BMI/CS 776
Lecture #17:
Pattern Matching - Suffix trees

Colin Dewey

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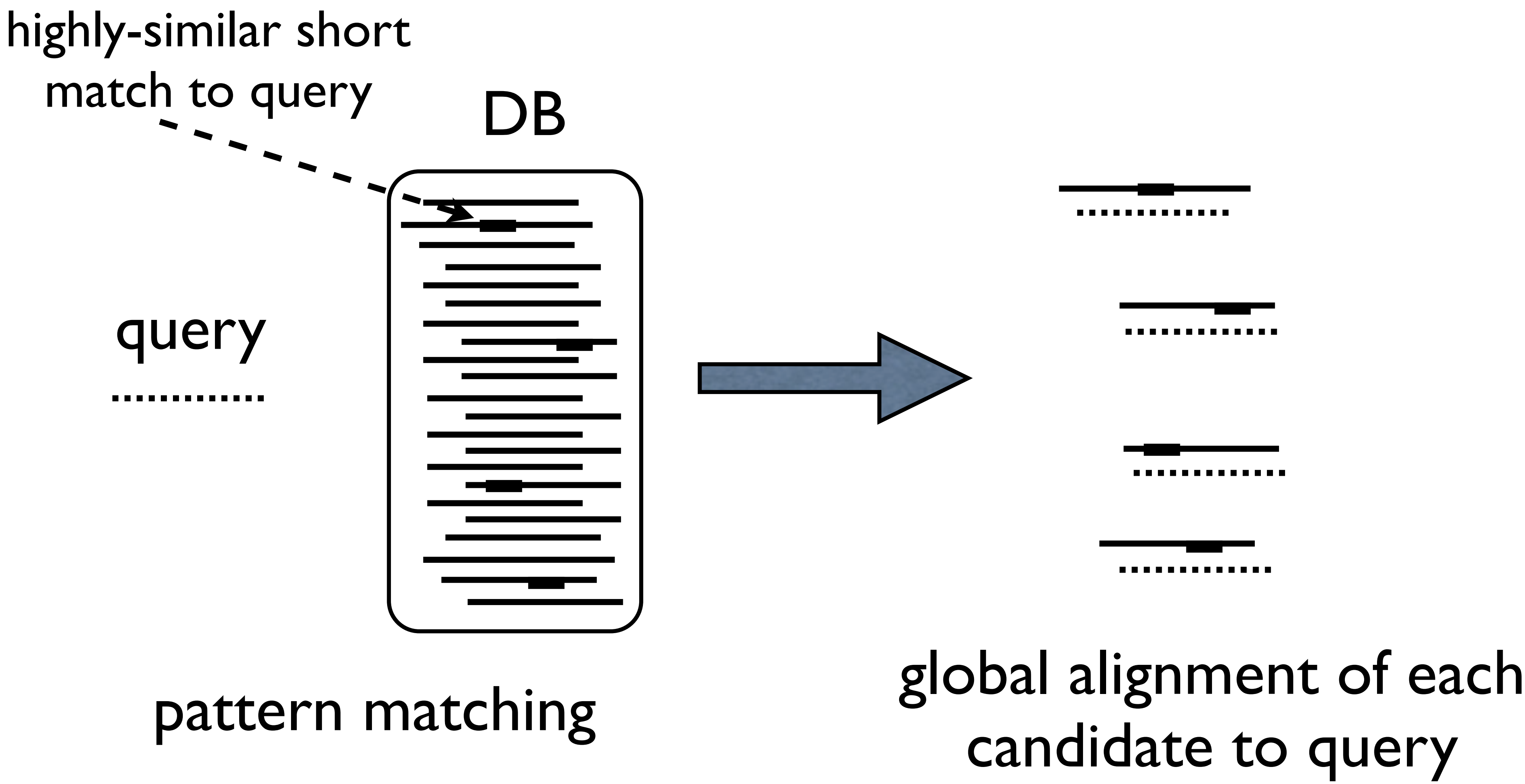
Alignment vs pattern matching

- Global sequence alignment
  - Input: n ≥ 2 relatively short sequences
  - Homology assumptions: homologous along entire length, colinear
  - Goal: determine homologous positions
- Pattern matching
  - Input: n ≥ 1 sequences (short or long)
  - Homology assumptions: none
  - Goal: find short exact/inexact substring (local) matches between or within input sequences

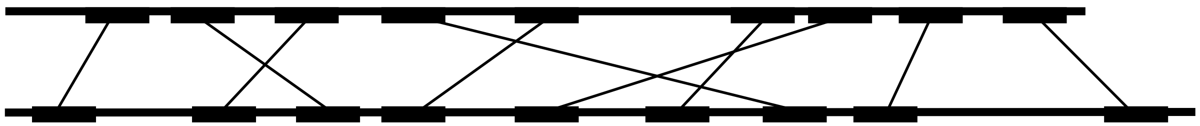
Why pattern matching?

