ADS: Algorithmen und Datenstrukturen 2 Teil VII: Suffix Trees

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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.
- ϵ denotes the empty string.
- strings are written by juxtaposition of characters:

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

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

where $A_0 = \{\epsilon\}$ and $A_{i+1} = \{aw \mid a \in A, w \in A^i\}$. • 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, $u, v, w \in A^*$:

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

Note, that by using ϵ every string may be particulated 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 $A = \{A, C, T, G\}$. 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 $0 \le i \le n-1$,

$$\bigcup_{i \le j \le n-1} s[i..j] \tag{2}$$

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

Hence, we need another way to represent this data.

Consider the string s = abab

string	а	b	а	b
position	0	1	2	3

Consider the string s = abab

string	а	b	а	b
position	0	1	2	3

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 O(n) suffixes!

Consider the string s = abab



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Consider the string S = abab

we observe substrings:



each substring is implicitly represented by at least one suffix

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Consider the string S = abab

we observe substrings:



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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 O(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 **b**ab\$ and **b**\$
- § is longest prefix of \$

This gives us three partial trees:







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



More on suffix tree construction later ...

formalities: suffix tree

Definition (suffix tree)

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

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

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

$$U = \{(s, i) \mid S\$[i..n-1] = s, 0 \le i \le n-1\}$$

- let getlcp(U) be a function evaluates the longest common prefix for all strings s in (s, i) ∈ U
- let insertEdge(α, u, β) be a function that inserts an edge with label u between the nodes α and β.
- let insertLeaf(α, u, i) be a function that attaches a leaf i with edge label u to α.

```
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 := \operatorname{getlcp}(P_a)
           \beta := \operatorname{topdown}(P_a, |v|)
           insertEdge(\alpha, av, \beta)
       else if |P_a| = 1 then
           (s,i) := P_a
           attachLeaf(\alpha, as, i)
       end if
   end for
    return \alpha
```

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partition wrt. to first character not belonging to the lcp

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if there are >= 2 suffixes get lcp for the set call topdown insert edge

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       else if |P_a| = 1 then
           (s,i) := P_a
           attachLeaf(\alpha, as, i)
       end if
   end for
   return \alpha
```

partition wrt. to first character not belonging to the lcp

if there are >= 2 suffixes get lcp for the set call topdown insert edge

this suffix is unique we attach a leaf

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

- \rightarrow first call
 - $P_a = \{(bab\$, 0), (b\$, 2)\}$, getlcp $(P_a) = b$, | getlcp $(P_a) | = 1$

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

→ first call
•
$$P_a = \{(bab\$, 0), (b\$, 2)\}, \text{ getlcp}(P_a) = b, | \text{ getlcp}(P_a) | = 1$$

• $P_b = \{(ab\$, 1), (\$, 3)\}, \text{ getlcp}(P_b) = \epsilon, | \text{ getlcp}(P_b) | = 0$

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

→ first call
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$$P_a = \{(bab\$, 0), (b\$, 2)\}, \text{ getlcp}(P_a) = b, | \text{ getlcp}(P_a) | = 1$$

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→ second call

•
$$P_a = \{(b\$, 0)\} \Longrightarrow \mathsf{addLeaf}(\alpha_a, ab\$, 0)$$



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

→ first call
•
$$P_a = \{(bab\$, 0), (b\$, 2)\}, \text{ getlcp}(P_a) = b, | \text{ getlcp}(P_a) | = 1$$

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→ second call

•
$$P_a = \{(b\$, 0)\} \Longrightarrow \operatorname{addLeaf}(\alpha_a, ab\$, 0)$$

• $P_\$ = \{(\epsilon, 2)\} \Longrightarrow \operatorname{addLeaf}(\alpha_a, \$, 2)$



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

→ first call
•
$$P_a = \{(bab\$, 0), (b\$, 2)\}$$
, getlcp $(P_a) = b$, | getlcp $(P_a) | = 1$
• $P_b = \{(ab\$, 1), (\$, 3)\}$, getlcp $(P_b) = \epsilon$, | getlcp $(P_b) | = 0$
→ second call
• $P_a = \{(b\$, 0)\} \Longrightarrow addLeaf(\alpha_a, ab\$, 0)$

•
$$P_a = \{(b\mathfrak{H}, 0)\} \Longrightarrow \mathsf{addLeaf}(\alpha_a, ab\mathfrak{H}, 0)$$

• $P_{\mathfrak{h}} = \{(\epsilon, 2)\} \Longrightarrow \mathsf{addLeaf}(\alpha_a, \mathfrak{h}, 2)$

• \implies insertEdge(α , *ab*, α_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.

Growing trees

Question

Assume you have built a suffix tree for the string

aba\$

Which modifications are necessary to obtain the suffix tree for

aba<mark>ba</mark>\$

Can the old tree be of any use?

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], $0 \le i \le n-1$ 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:

- 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]
- 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 $max_{j \le |S|} lcp(av, S[j..n]) = \ell$ $\Rightarrow lcp(v, S[j..n]) = k \ge \ell - 1$ \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 a position within ST with p representing the substring $S[i+1..i+\ell-1]$. p may be on an edge or a vertex.

