Suffix trees

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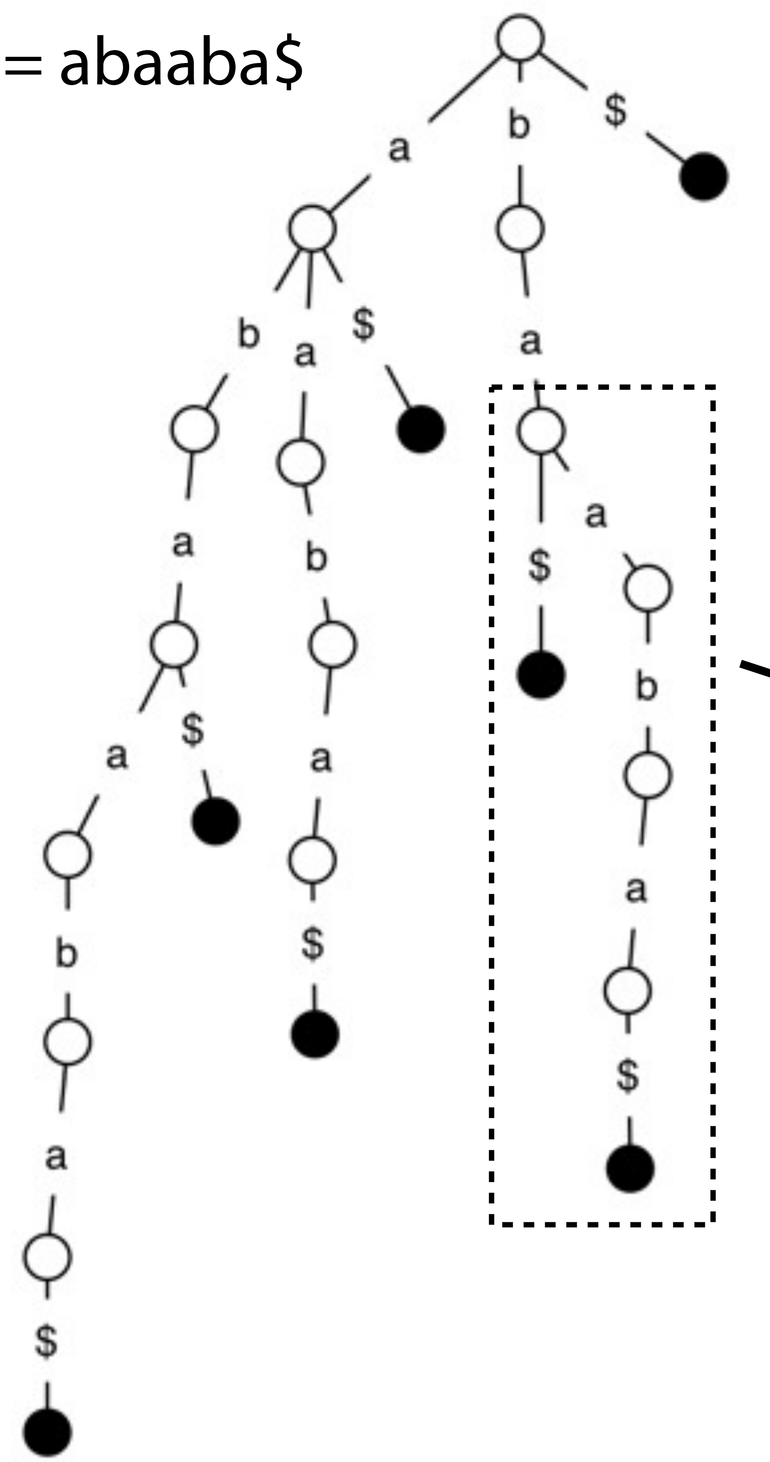
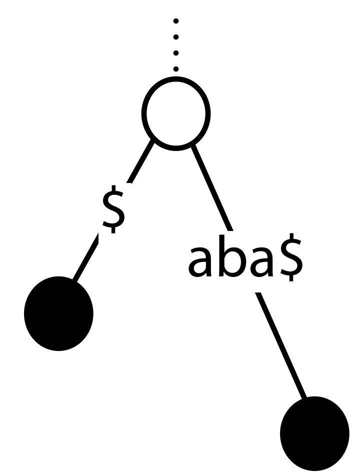
Suffix trie: making it smaller

