$, 2), (b\$, 3), (\$, 4)\}$

- $P_a = \{(bab\$, 0), (b\$, 2)\}$ ,  $\text{getlcp}(P_a) = 1$ 
  - $P_a = \{(b\$, 0)\} \rightarrow \text{addLeaf}(\alpha_a, ab\$, 0)$

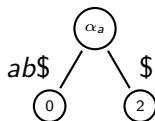




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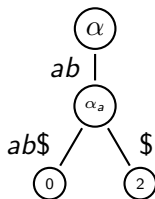
- $P_a = \{(bab\$, 0), (b\$, 2)\}$ ,  $\text{getlcp}(P_a) = 1$ 
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  - $P_\$ = \{(\epsilon, 2)\} \rightarrow \text{addLeaf}(\alpha_a, \$, 2)$



# naive construction: example

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  - $P_\$ = \{(\epsilon, 2)\} \rightarrow \text{addLeaf}(\alpha_a, \$, 2)$
- $\rightarrow \text{insertEdge}(\alpha, ab, \alpha_a)$



Can you continue this example?

## naive construction: complexity

The naive construction does not perform very well

- complexity of naive suffix tree construction is  $O(n^2)$ . Proof?

We can do better:

- Ukkonen has devised an online construction algorithm that runs in  $O(n)$ .
- McCreight's  $O(n)$ -algorithm also runs slightly faster in practice.

# McCreight's algorithm

- The idea: successively merge  $ST(S[i..n])$  with  $ST(S[i+1..n])$ ,  $i \in [0, n]$
- exploits the properties of longest common prefixes

## Definition (head)

The  $head(i)$  of some suffix  $S[i..n]$ ,  $0 \leq i \leq n-1$  is the longest common prefix of with  $S[j..n]$ , where  $j < i$ .

## Definition (tail)

The  $tail(i)$  is simply the rest:  $S[i..n] = head(i)tail(i)$

# heads up: McCreight's trick

To appreciate the trick we need to understand the following observation:

- 1 Once the suffix tree for  $S[0..n]..S[i..n]$  is build, we need to **update only those parts of ST that are “affected”** by introducing the suffix  $S[i + 1..n]$
- 2 Only parts beyond the head, ie. within the tail, may be “affected”.

# heads up: McCreight's trick

## Beweis.

Let  $ST(S)$  be as suffix tree of a string  $S$ . Assume the string  $av$  has a prefix implicitly represented in  $ST(S)$ . Hence, there is a search-path from the root to some edge or node (leaf?)

$\Rightarrow$  the search-path is of length  $\max_{j \leq |S|} lcp(av, S[j..n]) = \ell$

$\Rightarrow lcp(v, S[j..n]) = k \geq \ell - 1$

$\Rightarrow$  substring  $v[0..\ell-1]$  is also implicitly represented by  $ST(S)$

$\Rightarrow$  only suffix tree modifications below internal nodes or edge labels representing  $v[\ell-1..n]$  are necessary □

Hence, finding an inexpensive way to locate the head yields an inexpensive algorithm. Let's pretend we've found it:

**magic(head(i))** delivers  $p \in ST$  with  $p$  representing the substring  $S[i+1..i+\ell-1]$ .

# linear construction: algorithm M

```
Require: initial suffix tree for  $S[0..n-1]$   
for  $i$  in 0 to  $n - 2$  do  
  if  $\text{head}(i) = \epsilon$  then  
     $\text{head}(i+1) := \text{scan}(\epsilon, S[i+1..n])$   
    if  $\text{head}(i+1) \in E$  then  
       $\text{addNode}(\text{head}(i+1))$   
    end if  
     $\text{addLeaf}(\text{head}(i+1), \text{tail}(i+1), i+1)$   
  else  
     $p := \text{magic}(\text{head}(i))$   
    if  $p \in E$  then  
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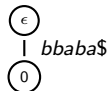
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```

$i$	0
$S[i+1..n]$	baba\$
$\text{head}(i)$	$\epsilon$
$\text{tail}(i)$	bbaba\$





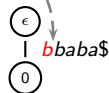
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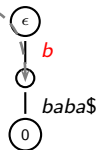
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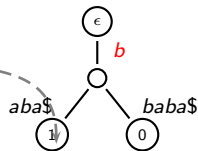
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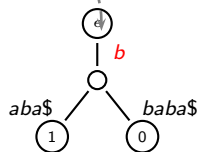
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$S[i+1..n]$	aba\$
$\text{head}(i)$	b
$\text{tail}(i)$	aba\$



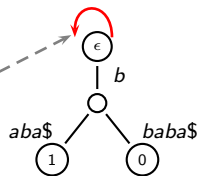
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    if  $p \in E$  then
       $\text{head}(i+1) = p$ 
    else if  $p \in V$  then
       $\text{head}(i+1) = \text{scan}(p, \text{tail}(i))$ 
    end if
    if  $\text{head}(i+1) \in E$  then
       $\text{addNode}(\text{head}(i+1))$ 
    end if
     $\text{addLeaf}(\text{head}(i+1), \text{tail}(i+1), i+1)$ 
  end if
end for

