Pattern Matching with Suffix Trees

BMI/CS 776
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Goals for Lecture

the key concepts to understand are the following

- the pattern matching task
- the suffix tree representation
- using a suffix tree to find matching strings
- the naïve O(m^2) approach to building a suffix tree
- Ukkonen's O(m) approach to building a suffix tree

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

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

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

Suffixes

S = "banana$"

suffixes of S

$

a$

na$

ana$

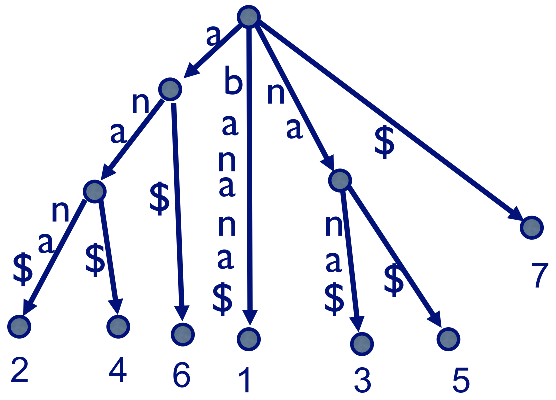
nana$

anana$

banana$

Suffix Tree Example

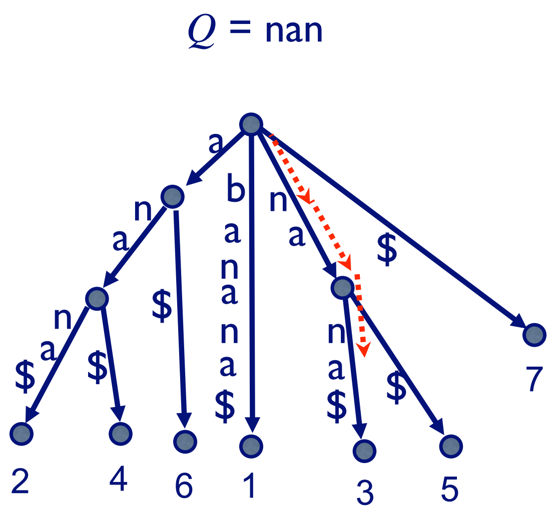
- S = "banana$"
- add '$' to end so that suffix tree exists (no suffix is a prefix of another suffix)