T = abaaba$



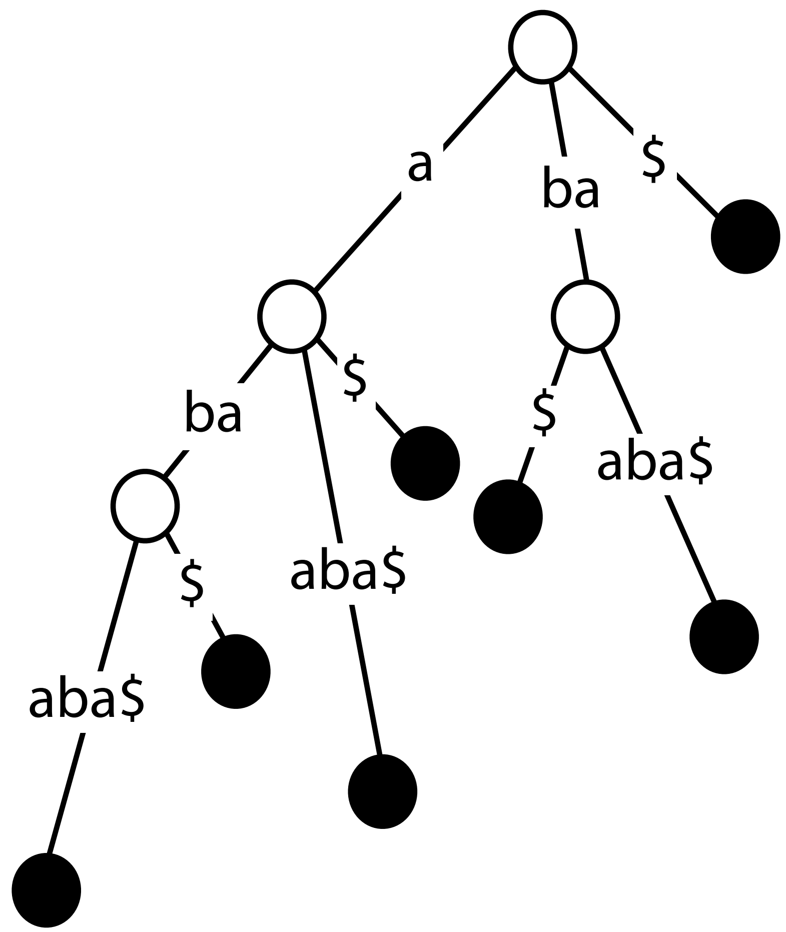
Idea 1: Coalesce non-branching paths into a *single edge* with a *string* label



Reduces # nodes, edges,
guarantees internal nodes have >1 child

Suffix tree

T = abaaba$



With respect to m:

