Winter School St. Petersburg

Suffix Trees

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Introduction

Usage

☞ Solving many string problems in linear time

History

- **String algorithms**
  ☞ Knuth-Morris-Pratt, Boyer-Moore, Aho-Corasick
- **Suffix tree algorithms**
  – 1973 P.Weiner: first linear construction algorithm
  – 1976 E.M.McCreight:
  more space-efficient algorithm
  – 1993 E. Ukkonen: conceptually different approach

Outline

1. **Data Structures**
   - ☞ Suffix tries and trees
2. **Construction Algorithms**
   - Naïve algorithm
   - Algorithms of Weiner, McCreight & Ukkonen
3. **Examples of Use**
   - Exact string matching problems
   - Longest common substring
   - Assembly of Strings
4. **Conclusion**

Data Structures I

Preliminaries

Notations			
Σ	finite, non empty alphabet	$S=s_1s_2\ldots s_n$	arbitrary string
α, β, γ	possibly empty strings	$\|S\|=n$	length of S

Definitions	
$S[i..j]=s_is_{i+1}\ldots s_j$	**substring** of S
$S[1..i]$	**prefix** of S that ends at position i
$S_i=S[i..n]$, $1\leq i \leq n+1$	**suffix** of S that starts at position i
S_{n+1}	empty string ε
$S(i)$	character at position i in S
$\sigma(S)=\{S_i \mid 1 \leq i \leq \|S\|\}$	set of all suffixes of S

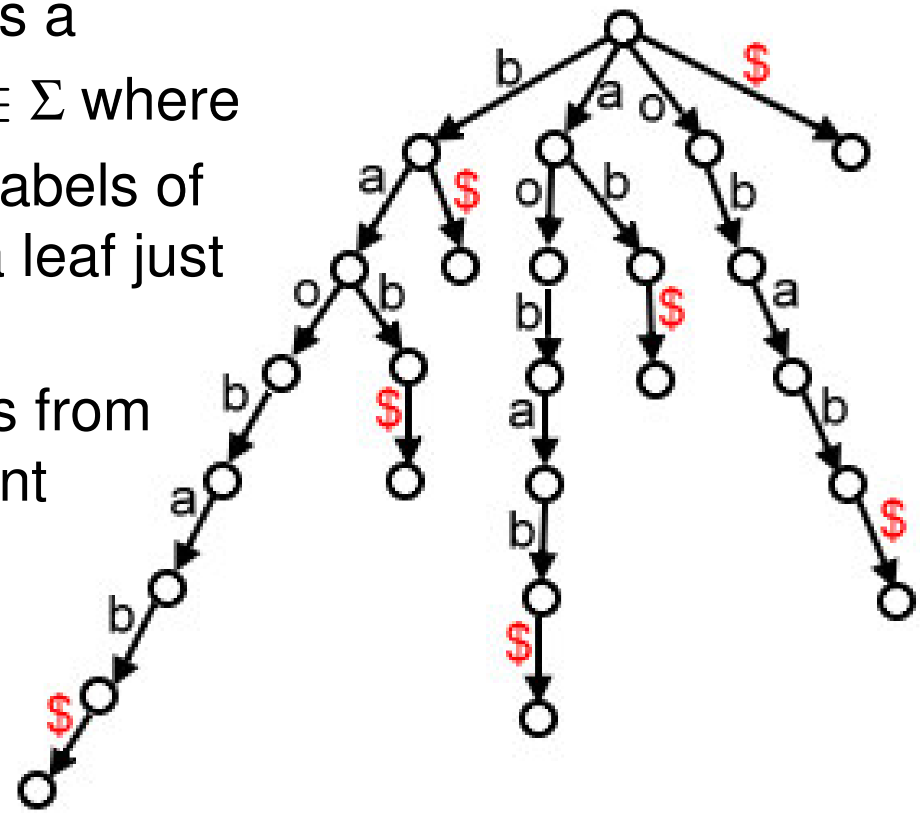
Data Structures II

Suffix Trie

Definition

A suffix trie for a string $S \subseteq \Sigma^n$ is a directed tree with edge labels $\in \Sigma$ where

- The concatenation of the labels of all paths from the root to a leaf just give $\sigma(S)$.
- The labels of sibling edges from one node start with different characters.
- Atomic tree



Termination Symbol $

No suffix must be prefix of another suffix.