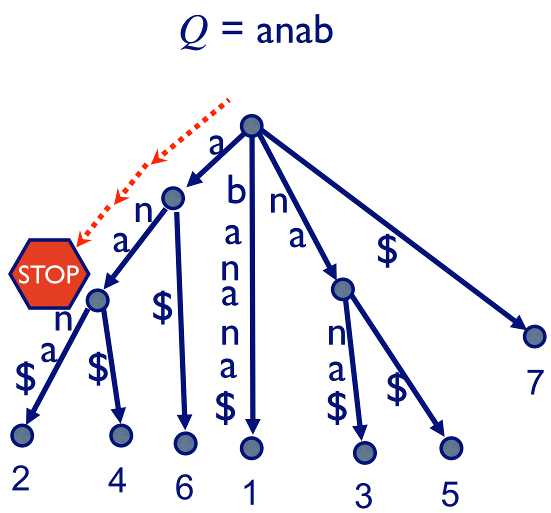
Solving the Substring Problem

- 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



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

Suffix Tree Example

- S = "banana$"
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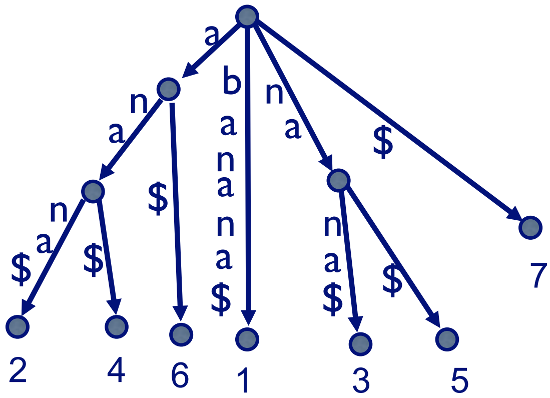
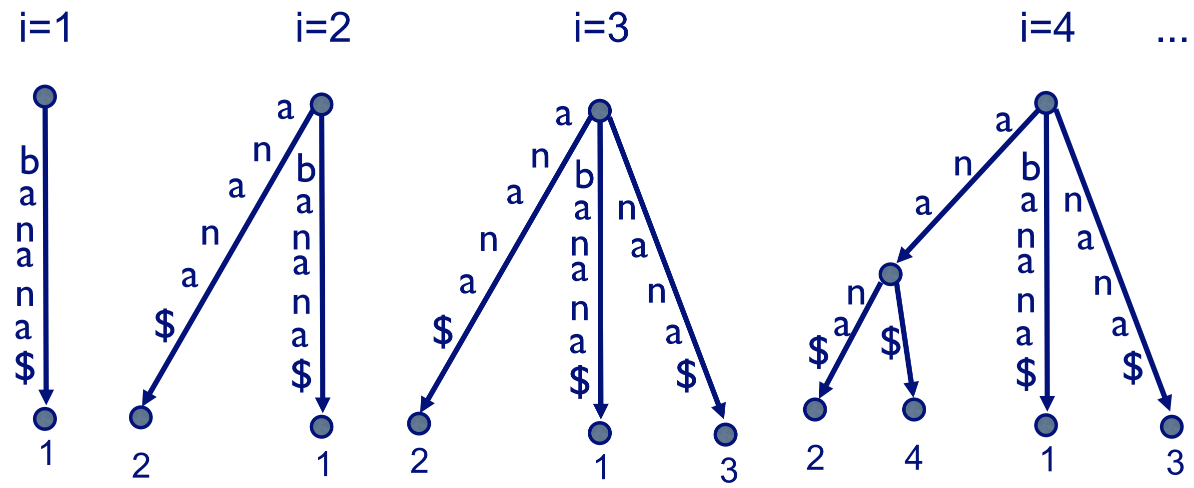


Naive Suffix Tree Building

- 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 $S_{i...m}$ to T by finding longest matching prefix of $S_{i...m}$ in T and branching from there

each step is O(m)

O(m^2) Suffix Tree Building

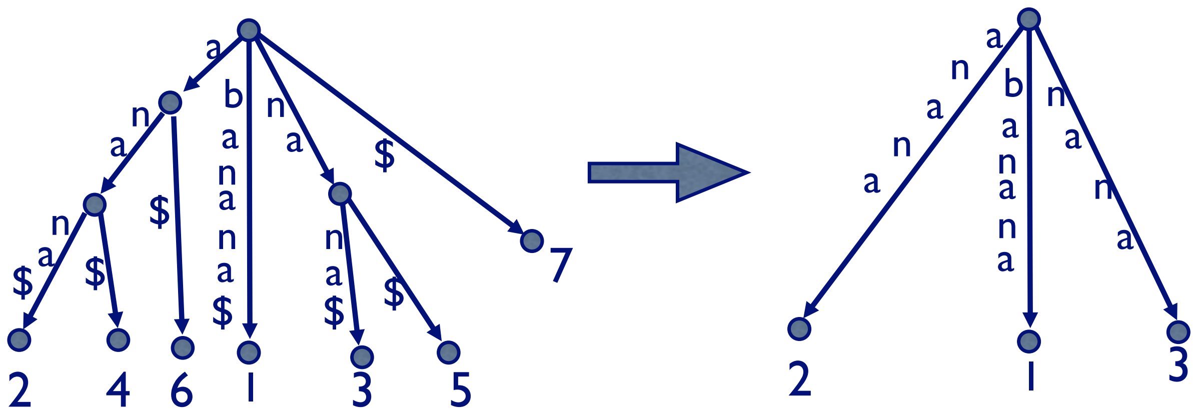


Ukkonen's O(m) Algorithm

- 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 $I_1, \ldots$, 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