How many leaves? ***m***

How many non-leaf nodes? **≤ *m* - *1***

≤ 2m -1 nodes total, or $O(m)$ nodes

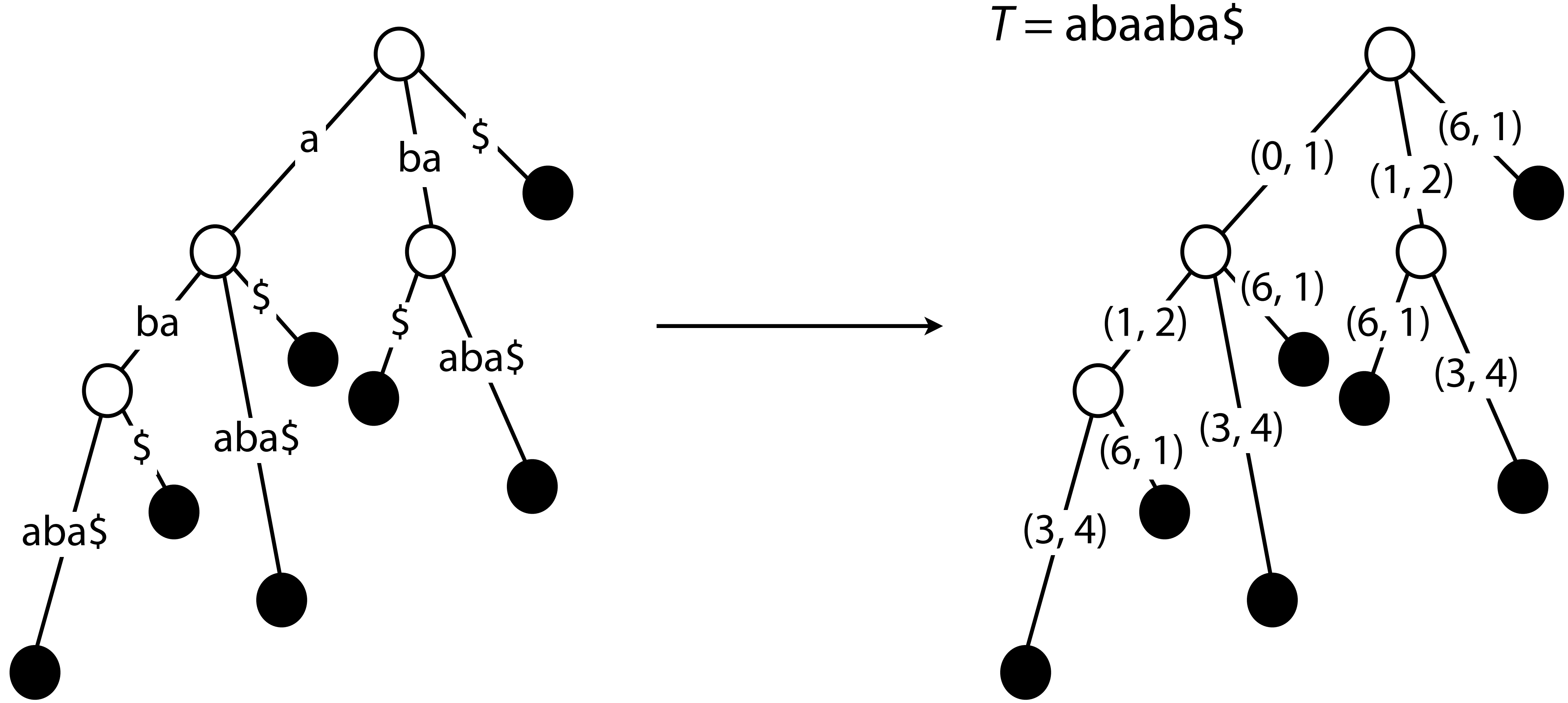
Is the total size $O(m)$ now?