- Applications:
  - Database search - short query, large DB
  - Alignment of long sequences - exact global alignment no longer feasible
  - Alignment of rearranged/duplicated sequences - no longer global alignment
- Key idea:
  - Short local matches can *seed* longer global alignments

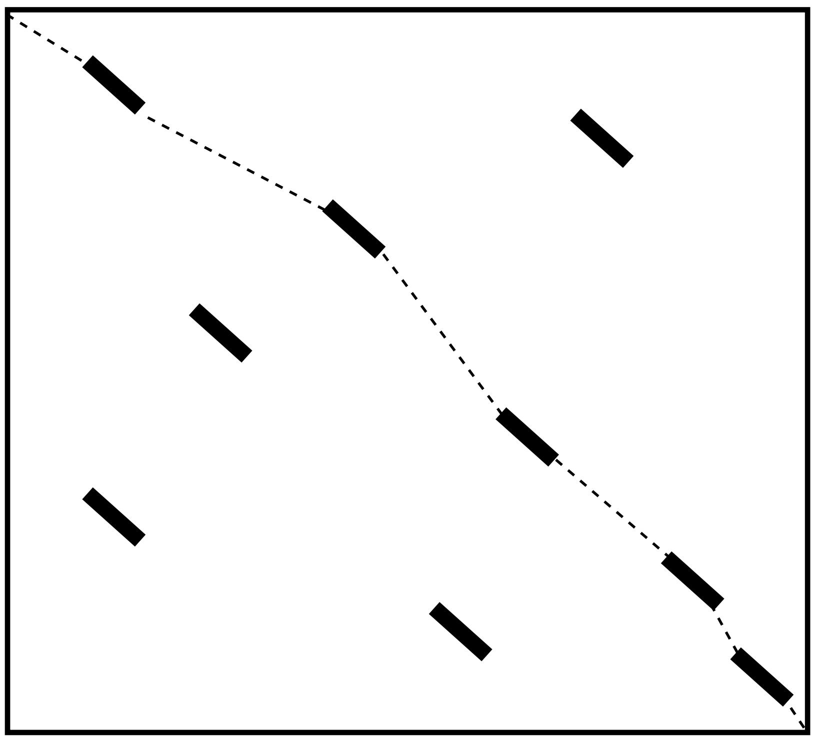
Database search



Global alignment of long sequences

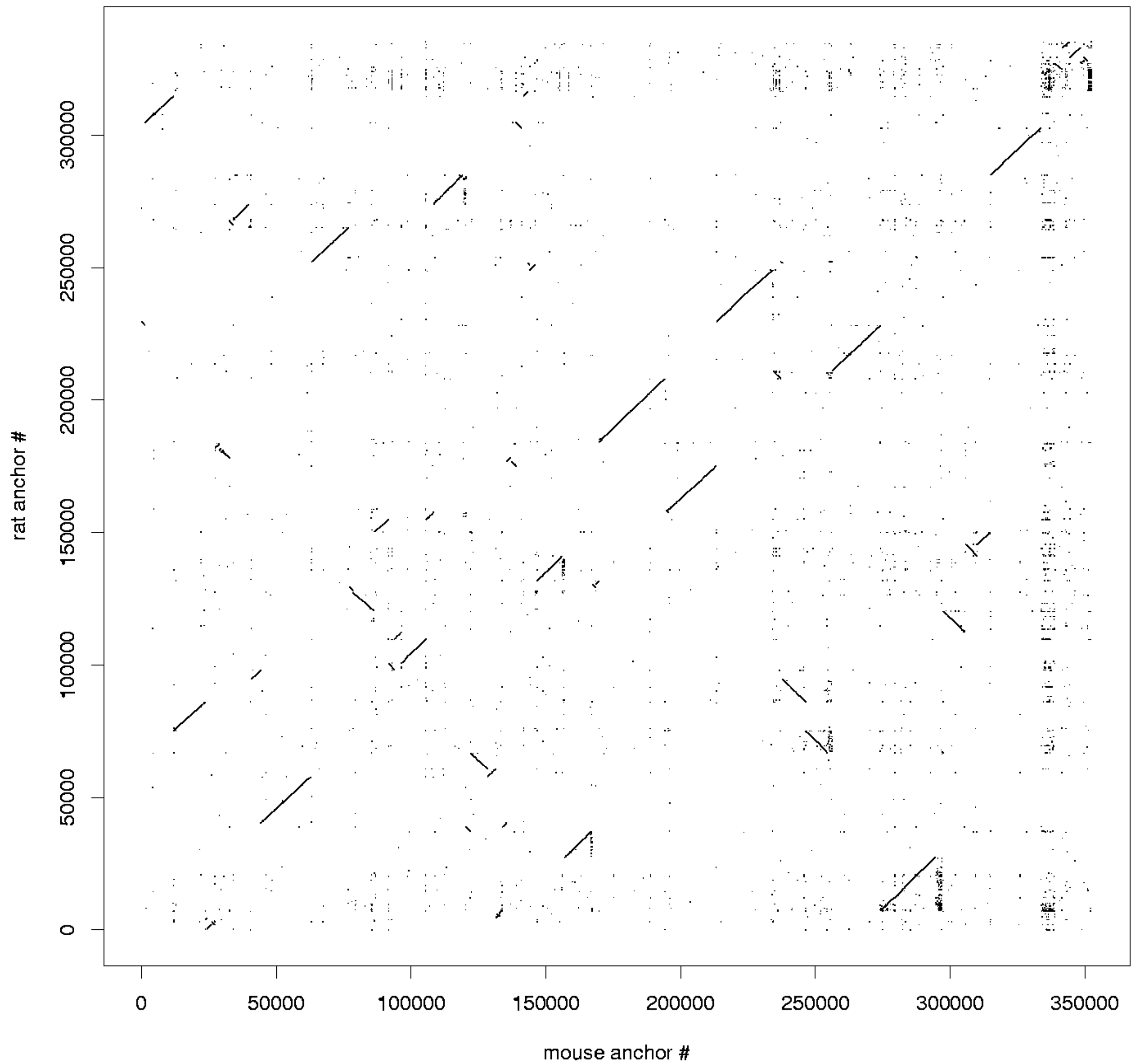


Find seed matches using pattern matching



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

