Pattern Matching with Suffix Trees

BMI/CS 776
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Alignment vs. Pattern Matching

- global sequence alignment
  - input: $n \geq 2$ relatively short sequences
  - homology assumptions: homologous along entire length, colinear
  - goal: determine homologous positions

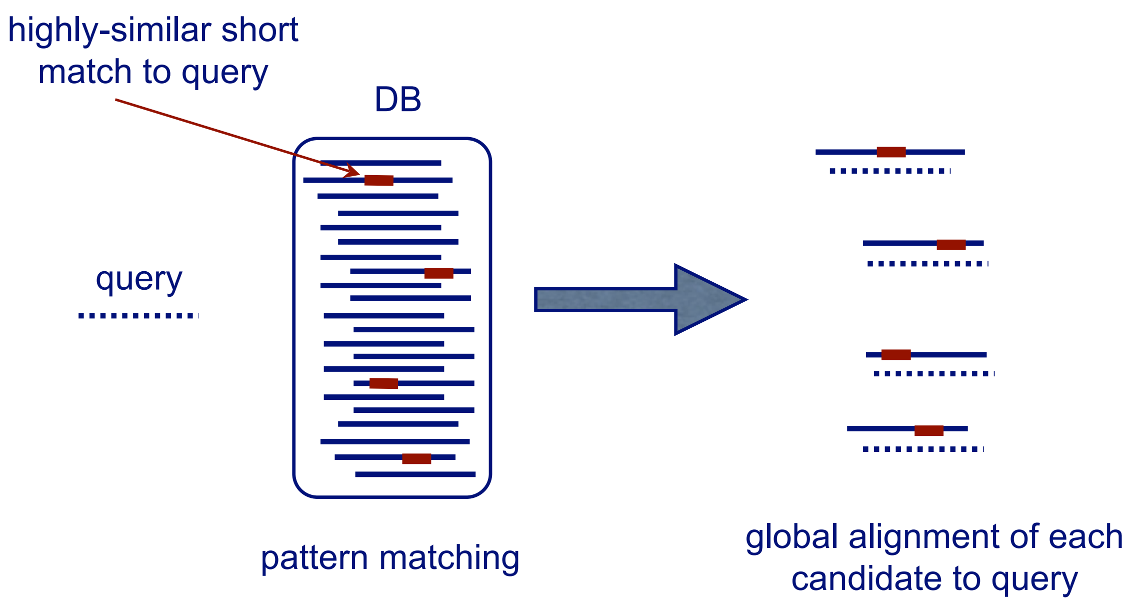
- pattern matching
  - input: $n \geq 1$ sequences (short or long)
  - homology assumptions: none
  - goal: find short exact/inexact substring (local) matches between or within input sequences

Why pattern matching?

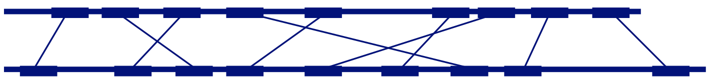
- applications:
  - database search - short query, large DB
  - alignment of long sequences - exact global alignment no longer feasible
  - alignment of rearranged/duplicated sequences - no longer a global alignment task