No: total length of edge labels is quadratic in m

Suffix tree

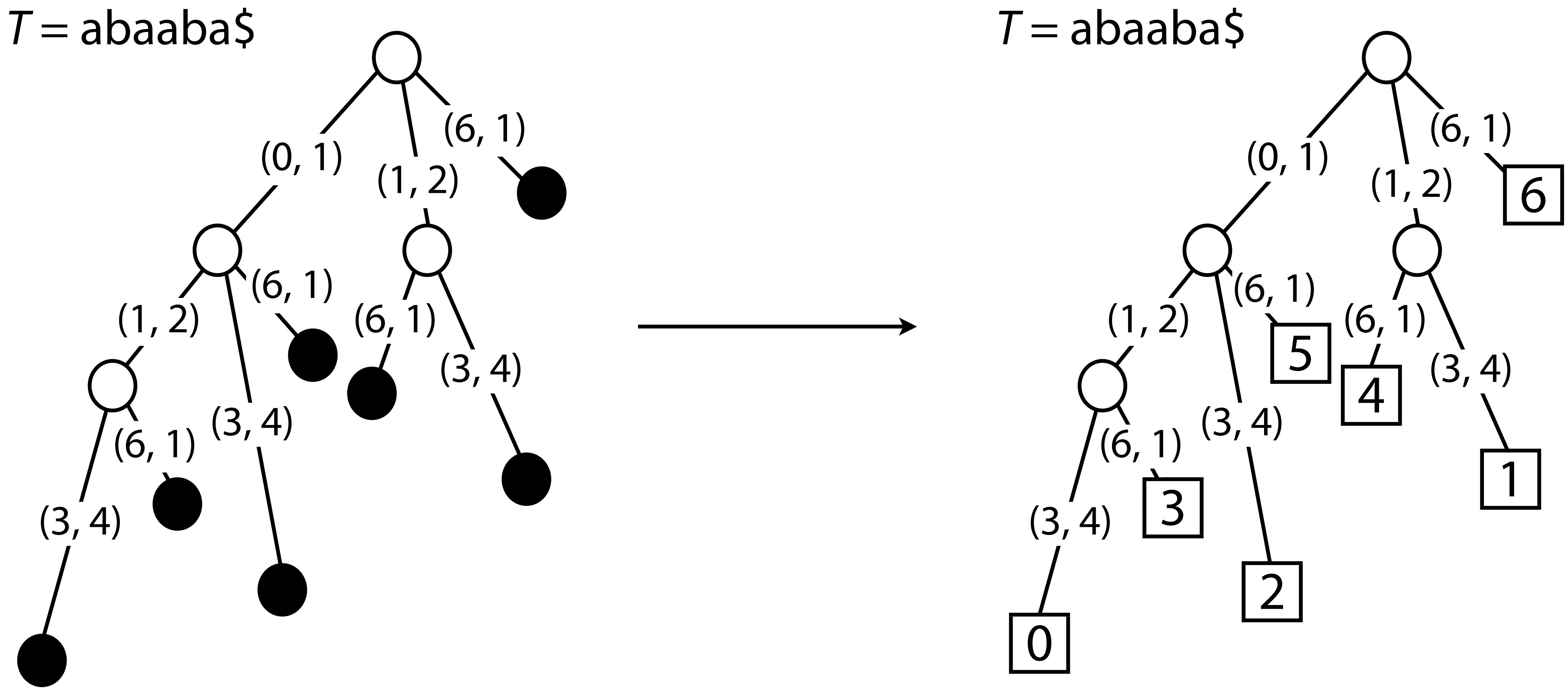
T = abaaba\$

Idea 2: Store T itself in addition to the tree. Convert tree's edge labels to (offset, length) pairs with respect to T.