Data Structures III

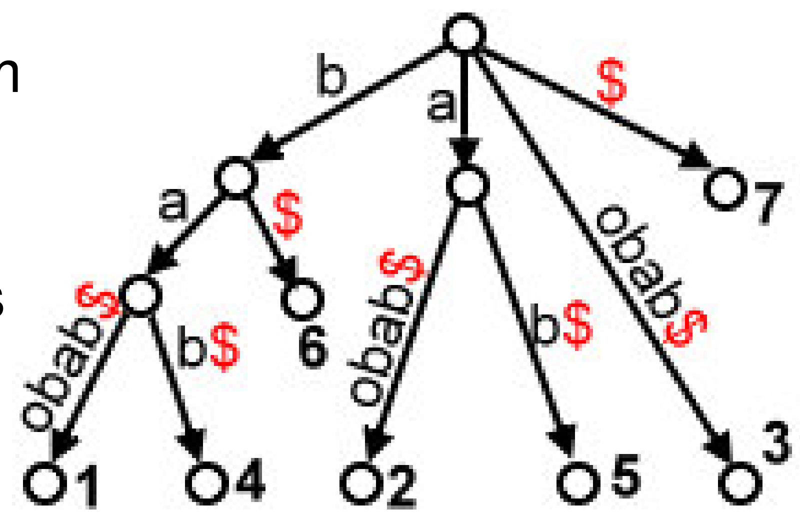
Suffix Tree

Definition

A suffix tree $\mathcal{T}$ for a string $S \subseteq \Sigma^n$ is a compact suffix trie.

This means

- $\mathcal{T}$ has exactly n leaves numbered 1 to n.
- The concatenation of the labels from the root to a leaf i spells out S_i. ($\rightarrow$ all paths give $\sigma(S)$)
- The labels of sibling edges from one node start with different characters.
- Every node except the root has at least two children. ($\rightarrow$ compact)



More Definitions

Paths and Labels

- A path is a downwards connected sequence of edges.
- The label of a path is the concatenation of the edge labels on the path.
- The path-label of node n is the concatenation of the edge labels on the path to node n. ($\rightarrow$ path-label of leaf i is S_i)

Reference pair (n, α) of s

n: node on the path to s

α: concatenation of edge-labels from n to s

s not necessarily a node

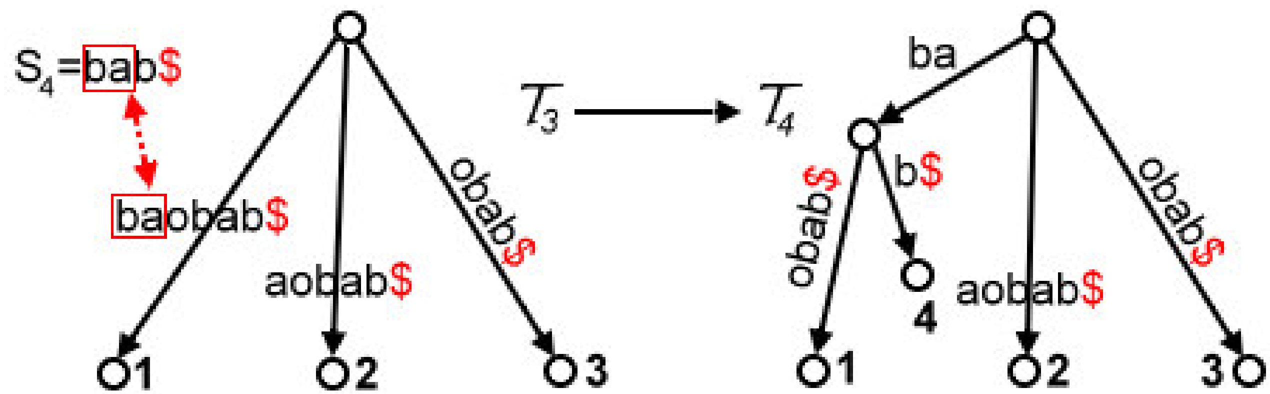
Canonical reference pair

n: last node on the path to s

A naïve algorithm

Suffix tree for S

- Start: single edge S[1..n]\$=S_1\$ $\rightarrow$ Tree $\mathcal{T}_1$
- Successive adding of S[i..n]\$=S_i\$, i from 2 to n+1
  $\mathcal{T}_{i-1} \rightarrow \mathcal{T}_i$