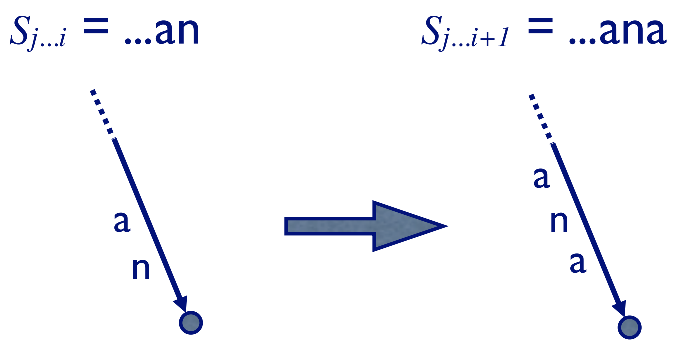
for i from 1 to m - 1 // phase i

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

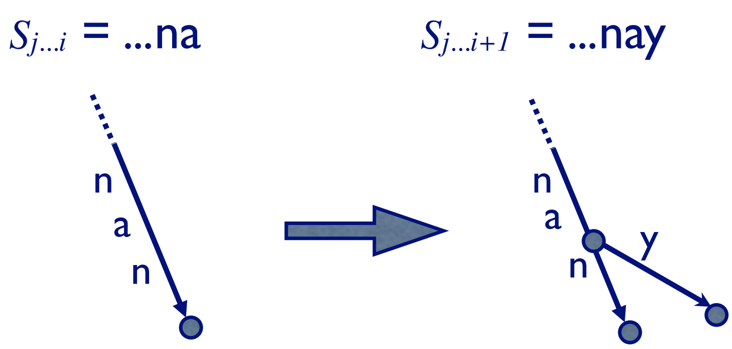
Suffix Extension Rule 1.

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



Suffix Extension Rule 2.

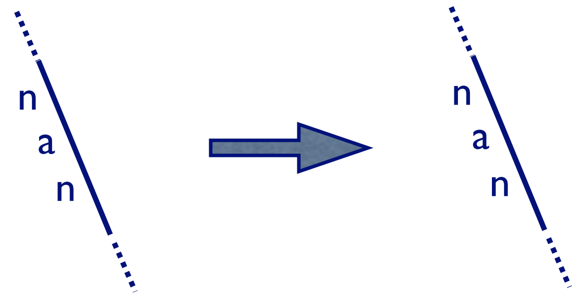
2. if there are paths continuing from path $S_{j...i}$ in the tree, but none starting with S_{i+1}, then create a new leaf edge with label S_{i+1} at the end of path $S_{j...i}$ (creating a new internal node if $S_{j...i}$ ends in the middle of an edge)



Suffix Extension Rule 3.

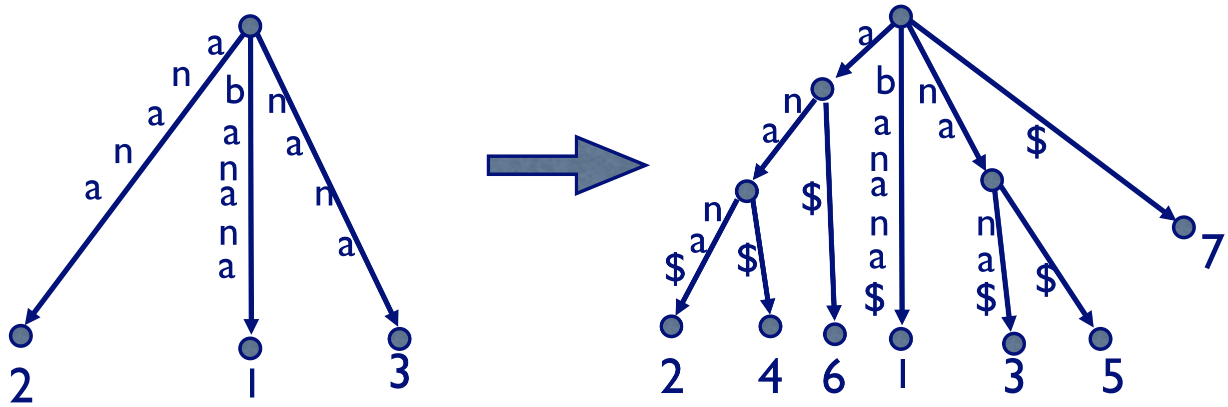
3. if there are paths continuing from path $S_{j\ldots i}$ in the tree, and one starts with S_{i+1}, then do nothing