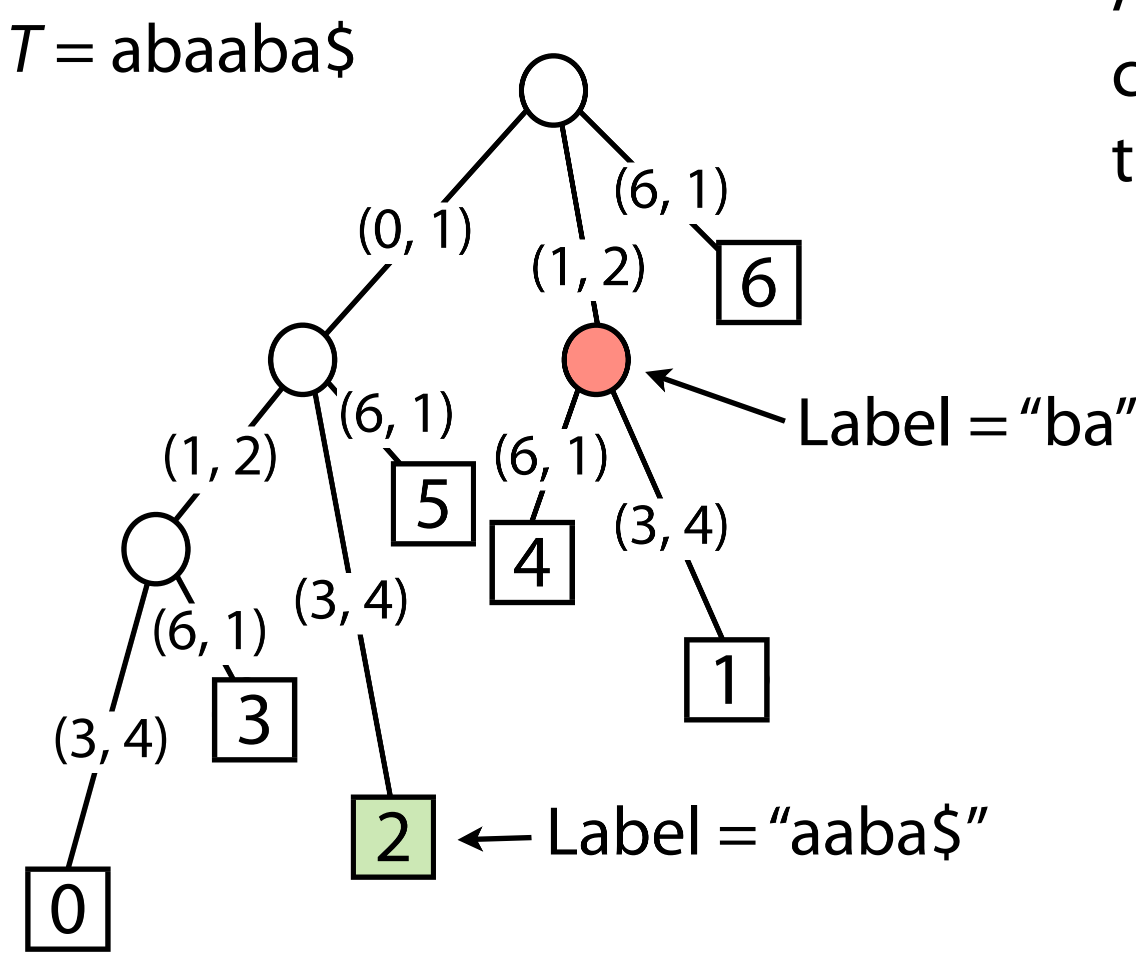


Space required for suffix tree is now $O(m)$

Suffix tree: leaves hold offsets



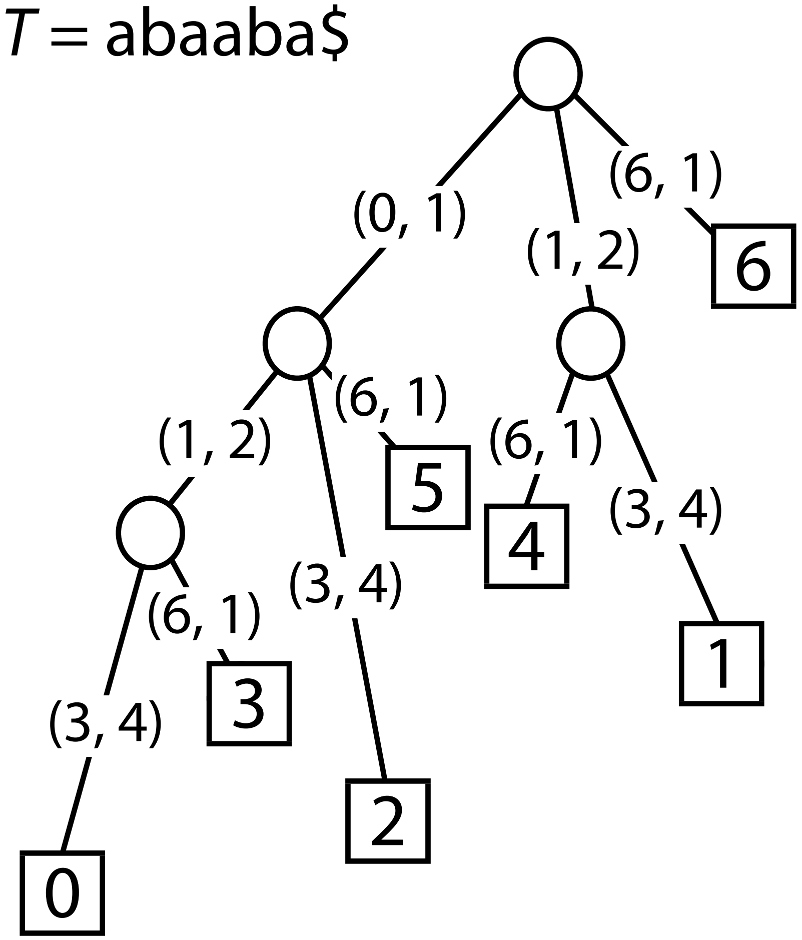
Suffix tree: labels



Again, each node's *label* equals the concatenated edge labels from the root to the node. These aren't stored explicitly.

Suffix tree: labels

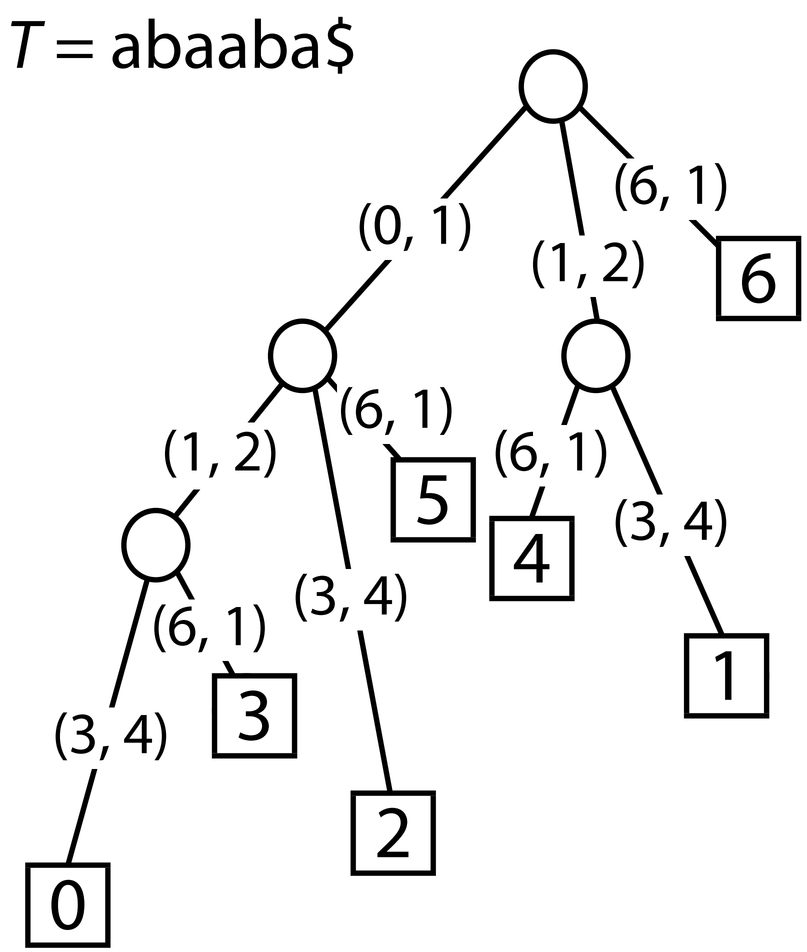
T = abaaba$



Because edges can have string labels, we must distinguish two notions of "depth"

- **Node** depth: how many edges we must follow from the root to reach the node
- **Label** depth: total length of edge labels for edges on path from root to node

Suffix tree: space caveat



Minor point:

We say the space taken by the edge labels is O(m), because we keep 2 integers per edge and there are O(m) edges

To store one such integer, we need enough bits to distinguish m positions in T, i.e. ceil($\log_2 m$) bits. We usually ignore this factor, since 64 bits is plenty for all practical purposes.