- key idea: short local matches can *seed* longer global alignments

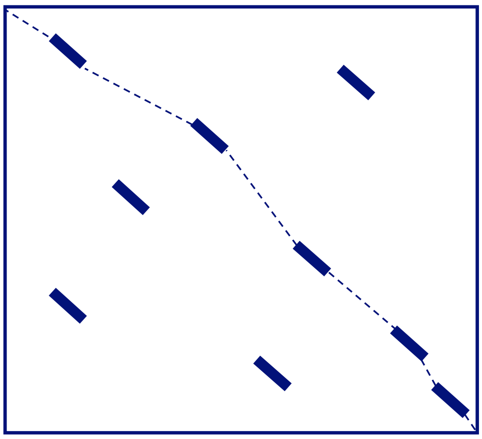
Database Search



Global Alignment of Long Sequences



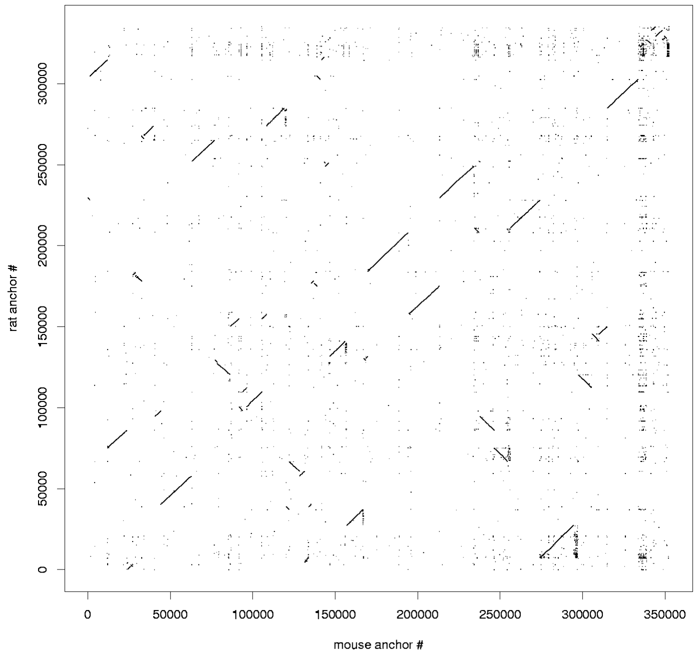
find seed matches using pattern matching



sparse dynamic programming with seed matches

Alignment of Rearranged Sequences

whole-genome dot plot



each dot represents a seed match between genome sequences

Suffix Trees

- substring problem:
  - given text S of length m
  - preprocess S in $O(m)$ time
  - such that, given query string Q of length n, find occurrence (if any) of Q in S in $O(n)$ time
- suffix trees solve this problem, and others

History of Suffix Trees

- Weiner (1973): first linear time algorithm for suffix tree construction
  - "the algorithm of 1973" (Knuth)
- McCreight (1976): space efficient version of algorithm

this lecture

- Ukkonen (1995): simple, elegant algorithm, with "online" property

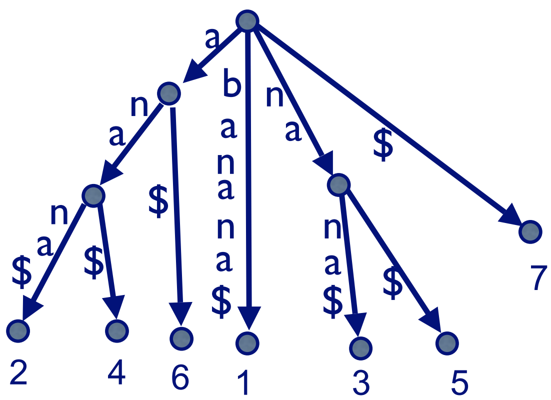
Suffix Tree Definition

- a suffix tree T for a string S of length m is tree with the following properties:
  - *rooted* and *directed*
  - m leaves, labeled 1 to m
  - each edge labeled by a substring of S
  - concatenation of edge labels on path from root to leaf i is suffix i of S (we will denote this by $S_{i...m}$)
  - each internal non-root node has at least two children
  - edges out of a node must begin with different characters

key property

Suffix Tree Example

- S = "banana$"
- add '$' to end so that suffix tree exists (no suffix is a prefix of another suffix)