- Very important for pattern matching
- Substring problem:
  - Given text T of length m
  - Preprocess T in $O(m)$ time
  - Such that, given query string S of length n, find occurrence (if any) of S in T in $O(n)$ time
- Suffix trees solve this problem, and many more

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

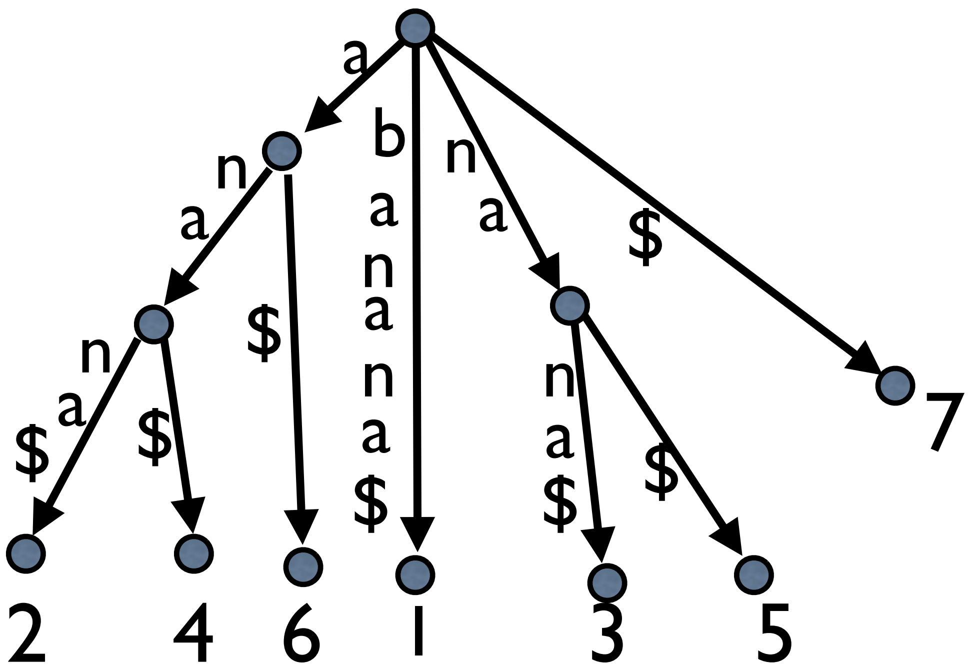
- A suffix tree *T* for a string *S* of length *m* is tree with the following properties:
  - *rooted* and *directed*
  - *m* leaves, labeled 1 to *m*
  - Each edge labeled by a substring of *S*