```
Require: tree for the suffix S$[0..n-1]
  for i in 0 to n-2 do
      if head(i) = \epsilon then
         head(i+1) := scan(ST(\epsilon), S[i+1..n])
         if head(i+1) ends in edge then
            addNode(head(i+1))
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
     else
         p := magic(head(i))
         if p ends in edge then
            head(i+1) = p
         else if p ends in vertex then
            head(i+1) = scan(ST(p), tail(i))
         end if
         if head(i + 1) ends in edge then
            addNode(head(i+1))
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
      end if
  end for
```

0

```
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  for i in 0 to n-2 do
      if head(i) = \epsilon then
         head(i+1) := scan(ST(\epsilon), S[i+1..n])
                                                            S[i+1..n]
                                                                          baba$
         if head(i+1) ends in edge then
                                                            head(i)
            addNode(head(i+1))
                                                            tail(i)
                                                                         bbaba$
         end if
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  end for
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```
Require: tree for the suffix S$[0..n-1]
  for i in 0 to n-2 do
      if head(i) = \epsilon then
                                                                               0
         head(i+1) := scan(ST(\epsilon), S[i+1..n])
                                                             S[i+1..n]
                                                                          baba$
         if head(i+1) ends in edge then
                                                             head(i)
            addNode(head(i+1))
                                                            tail(i)
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                                                                             baba$
                                                               aba$
         else if p ends in vertex then
                                                                            0
            head(i+1) = scan(ST(p), tail(i))
         end if
         if head(i + 1) ends in edge then
                                                         S[i + 1..\ell - 1] not yet in tree
            addNode(head(i+1))
                                                             \Rightarrow magic(head(i)) = \epsilon
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
      end if
   end for
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                                                                          aba$
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                                                                               ba$
                                                                S[i+1..n]
         if head(i+1) ends in edge then
                                                                head(i)
            addNode(head(i+1))
                                                                tail(i)
                                                                             aba$
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
                                                                       \epsilon
      else
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                                                             aba
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                                                                     aba$
                                                                                   baba$
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                                                                           ba$
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                                                              tail(i)
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            head(i+1) = p
                                                                               baba$
         else if p ends in vertex then
                                                                              0
            head(i+1) = scan(ST(p), tail(i))
                                                                           ba$
         end if
                                                                          1
         if head(i + 1) ends in edge then
            addNode(head(i+1))
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
      end if
  end for
```