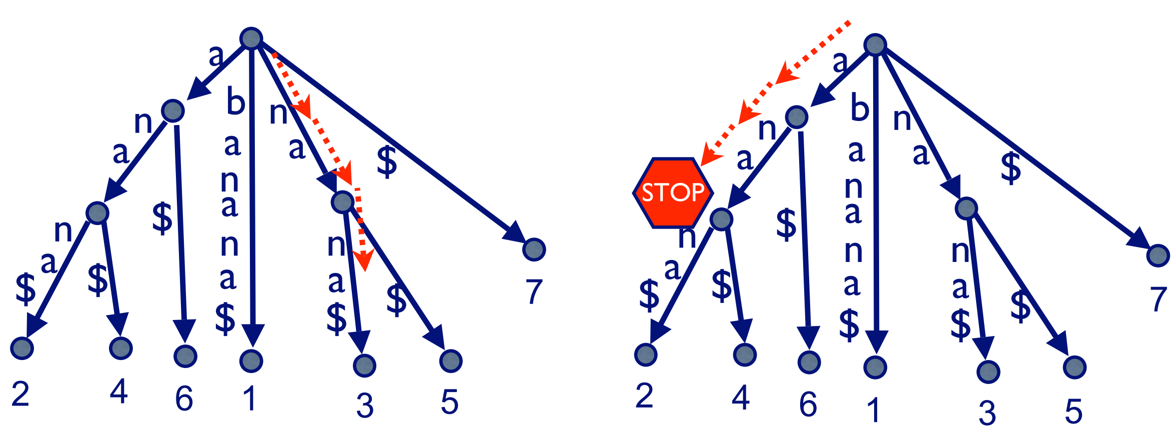
Solving the Substring Problem

- assume we have suffix tree T
- FindMatch(Q, T):
  - follow (unique) path down from root of T according to characters in Q
  - if all of Q is found to be a prefix of such a path return label of some leaf below this path
  - else, return no match found

Solving the Substring Problem

Q = nan

Q = anab



return 3

return no match found

Runtime of Substring Problem with Suffix Tree

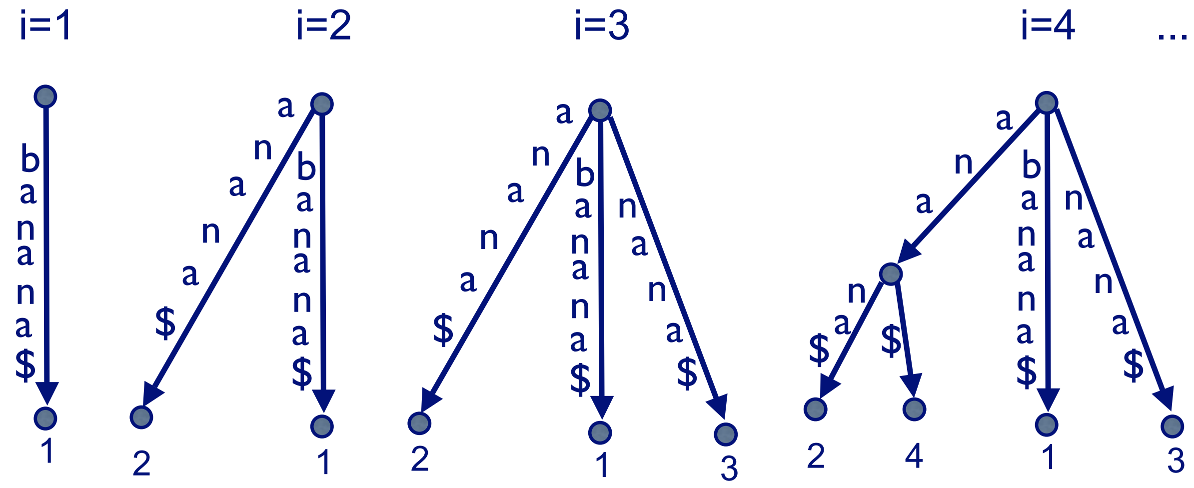
- finite alphabet: $O(1)$ work at each node
- edges out of each node start with unique characters: unique path from root
- size of tree below end of path: $O(k)$, k = number of suffixes starting with Q
- $O(n + k)$ time to report all k matching substrings
- $O(n)$ to report just one with an additional trick

Naive Suffix Tree Building

- now we need a $O(m)$ time algorithm for building suffix trees
- naive algorithm is $O(m^2)$:
  - $T \leftarrow$ empty tree
  - for i from 1 to m:
    - add suffix $S_{i\ldots m}$ to T by finding longest matching prefix of $S_{i\ldots m}$ in T and branching from there