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

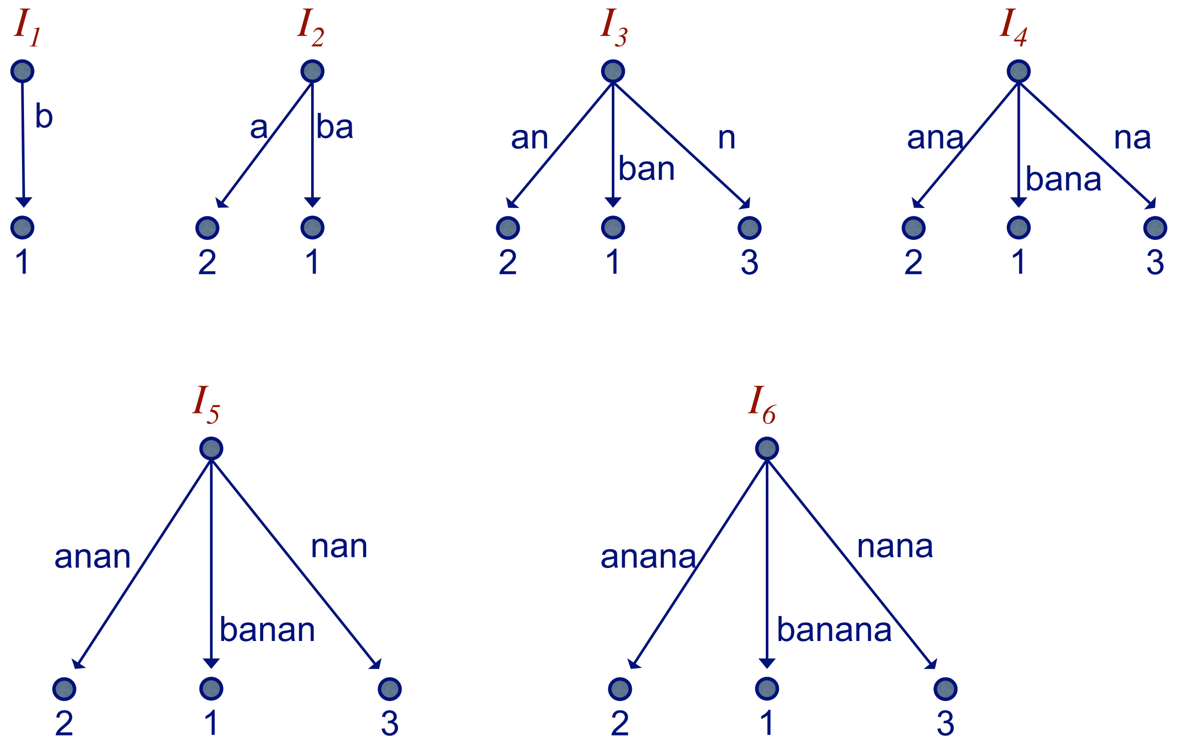


Conversion to Suffix Tree

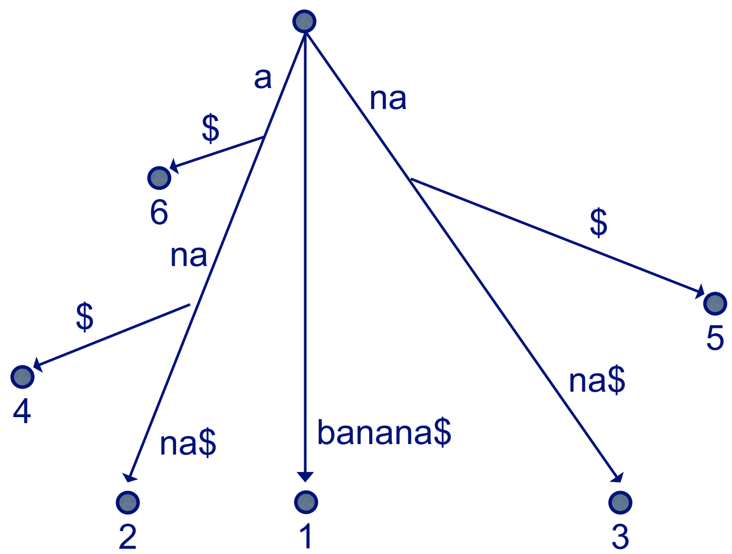
- convert implicit suffix tree at end of algorithm into true suffix tree
- simply run algorithm for one more iteration with $ final character
- traverse tree to label leaf edges with positions