key property

  - 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

Suffix tree example

- S = "banana$"
- Add '$' to end so that suffix tree exists

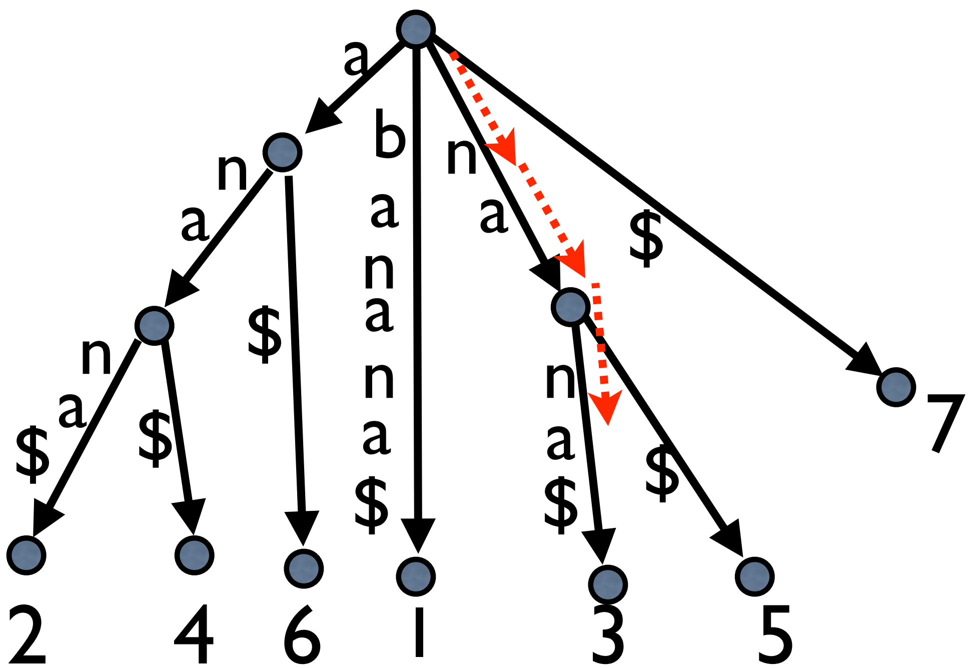


Solving the substring problem

- 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

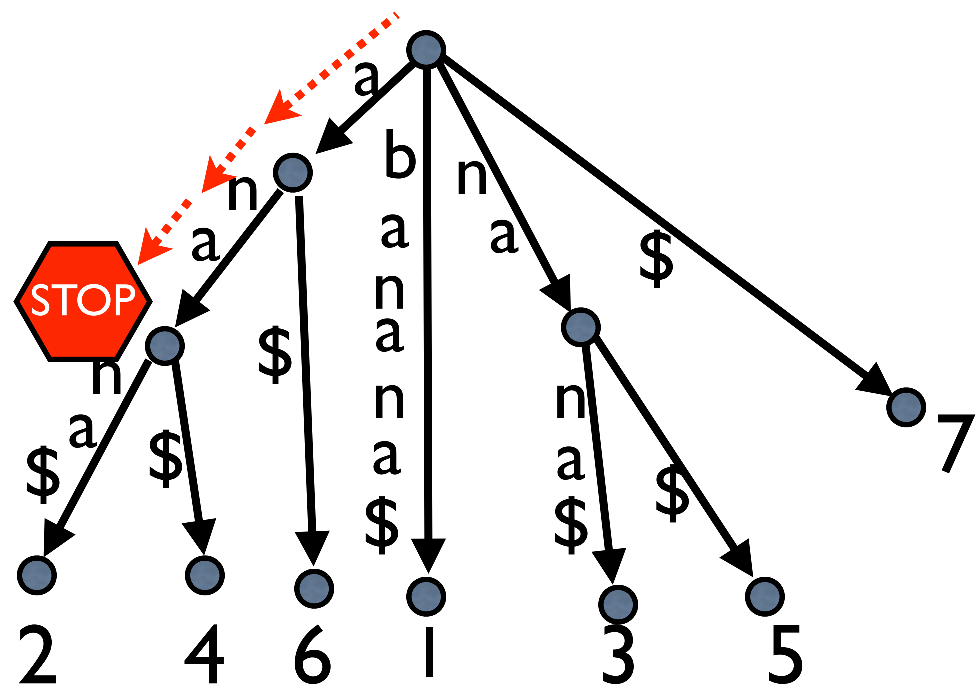
Solving the substring problem

Q = nan



return 3

Q = anab



return no match found