  - Find longest path from root in $\mathcal{T}_{i-1}$ matching a prefix of S_i.
  - Matching ends at node n (eventually new created).
  - Add new edge (n,i) labelled with unmatched suffix of S_i.

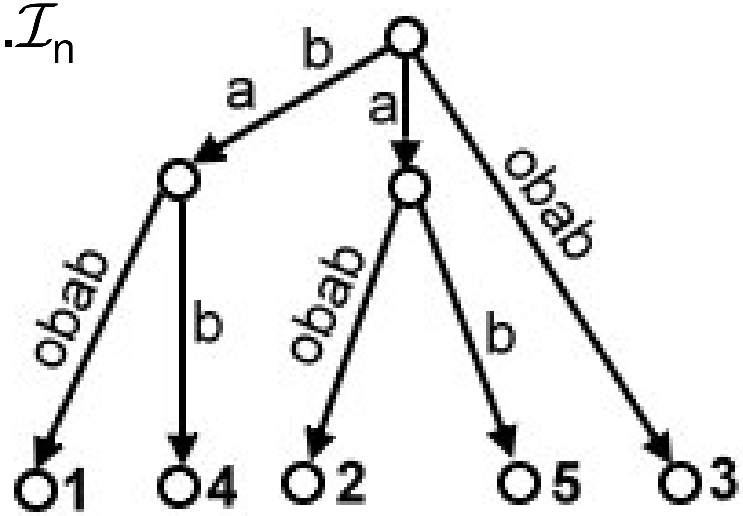
Time analysis

Inserting S_i takes $\mathcal{O}(|S_i|)$ time $\rightarrow$ Complexity: $\mathcal{O}(n^2)$

Ukkonen's Algorithm I

Proceeding

- Construction of suffix tree for string S in $\mathcal{O}(n)$ via implicit suffix trees $\mathcal{I}_1..\mathcal{I}_n$ $\rightarrow$ true suffix tree $\mathcal{T}$
- Start: $\mathcal{O}(n^3)$ method to build $\mathcal{T}$ $\rightarrow$ optimization to linear time



Implicit suffix trees

- Remove every occurrence of $\$$.
- Re-establish suffix-tree conditions.
- $\mathcal{I}_i$ implicit suffix tree for S[1..i]

($\mathcal{I}_n$ encodes all suffixes of S!)

Ukkonen's Algorithm II

Algorithm at a high level

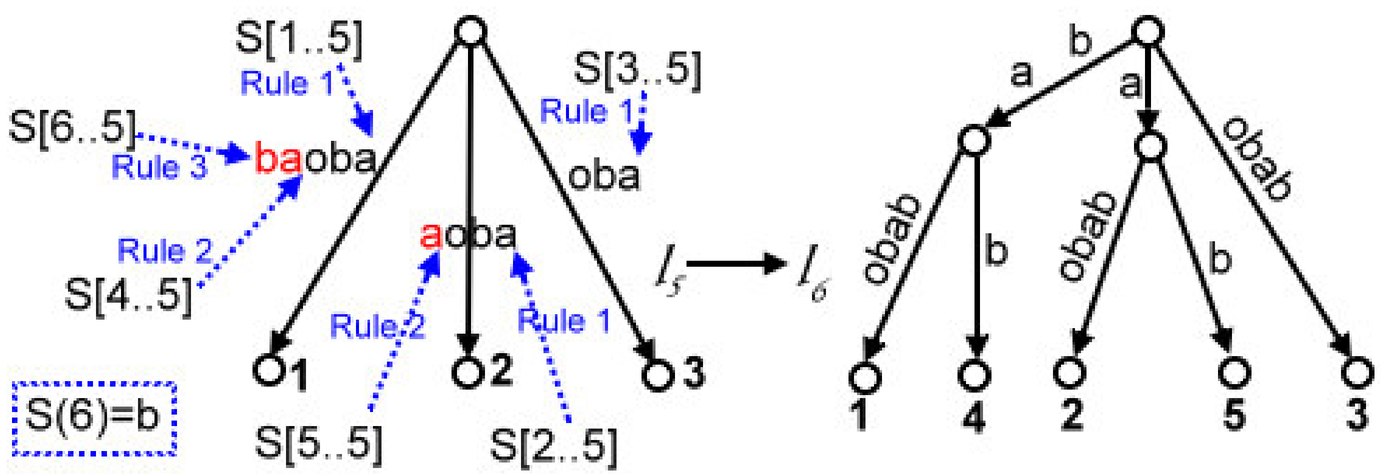
Construct implicit suffix tree $\mathcal{I}_1$.