each step is $O(m)$

O(m^2) Suffix Tree Building

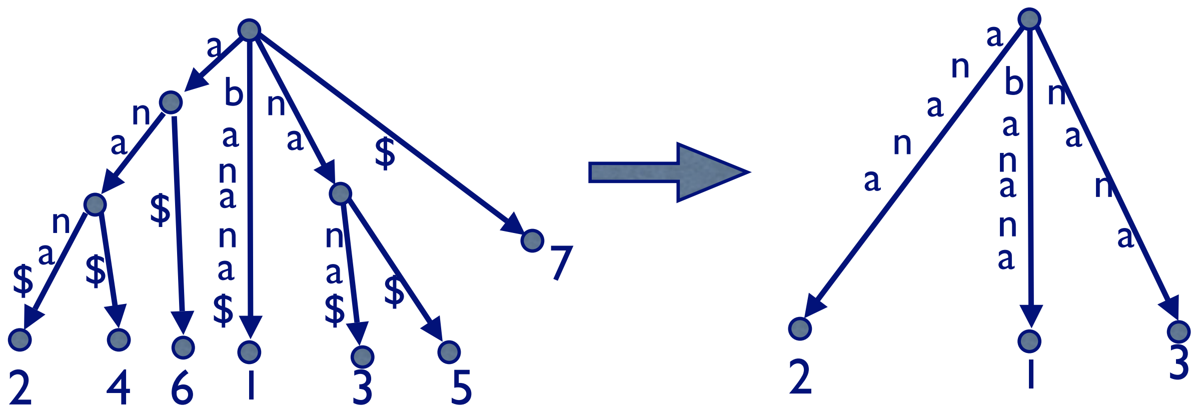


Ukkonen's O(m) Algorithm

- on-line algorithm
  - builds *implicit* suffix tree for each prefix of string S
  - implicit suffix tree of $S_{1\ldots i}$ denoted I_i
  - builds I_1, then I_2 from I_1,..., then I_m from I_{m-1}
- basic algorithm is O(m^3), but with a series of tricks, it is O(m)

Implicit Suffix Tree

- Suffix tree → implicit suffix tree
  - remove $ characters from labels
  - remove edges with empty labels
  - remove internal nodes with < 2 children



Ukkonen's Algorithm Overview

construct I_1

for i from 1 to m - 1:

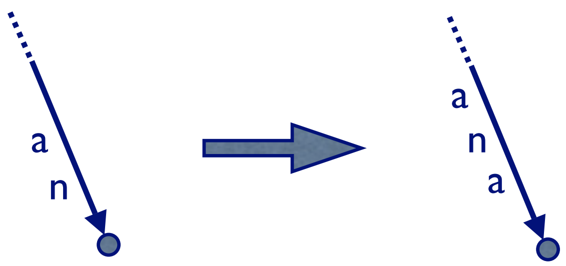
    for j from 1 to $i + 1$:

- find end of path from root labeled $S_{j...i}$
- add character S_{i+1} to the end of this path in the tree, if necessary

Suffix Extension Rule 1.

1. if path $S_{j...i}$ in tree ends at leaf, add character S_{i+1} to end of label of edge into leaf

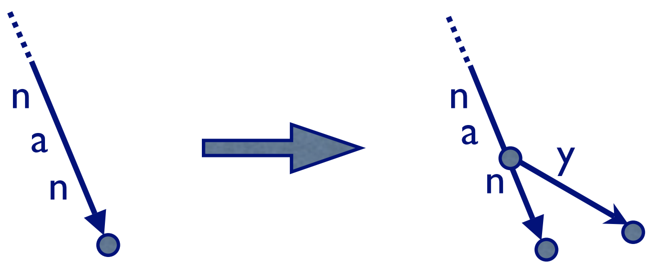
$S_{j...i}$ = ...an $\qquad$ $S_{j...i+1}$ = ...ana



Suffix Extension Rule 2.

2. if there are paths continuing from path $S_{j...i}$ in the tree, but none starting with S_{i+1}, then create a new leaf edge with label S_{i+1} at the end of path $S_{j...i}$ (creating a new internal node if $S_{j...i}$ ends in the middle of an edge)

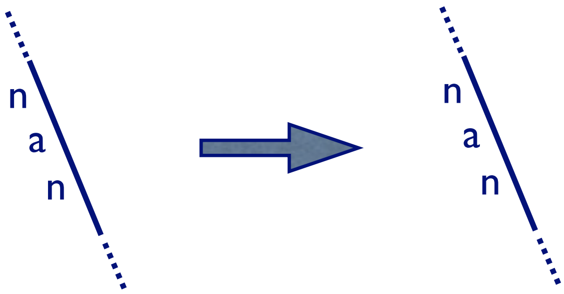
$S_{j...i}$ = ...na $\qquad$ $S_{j...i+1}$ = ...nay



Suffix Extension Rule 3.