Runtime of substring problem with suffix tree

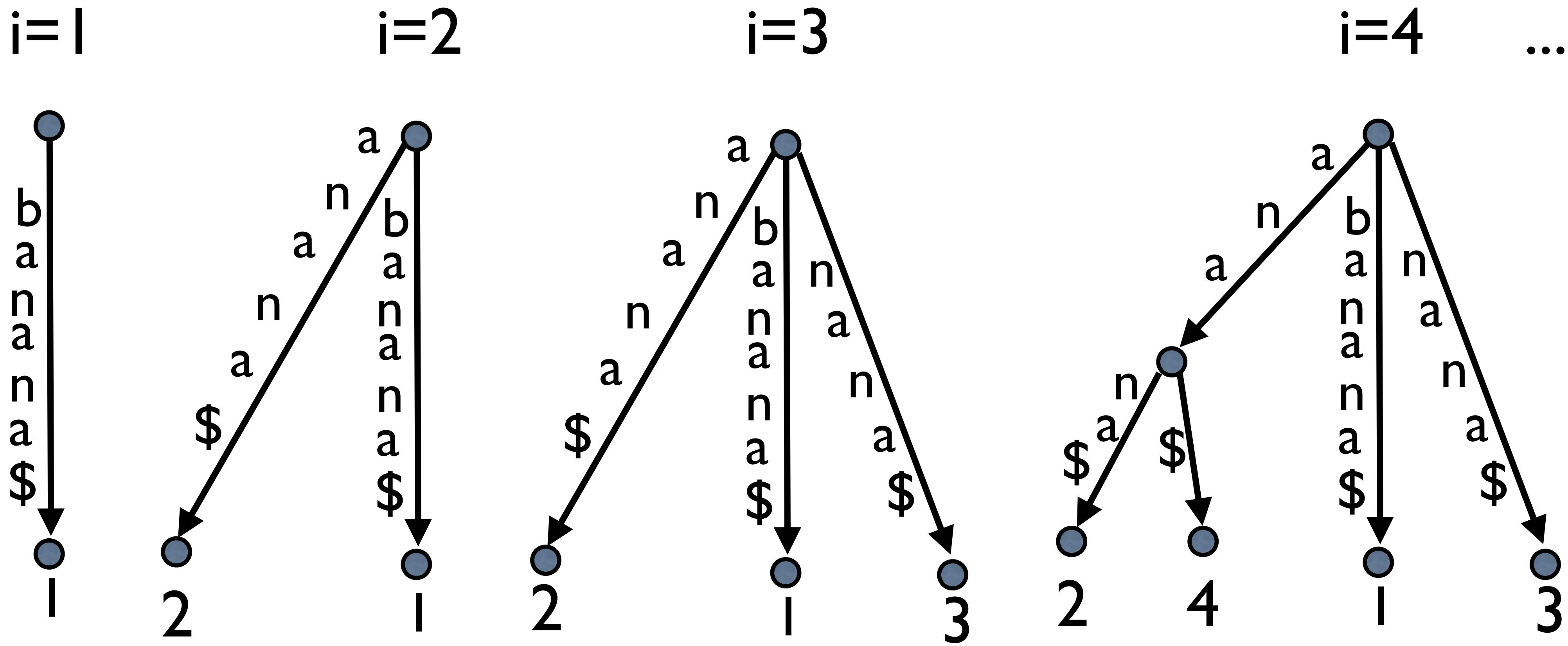
- Finite alphabet: $O(1)$ work at each node
- Edges out of each node start with unique characters: unique path from root
- Size of tree below end of path: O(k), k = number of suffixes starting with *Q*
- O(n + k) time to report all k matching substrings
- O(n) to report just one with an additional trick

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

O(m)