For i from 1 to n-1 { for j from 1 to i+1 {

1. find end of path from root labelled S[j..i] in $\mathcal{I}_i$
2. apply appropriate **extension rule** (S[j..i+1] in tree)
   1. S[j..i] ends at leaf $\rightarrow$ add S(i+1) to edge label
   2. No path from end of S[j..i] starts with S(i+1) $\rightarrow$ add new leaf edge labelled S(i+1) and leaf node j
   3. $\exists$ path from S[j..i] beginning with S(i+1) $\rightarrow$ do nothing

} \\extension

} \\phase



Time

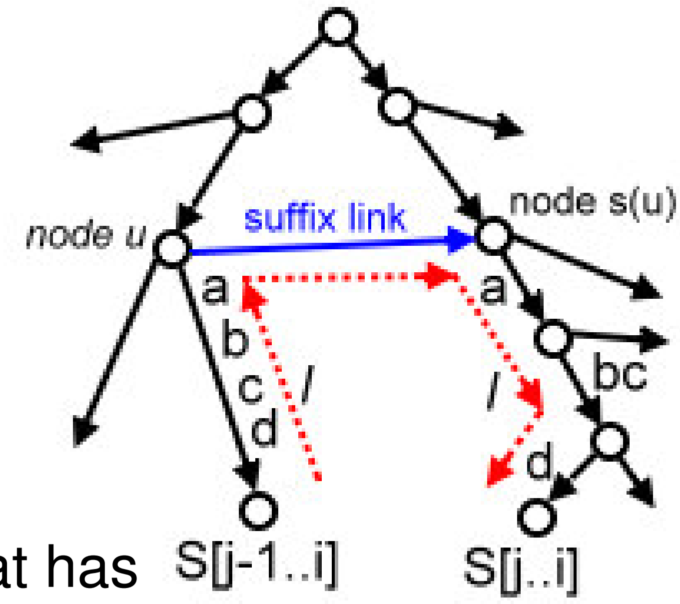
$\mathcal{O}(n^3)$

Ukkonen's Algorithm III

Suffix Links

Definition

Suffix link (u, s(u)) is a pointer from internal node u labelled xα to node s(u) labelled α.



Single Extension Algorithm

1. Find first node u up from S[j-1..i] that has suffix link or is root (at most one edge up!)
2. If u $\neq$ root: walk down from s(u) following path for α.
   If u = root: walk down from root following path for S[j..i].
3. Apply appropriate extension rule $\rightarrow$ S[j..i]S(i+1) in the tree
4. If new internal node w was created, create suffix link (w, s(w))

Time complexity

Worst case not yet improved: $\mathcal{O}(n^3)$

Ukkonen's Algorithm IV

Problem:

Down-walking along path labelled α costs $\mathcal{O}(|\alpha|)$ time

Trick 1: Skip/Count

- Skip edge if |unmatched part of α| > |edge label|
- **Time complexity**
  Traversing of edge $\mathcal{O}(1) \rightarrow$ down-walk in $\mathcal{O}$(#nodes)
  $\rightarrow$ 1 phase in $\mathcal{O}(n) \rightarrow$ algorithm in $\mathcal{O}(n^2)$

Edge-label compression

- Time for algorithm $\geq$ size of its output ($\Theta(n^2)$)
  $\rightarrow$ different representation scheme for edge labels
- **Pair of indices (i,j)**
  i beginning position of substring in S
  j ending position of substring in S