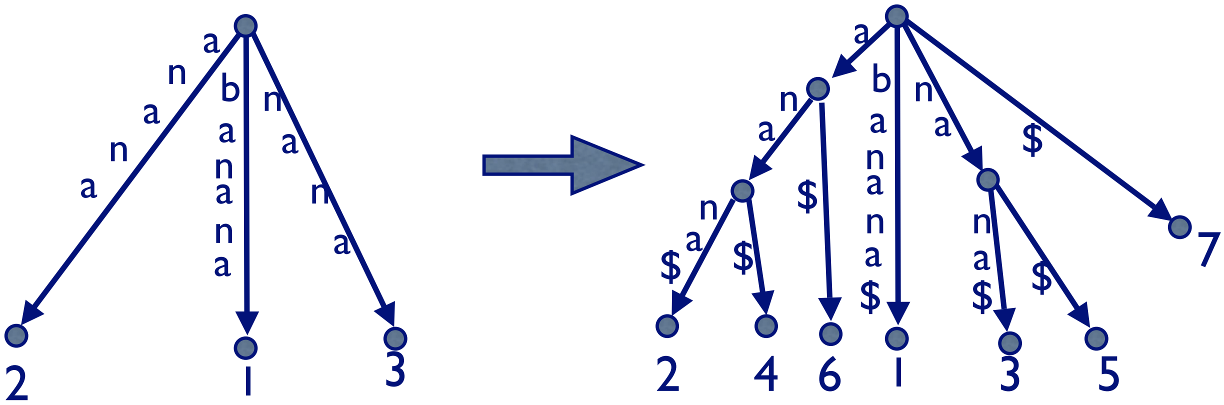
3. if there are paths continuing from path $S_{j...i}$ in the tree, and one starts with S_{i+1}, then do nothing