O(m²) suffix tree building

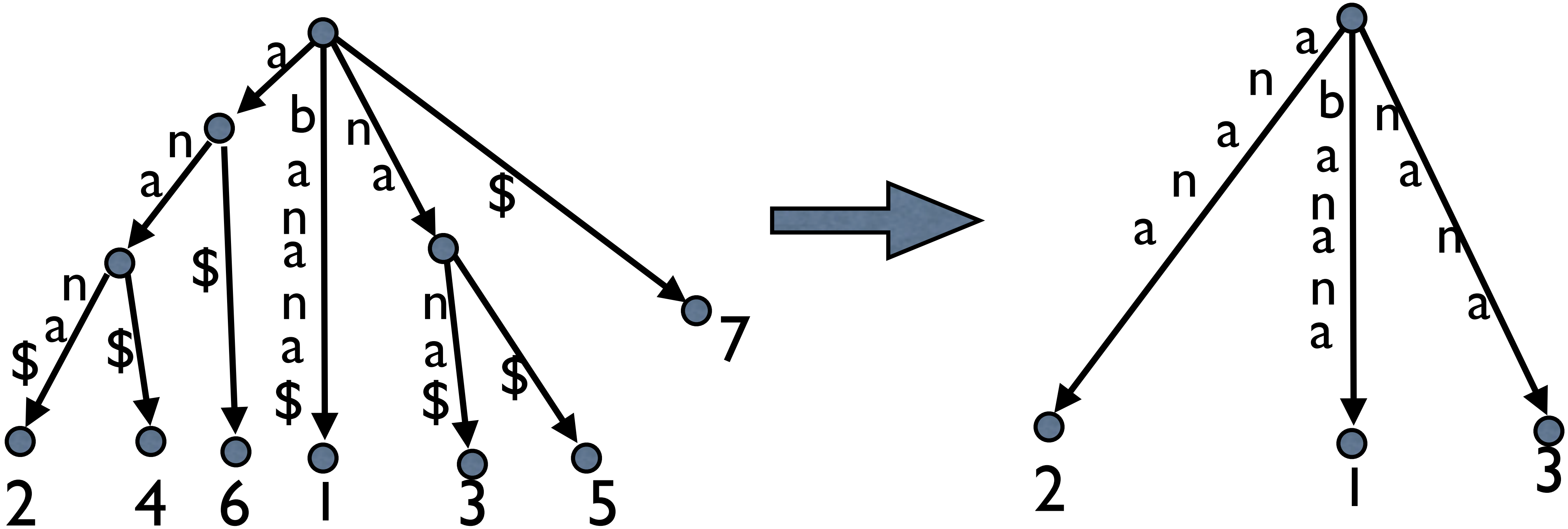


Ukkonen's O(m) algorithm

- On-line algorithm
  - Builds implicit suffix tree for each prefix of string S
  - Implicit suffix tree of $S_{1...i}$ 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 without two children

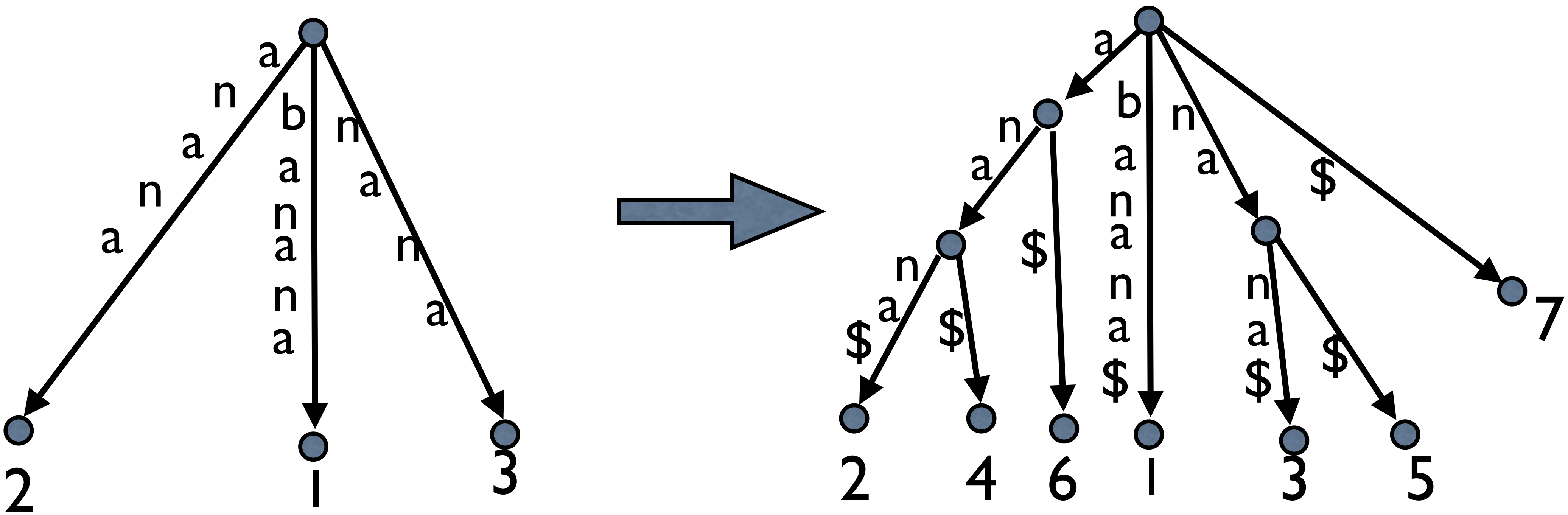


Ukkonen's algorithm overview

- Construct I_1
- For i from 1 to m - 1:
  - For j from 1 to i + 1:
    - Find end of path from root labeled $S_{j\ldots i}$
    - Add character S_{i+1} to the end of this path in the tree, if necessary (suffix extension)

Conversion to suffix tree

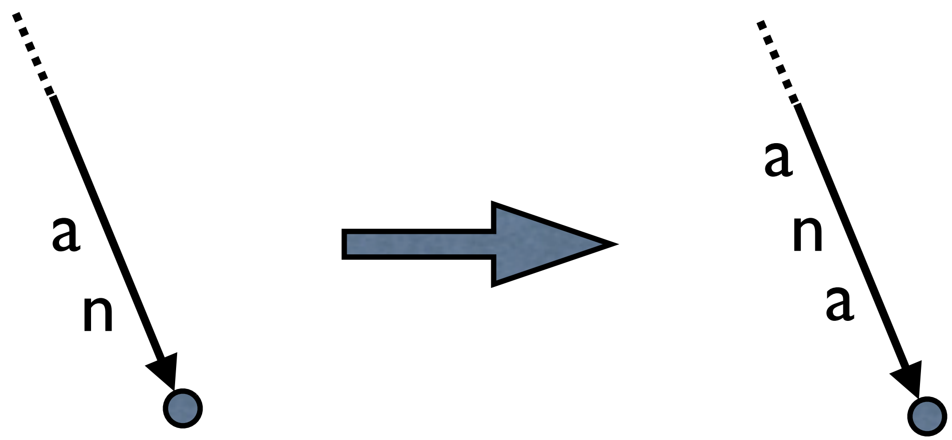
- Convert implicit suffix tree at end of algorithm into true suffix tree
- Simply run algorithm for one more iteration with $ final character
- Traverse tree to label leaf edges with positions