Ukkonen's Algorithm V

Trick 2: Rule 3 is a show stopper

- If rule 3 applies for S[j..i] it also applies for any S[k..i], k>j **(Implicit extensions)**
- End phase after first extension j* where rule 3 applies

Trick 3: Once a leaf, always a leaf

- j_i = # initial extensions in phase i where rule 1 or 2 applies $\rightarrow j_i \leq j_{i+1}$
- In phase i+1 do
  - Label new created leaf-edges (n,e) $\rightarrow$ S[n..i+1]
    (e global symbol denoting current end)
  - In extensions 1 to j_i only increment e $\rightarrow$ rule 1 for leaf-edges

Combination

In phase i+1 explicit extensions only from

- Extension j_i+1 = active point to
- Extension j* = end point

Ukkonen's Algorithm VI

Single phase algorithm

1. Increment index e to i+1
2. Explicitly compute successive extensions (using SEA) starting at j_i+1 until first extension j* where rule 3 applies (or until all extensions are done)
3. Set j_i+1 to j*-1 to prepare for next phase.

Time complexity

Suffix Links + Edge Compression + Trick 1-3 allows construction of suffix tree for String S in $\mathcal{O}(|S|)$.

Creating the true suffix tree

Conversion in $\mathcal{O}(|S|)$.

1. Add termination symbol $ to end of S.
2. Let Ukkonen's algorithm continue with extended string.
3. Replace each index e on every leaf edge with n.

McCreight's Algorithm I

Definitions

- $\mathcal{T}_i$: intermediate suffix tree encoding suffixes S_1 to S_{i-1}
- McHead(i): longest prefix of S_i that is also prefix of S_j, j<I
- McTail(i): S_i-McHead(i)

Proceeding

The "Algorithm M" inserts suffixes in order from S_1 to S_n.

$\mathcal{T}_i \rightarrow \mathcal{T}_{i+1}$

- Find end of path labelled McHead(i)
- n = node labelled McHead(i) (eventually new created)
- Add new leaf i and new edge (n,i) labelled McTail(i)

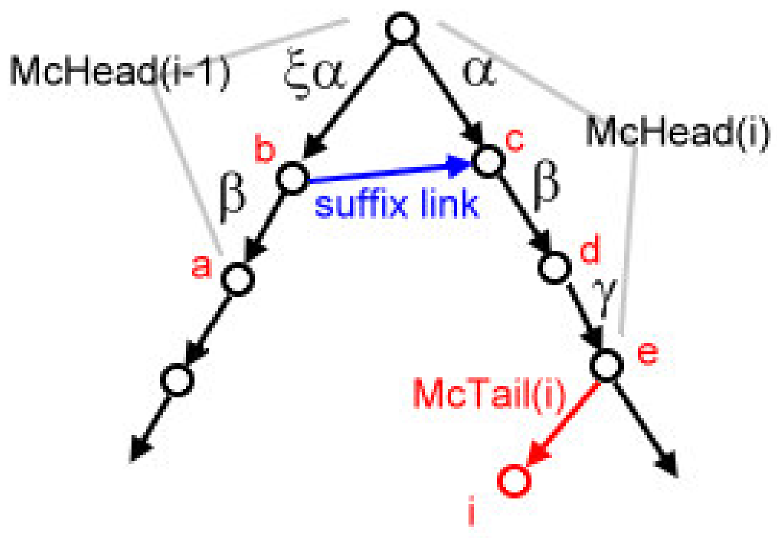
More efficiency

- Edge compression, suffix links
- Lemma: McHead(i-1) = $x\delta \Rightarrow \delta$ is a prefix of McHead(i)

McCreight's Algorithm II

Step i of "Algorithm M"

1. Starting from McHead(i-1)=$\xi\alpha\beta$ walk upwards till first node a (labelled $\xi\alpha$); if a = root go to 3.
2. Follow suffix link to node c (labelled α)
3. "Rescanning": walk downwards along path labelled β using skip/count trick $\rightarrow$ node d
4. Add suffix link (a,d)
5. "Scanning": search downwards along path labelled γ (unknown length!) $\rightarrow$ node e
6. Add leaf i and edge (e,i)