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)

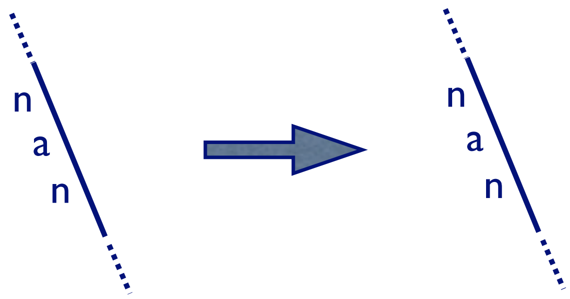
- e is a global index that is updated in constant time on each phase

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

    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 $S_{j...i+1}$ is already in the tree

Explicit Operations

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

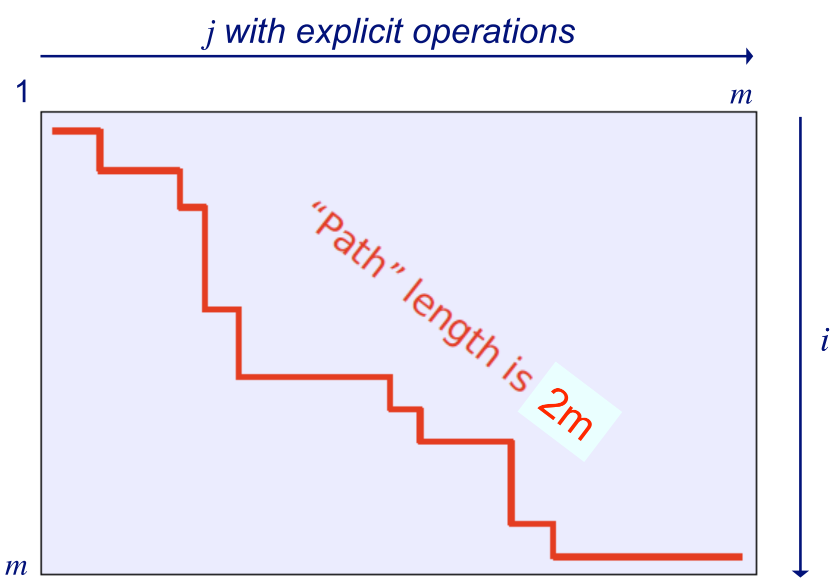
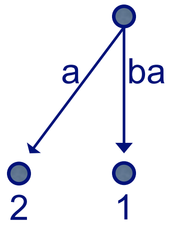
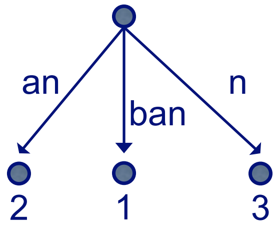


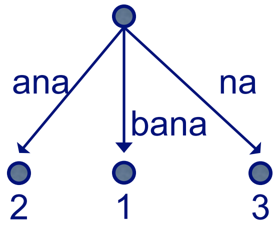
Figure from Aarhus Universitet course on String Algorithms

Example Revisited

phase (i)		j	extension	rule
1	$j_L \longrightarrow$	1	ba	1
		2	a	2
	$j_R \longrightarrow$			
2		1	ban	1
	$j_L \longrightarrow$	2	an	1
		3	n	2
	$j_R \longrightarrow$			
3		1	bana	1
		2	ana	1
	$j_L \longrightarrow$	3	na	1
	$j_R \longrightarrow$	4	a	3