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

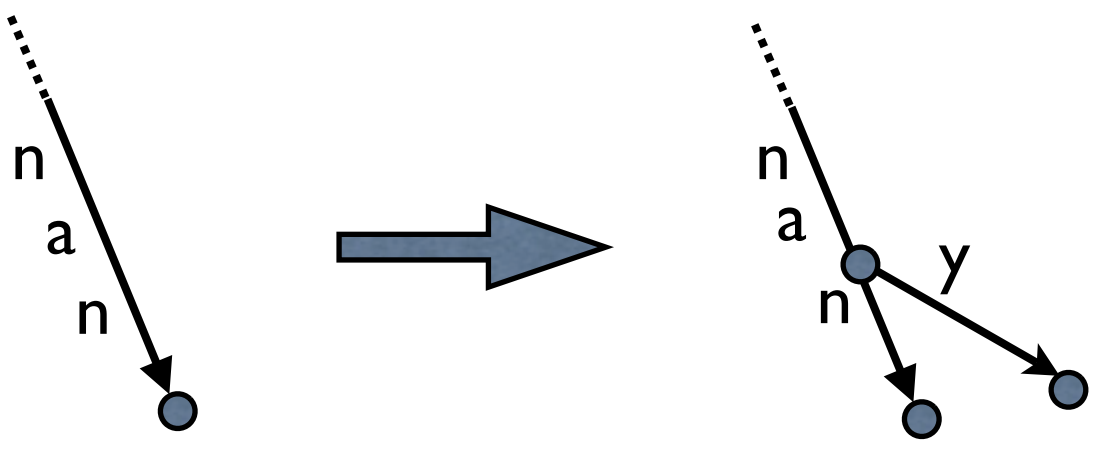
$S_{j...i}$ = ...an $\qquad\qquad$ $S_{j...i+1}$ = ...ana



Suffix extension rule II

II. If there are paths continuing from path $S_{i...j}$ 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 $S_{i...j}$ (creating a new internal node if $S_{i...j}$ ends in the middle of an edge)

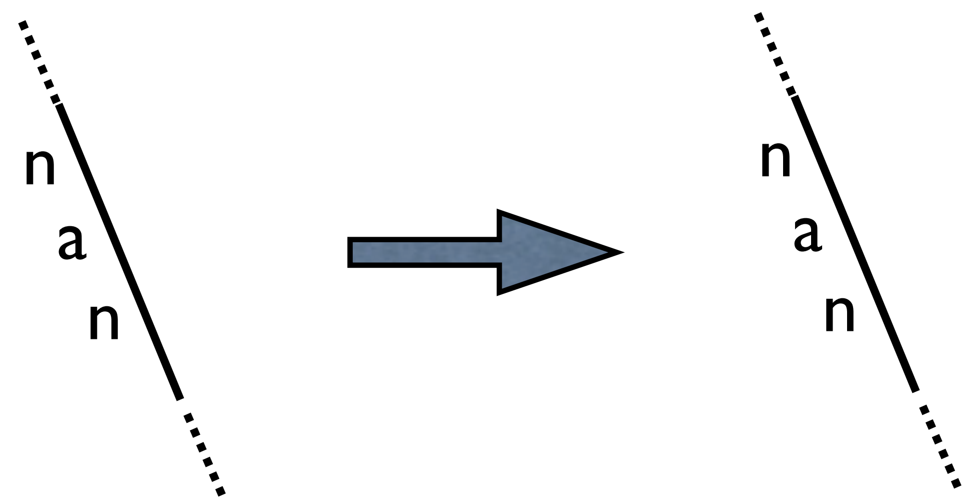
$S_{j...i}$ = ...na $\qquad\qquad$ $S_{j...i+1}$ = ...nay