Time complexity

Rescanning and scanning
in $\mathcal{O}(1)$ $\rightarrow \mathcal{O}(n)$

Weiner's Algorithm I

Definitions

- $\mathcal{W}_i$: suffix tree for S_i=S[i..n]$
- WHead(i): longest prefix of S_i that is also prefix of S_j,j>i

Proceeding

Build $\mathcal{W}_{n+1}$ = edge (root, n+1) labelled $

For i from n to 1 do

- Find WHead(j) in $\mathcal{W}_{\mathbf{j+1}}$
- w = node labelled WHead(j) (eventually new created)
- Create new leaf j and edge (w,j) labelled S[j..n]-WHead(j)

More efficiency

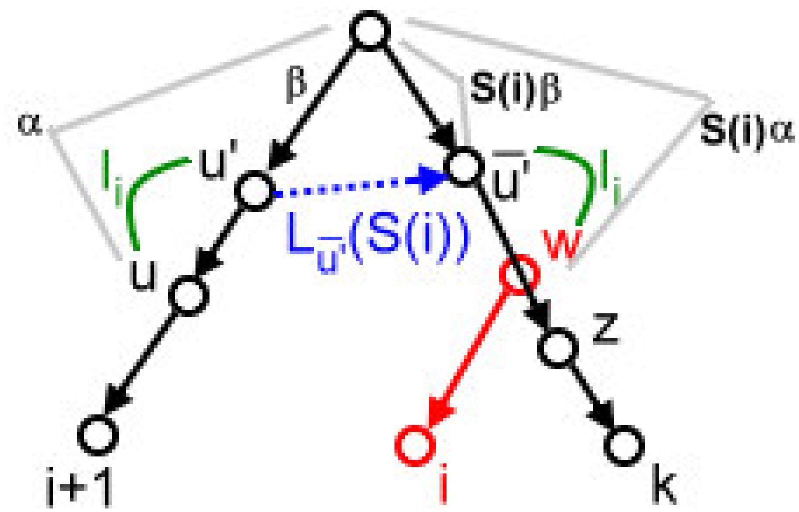
- Edge compression
- 2 vectors: Indicator Vector $\mathcal{I}_u$(x) and Link Vector $\mathcal{L}_u$(x)

Weiner's Algorithm II

The Vectors

- $\mathcal{I}_u(x)=1 \Leftrightarrow$ u labelled α & $\exists$ partial path in $\mathcal{W}$ labelled $x\alpha$
- $\mathcal{L}_u(x)=\uparrow \hat{u} \Leftrightarrow \hat{u}$ labelled $x\alpha$ & u labelled α; otherwise $\mathcal{L}_{\mathbf{u}}(x)$=null

Vector Usage



$\mathcal{W}_{i+1} \rightarrow \mathcal{W}_i$:

- Start at leaf i+1, find first u with $\mathcal{I}_u(S(i))=1$ (u labelled α)
- Continue till first u' with $\mathcal{L}_{u'}(S(i)) \neq$ null (l_i = |u-u'|)
  - u, u' don't exist $\rightarrow \mathcal{W}$Head(i)=ε
  - u, u' exist $\rightarrow$ WHead(i)=S(i)α & WHead(i) ends l_i chars below $\hat{u}$
  - u exists, u' doesn't $\rightarrow$ WHead(i) ends l_i chars below root

Time complexity

Head (i) found in $\mathcal{O}(1) \rightarrow$ Complexity of algorithm $\mathcal{O}(n)$

Exact string matching

Exact string matching

- **Find all occurrences for pattern P in text T:**
  Build suffix tree in $\mathcal{O}(|T|)$ and match P along unique path $\mathcal{O}(|P|)$.
  - P exhausted: numbers of leaves below are starting points for P
  - mismatch: P does not occur
- **Comparison with KMP and BM algorithms**
  - P and T fix; P fix $\rightarrow$ same time and space bound
  - fixed T and varying Ps $\rightarrow$ $\mathcal{O}(|T|) + \Sigma_P \mathcal{O}(|P|+|\#\text{occurrences of } P|)$
  $\rightarrow$ vastly better performance