$S_{j...i}$ = ...na $S_{j...i+1}$ = ...nan

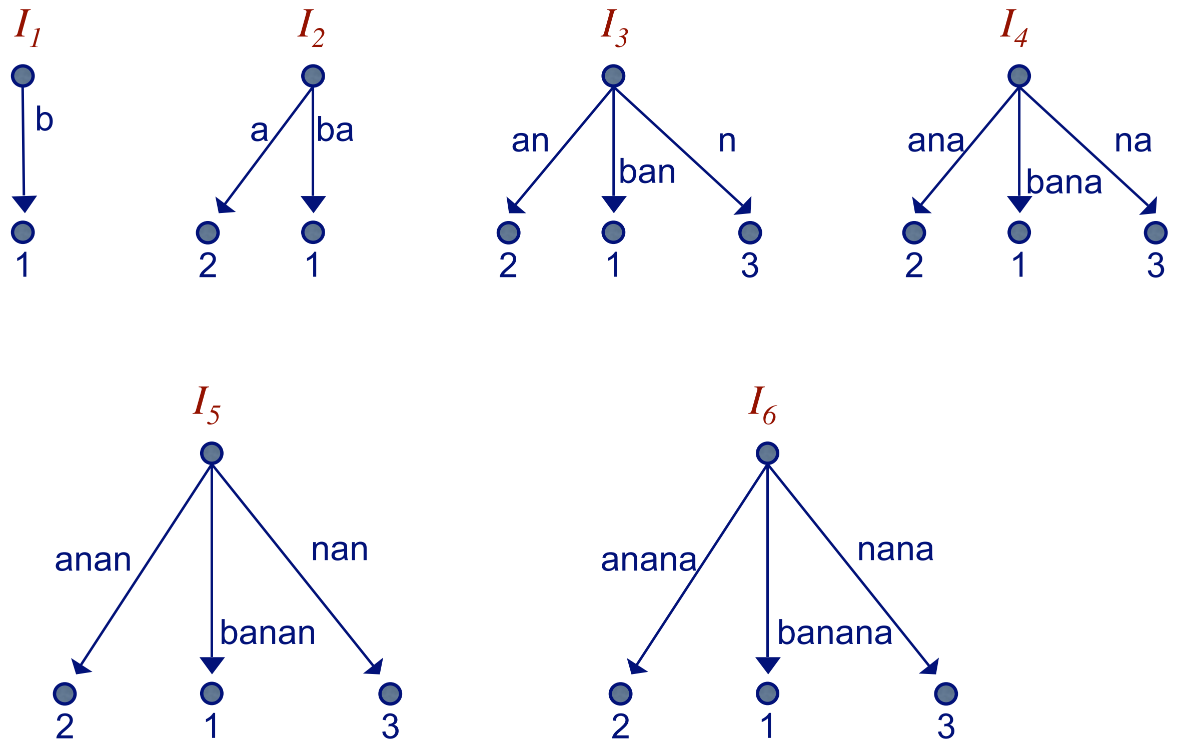


Conversion to Suffix Tree

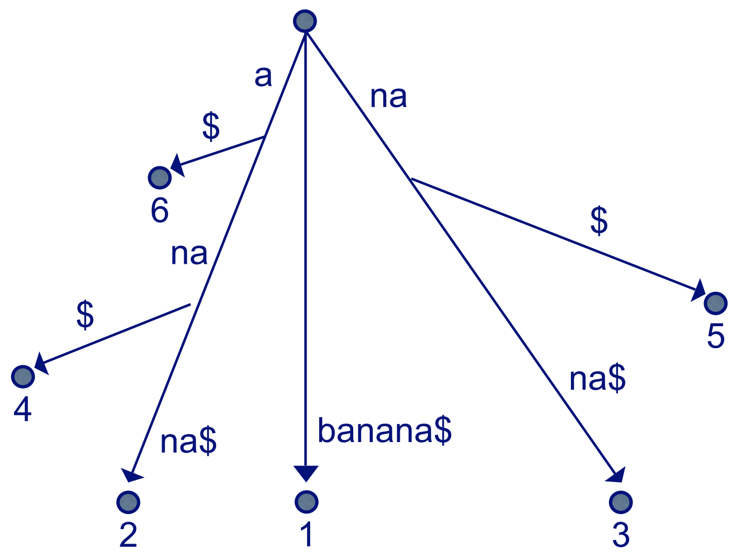
- convert implicit suffix tree at end of algorithm into true suffix tree
- simply run algorithm for one more iteration with $ final character
- traverse tree to label leaf edges with positions



Example



Example (Continued)



Key Idea 1:
Leaves ⇒ Free Operations

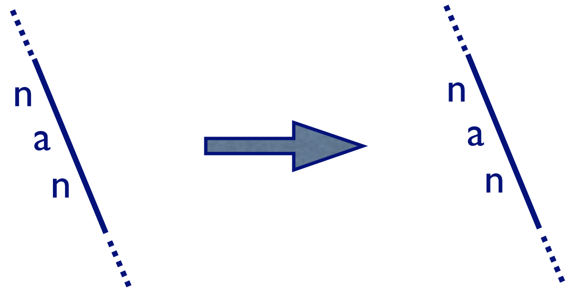
- *once a leaf always a leaf*: when a leaf edge is created on phase p, label the edge with (p,e)
- e is a global index that is updated in constant time on each phase

Key Idea 2:
Existing Strings ⇒ Free Operations

- if suffix extension rule 3 applies to extension j, it will apply in all further extensions in phase; therefore end phase early

3. if there are paths continuing from path $S_{j...i}$ in the tree, and one starts with S_{i+1}, then do nothing

$S_{j...i}$ = ...na $\qquad$ $S_{j...i+1}$ = ...nan



Ukkonen's Algorithm with Implicit Free Operations

construct I_1

for i from 1 to m - 1:

  for $j_L < j < j_R$:

    find end of path from root labeled $S_{j \ldots i}$

    add character S_{i+1} to the end of this path

- j_L in iteration i is the last leaf inserted in iteration i-1
- j_R in iteration i is the first index where $S_{j \ldots i+1}$ is already in the tree