Similar argument for the pointers / references used to distinguish tree nodes.

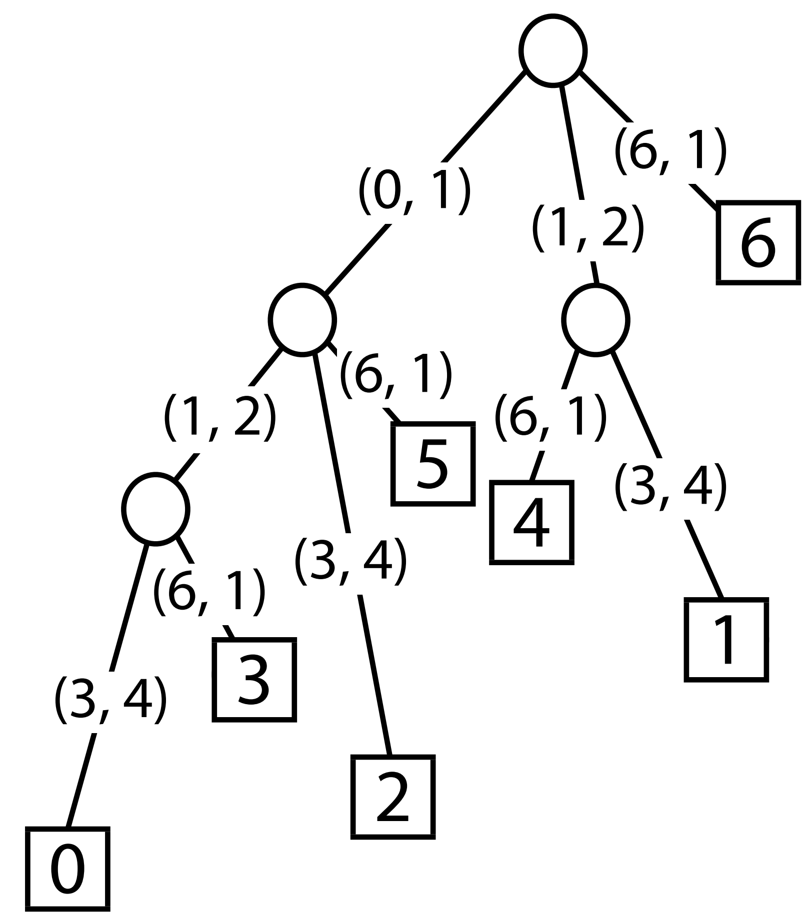
Suffix tree: building

Naive method 1: build a suffix trie, then coalesce non-branching paths and relabel edges

Naive method 2: build a single-edge tree representing only the longest suffix, then augment to include the 2nd-longest, then augment to include 3rd-longest, etc