```
Require: tree for the suffix S$[0..n-1]
   for i in 0 to n-2 do
      if head(i) = \epsilon then
                                                                               3
         head(i+1) := scan(ST(\epsilon), S[i+1..n])
                                                                              a$
                                                                 S[i+1..n]
         if head(i+1) ends in edge then
                                                                 head(i)
                                                                              ba
            addNode(head(i+1))
                                                                 tail(i)
                                                                               $
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
      else
         p := magic(head(i))^{-1}
                                                            aba
         if p ends in edge then
            head(i+1) = p
                                                                                 baba$
         else if p ends in vertex then
                                                                                0
            head(i+1) = scan(ST(p), tail(i))
                                                                            ba$
         end if
                                                                   3
                                                                            1
         if head(i + 1) ends in edge then
            addNode(head(i+1))
         end if
                                                          S[i + 1..\ell - 1]=a in tree \Rightarrow
         addLeaf(head(i+1), tail(i+1), i+1)
                                                           p points to a-edge of root
      end if
   end for
```

```
Require: tree for the suffix S$[0..n-1]
   for i in 0 to n-2 do
      if head(i) = \epsilon then
                                                                             3
         head(i+1) := scan(ST(\epsilon), S[i+1..n])
                                                               S[i+1..n]
                                                                            a$
         if head(i+1) ends in edge then
                                                               head(i)
                                                                            ba
            addNode(head(i+1))
                                                               tail(i)
                                                                             $
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
      else
         p := magic(head(i))
         if p ends in edge then
            head(i+1) = p
                                                      ∕ba$
                                                                                  baba$
         else if p ends in vertex then
                                                            2
                                                                                 0
            head(i+1) = scan(ST(p), tail(i))
                                                                             ba$
         end if
                                                                    3
                                                                             1
         if head(i + 1) ends in edge then
            addNode(head(i+1))
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
      end if
   end for
```

```
Require: tree for the suffix S$[0..n-1]
  for i in 0 to n-2 do
      if head(i) = \epsilon then
                                                                             3
         head(i+1) := scan(ST(\epsilon), S[i+1..n])
                                                               S[i+1..n]
                                                                            a$
         if head(i+1) ends in edge then
                                                               head(i)
                                                                            ba
            addNode(head(i+1))
                                                               tail(i)
                                                                             $
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
     else
         p := magic(head(i))
         if p ends in edge then
            head(i+1) = p
                                                      ba$
                                                                                    baba$
         else if p ends in vertex then
                                                                 4
                                                         2
            head(i+1) = scan(ST(p), tail(i))
                                                                               ba$
         end if
         if head(i + 1) ends in edge then
            addNode(head(i+1))
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
      end if
  end for
```

```
Require: tree for the suffix S$[0..n-1]
  for i in 0 to n-2 do
      if head(i) = \epsilon then
         head(i+1) := scan(ST(\epsilon), S[i+1..n])
         if head(i+1) ends in edge then
            addNode(head(i+1))
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
     else
         p := magic(head(i))
         if p ends in edge then
            head(i+1) = p
         else if p ends in vertex then
            head(i+1) = scan(ST(p), tail(i))
         end if
         if head(i + 1) ends in edge then
            addNode(head(i+1))
         end if
         addLeaf(head(i+1), tail(i+1), i+1)
      end if
  end for
```

i	4
S[i+1n]	\$
head(i)	а
tail(i)	\$



What will happen now?

For some 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 $\mathsf{M}.$

Suffix trees: a stringology toolbox

string search

- Iongest common substrings (two strings)
- Iongest repeated substrings (one string)
- I for each suffix of a pattern, get length of the longest match
- Shortest unique substrings
- **()** ...

Abschlussveranstaltung SWT-Praktikum 2011

Im SWT-Praktikum stellen die studentischen Teams im 4. Semester ihre Fähigkeiten unter Beweis, ein größeres Software-Projekt im Umfang von etwa 1000 Mannstunden "nach den Regeln der Kunst" gemeinschaftlich zu planen und umzusetzen.

In der Abschlussveranstaltung

am 7. Juli 2011, 9:15 bis 10:45 Uhr im Hs 10

präsentieren die Teams in Vorträgen und Demonstrationen von je etwa 10 Minuten die Ergebnisse ihrer Arbeit der Öffentlichkeit.

Dazu sind alle Studenten des ersten Studienjahres, die sich bereits jetzt über die Anforderungen und Ergebnisse des SWT-Praktikums im 4. Semester informieren wollen, herzlich eingeladen.