Exact set matching

- **Task:** Find all k occurrences of a set of strings $\mathcal{P}$ in text T
-

Approach	**Tree**	**Search**	**Total**
Aho-Corasick	$\mathcal{O}(\Sigma\|P\|)$	$\mathcal{O}(\|T\|)$	$\mathcal{O}(\Sigma\|P\|+\|T\|+k)$
Suffix Trees	$\mathcal{O}(\|T\|)$	$\mathcal{O}(\Sigma\|P\|)$	$\mathcal{O}(\Sigma\|P\|+\|T\|+k)$

Longest common substring

Generalized suffix tree

- **Definition**:
  Tree which represents the suffixes of a set $\{S_1,S_{\mathbf{2}},\ldots S_{\mathbf{n}}\}$
- **Construction**: Variation of Ukkonen's algorithm
  1. Build tree for $S_1\$$
  2. Match $S_2\$$ against path in tree, first mismatch S[i+1]
     $\rightarrow$ tree encodes $\sigma(S_1)$ and implicitly $\sigma(S_{\mathbf{2}}[1..i])$
  3. Resume Ukkonen's algorithm on S_2 in phase i+1
  4. Repeat for each string

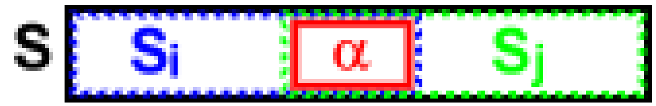
Longest common substring (lcs)

- **Proceeding**:
  - Build generalized suffix tree for S_1 and S_2
  - Mark internal nodes v with 1(2) if leaf in subtree of v represents suffix of $S_1(S_2)$
  - Search node marked 1 and 2 with longest path-label (= lcs)
- **Time complexity:** $\mathcal{O}(\Sigma\, |S_i|)$

String Assembly I

Introduction

- **Application:** DNA Analysis
- **Definition:** Superstring Problem
  For a given set of strings $\{S_1, S_2, \dots S_n\}$ find superstring S which contains every S_i as substring.
- **Solution:** Blending
  Assembling of two strings S_i, S_j as follows:
  Find longest suffix α of S_i which is prefix of S_j and create new string **blend** $(S_i,S_j) = S_i - \alpha + S_j = S_i - \mathbf{ov}(S_i,S_j) + S_j$



- GREEDY-Heuristic with Suffix Trees (Kosaraju/Delcher)
  $\rightarrow$ approximate solution for smallest S

String Assembly II

GREEDY-Heuristic with Suffix Trees

- **Generalized suffix tree $\mathcal{T}$:**
  - leaf numbers: (i, p) $\rightarrow$ suffix $S_1[p..|S_1|]$
  - implicit $\rightarrow$ \$ omitted, internal nodes can be leaves
  - substrings of other strings and copies of identical strings removed
- **Arrays & Sets:**
  - **chain** $\rightarrow$ already blended strings
  - **wrap** $\rightarrow$ unavailable suffixes and prefixes
  - $\mathbf{S_u}$ $\rightarrow$ suffixes available at node u
    initially $S_u = \{i|u \text{ has leaf number } (i,1)\}$
  - $\mathbf{P_u}$ $\rightarrow$ prefixes available at node u
    initially $P_u = \{i|u \text{ has leaf number } (i,d),\ d>1\}$

String Assembly III

Proceeding

1. Find node u with largest string-depth
2. Find pair(i,j) with
   - $i \in S_u$, $j \in P_u$
   - chain(i) = 0, wrap(i) $\neq$ j
3. Discard all i from S_u with chain(i) $\neq$ 0
4. Remove i from S_u and j from P_u and set
   - chain(i) = j
   - wrap(wrap(i)) = wrap (j), wrap(wrap(j)) = wrap (i)
5. Repeat 2. – 4. until no further blends are feasible
6. Union remaining P_u to set P of u's parent
7. Discard S_u and remove u from string-depth-order
8. Goto 1.
9. Generate superstring from chain array

Conclusion

Suffix Trees

☞ Implementation Details

Comparison of the algorithms

- Time
- Space
- Comprehensibility

Applications