Suffix extension rule III

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

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

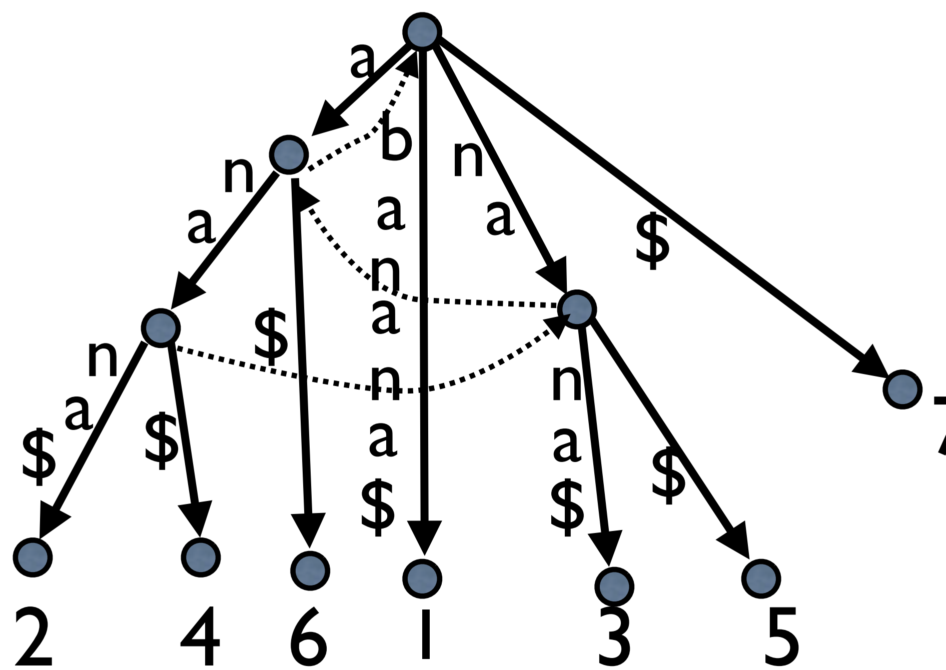


Suffix links

- How to find end of each suffix $S_{j...i}$?
- Could search down tree in O(i-j+1) time $\rightarrow$O(m^3) time total
- Better: create links between nodes corresponding to ends of similar suffixes
- With some additional tricks, get runtime to O(m^2) time total

Suffix link definition

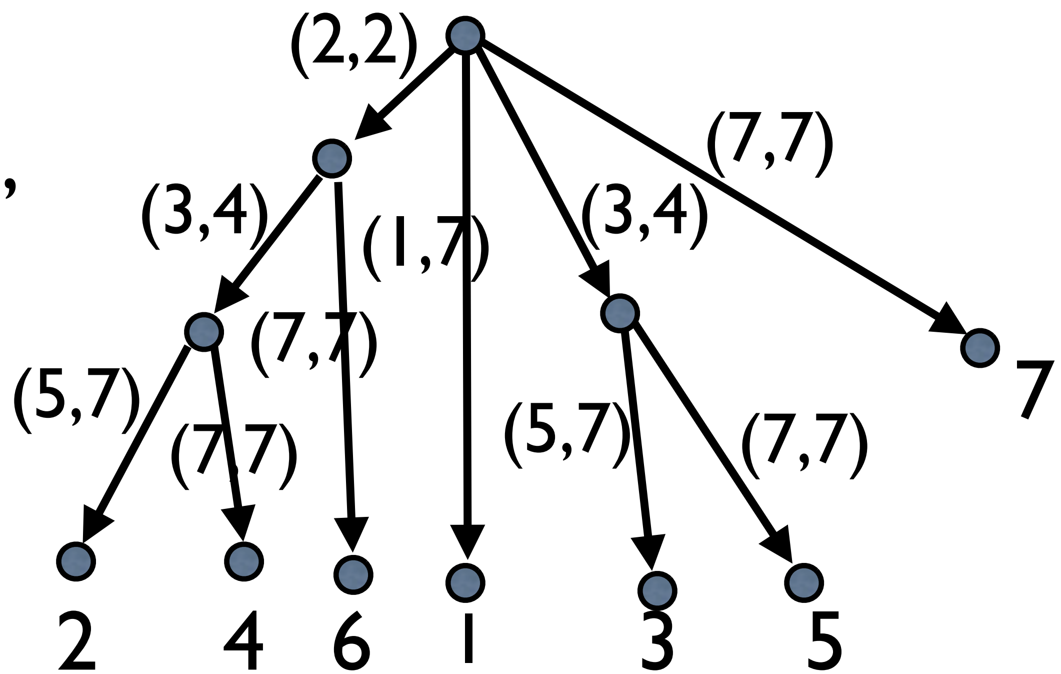
- A *suffix link* is a pointer from an internal node *v* to another node *s(v)* where
    - x is a character, α is a substring (possibly empty)
    - *v* has path-label xα
    - *s(v)* has path-label α



Edge-label compression

- Label edges with pair of indices into string rather than with explicit substring
- Makes space requirement only O(m)

S = "banana$"



Final runtime

- With a few more tricks and implementation details, Ukkonen's algorithm runs in time O(m)
- More details found in (Ukkonen, 1995) or book by Dan Gusfield (Gusfield, 1997)