```

$i$	1
$S[i+1..n]$	aba\$
$\text{head}(i)$	b
$\text{tail}(i)$	aba\$



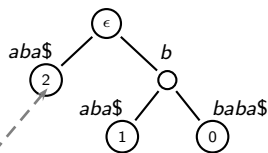
# linear construction: algorithm M

```

Require: initial suffix tree for  $S[0..n-1]$ 
for  $i$  in 0 to  $n - 2$  do
  if  $\text{head}(i) = \epsilon$  then
     $\text{head}(i+1) := \text{scan}(\epsilon, S[i+1..n])$ 
    if  $\text{head}(i+1) \in E$  then
       $\text{addNode}(\text{head}(i+1))$ 
    end if
     $\text{addLeaf}(\text{head}(i+1), \text{tail}(i+1), i+1)$ 
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     $\text{addLeaf}(\text{head}(i+1), \text{tail}(i+1), i+1)$ 
  end if
end for

```

$i$	1
$S[i+1..n]$	aba\$
$\text{head}(i)$	b
$\text{tail}(i)$	aba\$



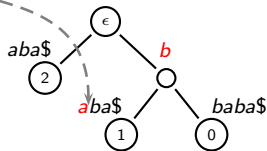
# linear construction: algorithm M

```

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    end if
     $\text{addLeaf}(\text{head}(i+1), \text{tail}(i+1), i+1)$ 
  end if
end for

```

$i$	2
$S[i+1..n]$	ba\$
$\text{head}(i)$	$\epsilon$
$\text{tail}(i)$	aba\$



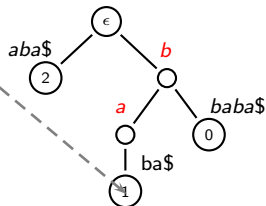
# linear construction: algorithm M

```

Require: initial suffix tree for  $S[0..n-1]$ 
for  $i$  in 0 to  $n - 2$  do
  if  $\text{head}(i) = \epsilon$  then
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       $\text{addNode}(\text{head}(i+1))$ 
    end if
     $\text{addLeaf}(\text{head}(i+1), \text{tail}(i+1), i+1)$ 
  end if
end for

```

$i$	2
$S[i+1..n]$	ba\$
$\text{head}(i)$	$\epsilon$
$\text{tail}(i)$	aba\$





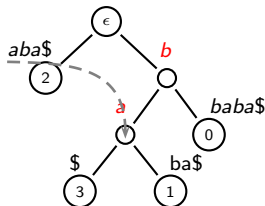
# linear construction: algorithm M

```

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  if  $\text{head}(i) = \epsilon$  then
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  end if
end for

```

$i$	2
$S[i+1..n]$	ba\$
$\text{head}(i)$	$\epsilon$
$\text{tail}(i)$	aba\$



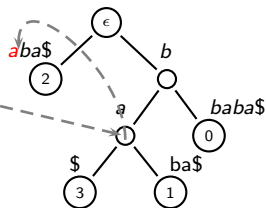
# linear construction: algorithm M

```

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  if  $\text{head}(i) = \epsilon$  then
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    if  $\text{head}(i+1) \in E$  then
       $\text{addNode}(\text{head}(i+1))$ 
    end if
     $\text{addLeaf}(\text{head}(i+1), \text{tail}(i+1), i+1)$ 
  end if
end for

```

$i$	3
$S[i+1..n]$	a\$
$\text{head}(i)$	ba
$\text{tail}(i)$	\$



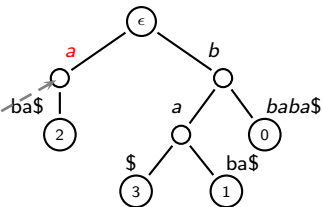
# linear construction: algorithm M

```

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    end if
     $\text{addLeaf}(\text{head}(i+1), \text{tail}(i+1), i+1)$ 
  end if
end for

```

$i$	3
$S[i+1..n]$	a\$
$\text{head}(i)$	ba
$\text{tail}(i)$	\$



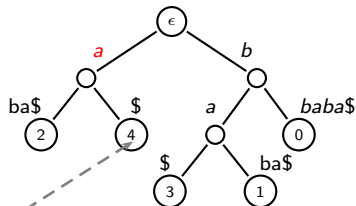
# linear construction: algorithm M

```

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  end if
end for

```

$i$	3
$S[i+1..n]$	a\$
$\text{head}(i)$	ba
$\text{tail}(i)$	\$



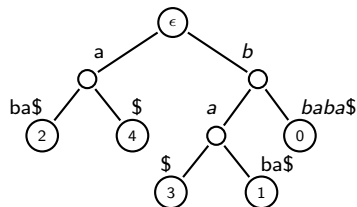
# linear construction: algorithm M

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for  $i$  in 0 to  $n - 2$  do
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    if  $\text{head}(i+1) \in E$  then
       $\text{addNode}(\text{head}(i+1))$ 
    end if
     $\text{addLeaf}(\text{head}(i+1), \text{tail}(i+1), i+1)$ 
  end if
end for

```

$i$	4
$S[i+1..n]$	\$
$\text{head}(i)$	a
$\text{tail}(i)$	\$



What will happen now?

# magic

For some  $\text{head}(i) = S[i..i+\ell]$ , the function **magic(head(i))** delivers a position  $p \in ST(S)$  with  $p$  representing the substring  $S[i+1..i+\ell-1]$ . It is realized using **suffix links**:

- suffix links are only defined on nodes
- to use suffix link, go back to parent node
- while going back remember all edge labels
- jump to another node via suffix link
- rematch the edge labels
- done. we reached the location for  $S[i+1..i+\ell-1]$ .

Suffix links can be updated during the construction of the suffix tree with algorithm M.

# Suffix trees: a stringology toolbox

- 1 string search
- 2 longest common substrings (two strings)
- 3 longest repeated substrings (one string)
- 4 for each suffix of a pattern, get length of the longest match
- 5 shortest unique substrings
- 6 ...