Explicit Operations

- for $j_L < j < j_R$, j is made a leaf
- once a leaf, always a leaf

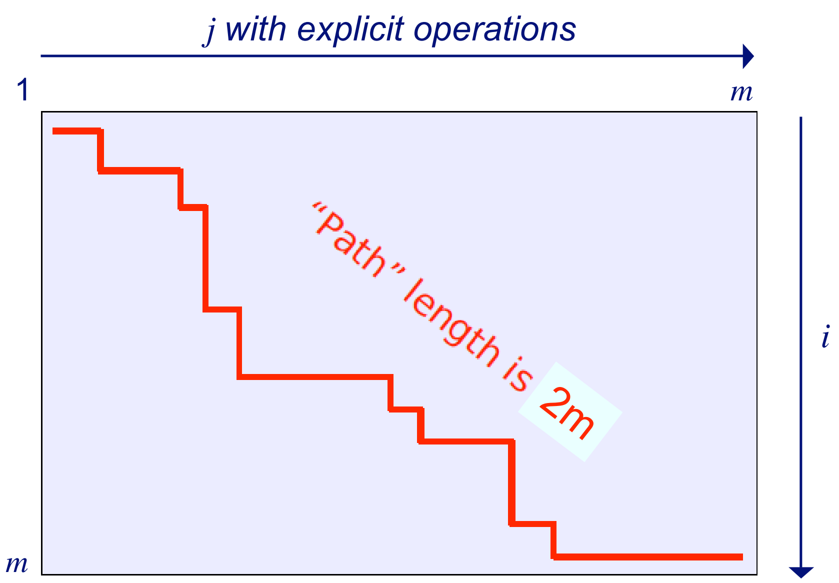


Figure from Aarhus Universitet course on String Algorithms

Ukkonen's Algorithm

construct I_1

for i from 1 to m - 1

  for $j_L < j < j_R$

    find end of path from root labeled $S_{j...i}$

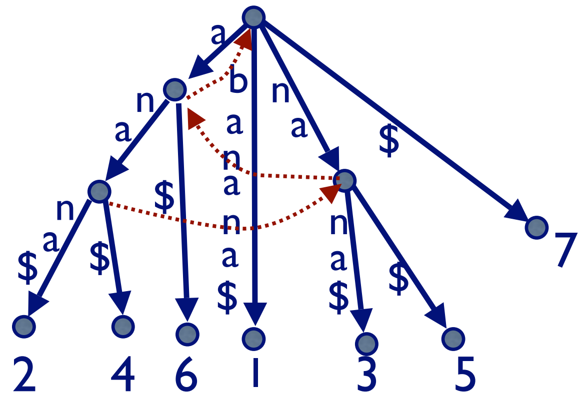
    add character S_{i+1} to the end of this path

$2m$ of these

can be done in constant time

Key Idea 3: Suffix Links

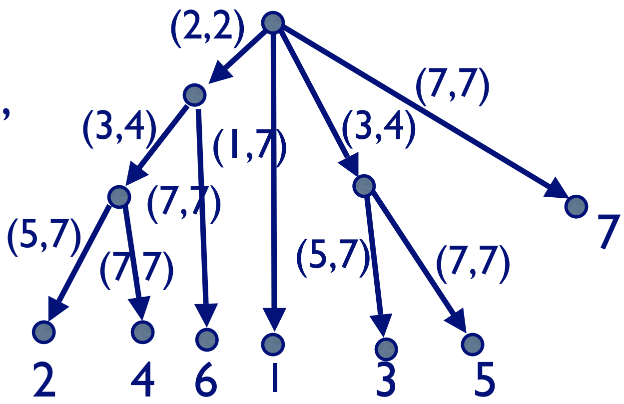
- how to find end of each suffix $S_{j...i}$?
- instead of searching down tree in O(i-j+1) time, use suffix links and some tricks
- a *suffix link* is a pointer from an internal node v to another node $s(v)$ where
  - x is a character, α is a substring (possibly empty)
  - v has path-label $x\alpha$
  - $s(v)$ has path-label α



Edge-Label Compression

- to get run time down to O(m) have to ensure that space is O(m)
- label edges with pair of indices into string rather than with explicit substring
- makes space requirement only O(m)

s = “banana$”



Final Runtime

- putting all of these tricks and implementation details together, Ukkonen’s algorithm runs in time O(m)
- more details found in (Ukkonen, 1995) or book by Dan Gusfield (Gusfield, 1997)