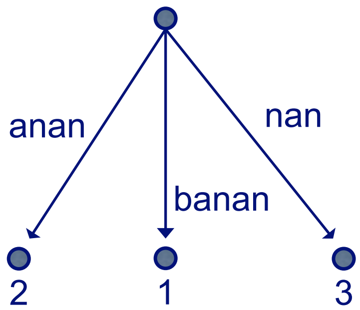


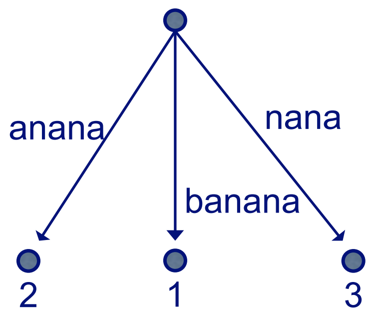




Example Revisited

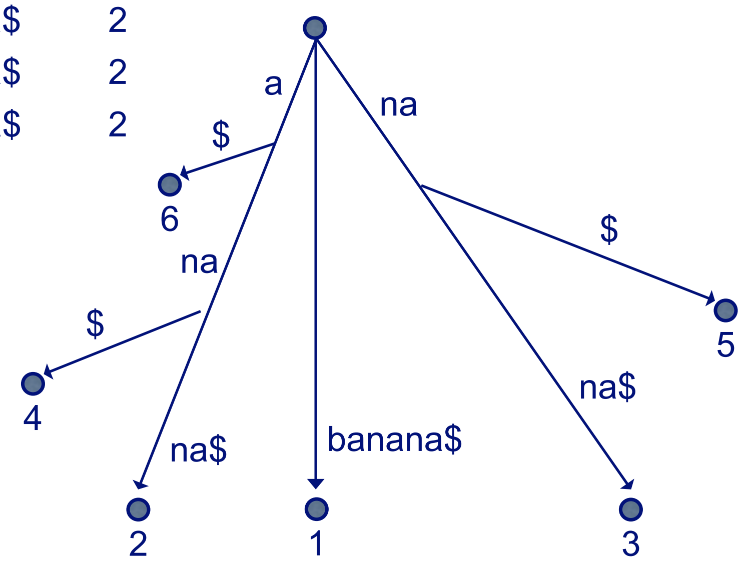
phase (i)		j	extension	rule
4		1	banan	1
		2	anan	1
	$j_L \longrightarrow$	3	nan	1
	$j_R \longrightarrow$	4	an	3
		5	n	3
5		1	banana	1
		2	anana	1
	$j_L \longrightarrow$	3	nana	1
	$j_R \longrightarrow$	4	ana	3
		5	na	3
		6	a	3





Example Revisited

phase (i)		j	extension	rule
6		1	banana$	1
		2	anana$	1
	$j_L \longrightarrow$	3	nana$	1
		4	ana$	2
		5	na$	2
		6	a$	2
	$j_R \longrightarrow$			



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 $S_{j..i}$

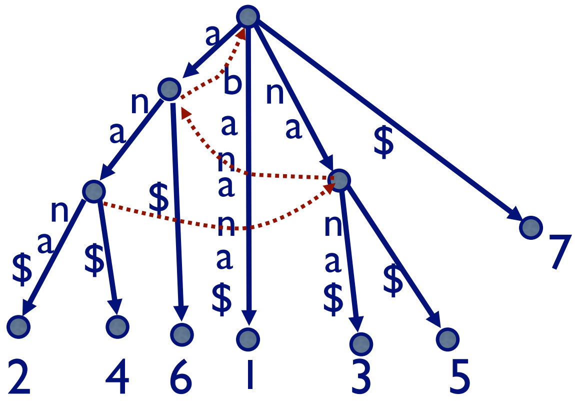
    add character S_{i+1} to the end of this path

$2m$ of these

can be done in constant time

Key Idea 3: Suffix Links

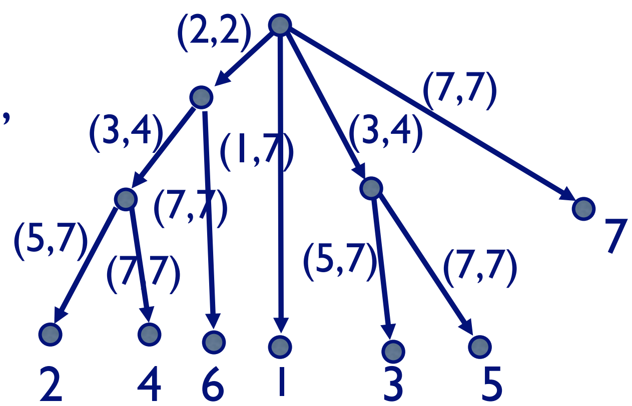
- how to find end of each suffix $S_{j..i}$?
- instead of searching down tree in O(i-j+1) time, use suffix links and some tricks
- a *suffix link* is a pointer from an internal node v to another node $s(v)$ where
  - x is a character, α is a substring (possibly empty)
  - v has path-label $x\alpha$
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