Both are $O(m^2)$ time, but first uses $O(m^2)$ space while second uses $O(m)$

Naive method 2 is described in Gusfield 5.4



Suffix tree: implementation

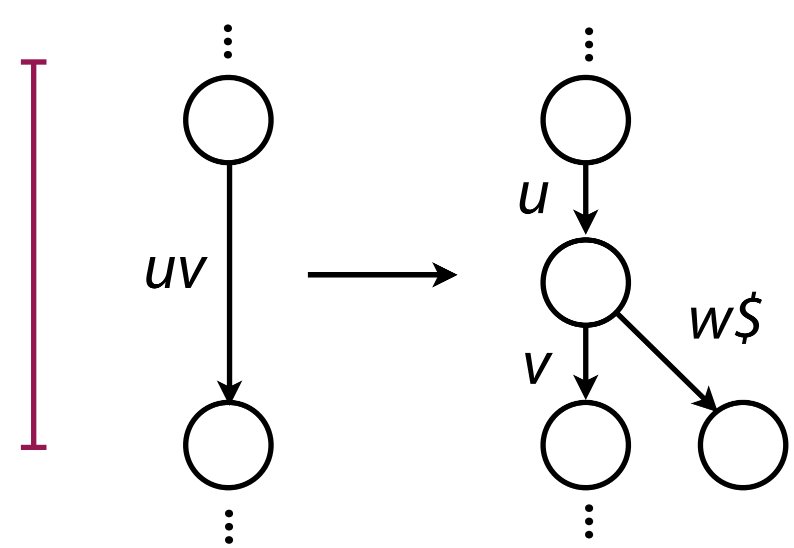
```
class SuffixTree(object):

    class Node(object):
        def __init__(self, lab):
            self.lab = lab # label on path leading to this node
            self.out = {}  # outgoing edges; maps characters to nodes

    def __init__(self, s):
        """ Make suffix tree, without suffix links, from s in quadratic time
            and linear space """
        s += '$'
        self.root = self.Node(None)
        self.root.out[s[0]] = self.Node(s) # trie for just longest suf
        # add the rest of the suffixes, from longest to shortest
        for i in xrange(1, len(s)):
            # start at root; we'll walk down as far as we can go
            cur = self.root
            j = i
            while j < len(s):
                if s[j] in cur.out:
                    child = cur.out[s[j]]
                    lab = child.lab
                    # Walk along edge until we exhaust edge label or
                    # until we mismatch
                    k = j+1
                    while k-j < len(lab) and s[k] == lab[k-j]:
                        k += 1
                    if k-j == len(lab):
                        cur = child # we exhausted the edge
                        j = k
                    else:
                        # we fell off in middle of edge
                        cExist, cNew = lab[k-j], s[k]
                        # create "mid": new node bisecting edge
                        mid = self.Node(lab[:k-j])
                        mid.out[cNew] = self.Node(s[k:])
                        # original child becomes mid's child
                        mid.out[cExist] = child
                        # original child's label is curtailed
                        child.lab = lab[k-j:]
                        # mid becomes new child of original parent
                        cur.out[s[j]] = mid
                else:
                    # Fell off tree at a node: make new edge hanging off it
                    cur.out[s[j]] = self.Node(s[j:])
```

$O(m^2)$ time, $O(m)$ space

Make 2-node tree for longest suffix

Add rest of suffixes from long to short, adding 1 or 2 nodes for each

Most complex case:



Suffix tree: implementation

```
(still in class SuffixTree)

    def followPath(self, s):
        """ Follow path given by s.  If we fall off tree, return None.  If we
            finish mid-edge, return (node, offset) where 'node' is child and
            'offset' is label offset.  If we finish on a node, return (node,
            None). """
        cur = self.root
        i = 0
        while i < len(s):
            c = s[i]
            if c not in cur.out:
                return (None, None) # fell off at a node
            child = cur.out[s[i]]
            lab = child.lab
            j = i+1
            while j-i < len(lab) and j < len(s) and s[j] == lab[j-i]:
                j += 1
            if j-i == len(lab):
                cur = child # exhausted edge
                i = j
            elif j == len(s):
                return (child, j-i) # exhausted query string in middle of edge
            else:
                return (None, None) # fell off in the middle of the edge
        return (cur, None) # exhausted query string at internal node
```

followPath: Given a string, walk down corresponding path. Return a special value if we fall off, or a description of where we end up otherwise.

```
    def hasSubstring(self, s):
        """ Return true iff s appears as a substring """
        node, off = self.followPath(s)
        return node is not None
```

Has substring? Return true iff **followPath** didn't fall off.

```
    def hasSuffix(self, s):
        """ Return true iff s is a suffix """
        node, off = self.followPath(s)
        if node is None:
            return False # fell off the tree
        if off is None:
            # finished on top of a node
            return '$' in node.out
        else:
            # finished at offset 'off' within an edge leading to 'node'
            return node.lab[off] == '$'
```

Has suffix? Return true iff **followPath** didn't fall off and we ended just above a "$".

Suffix tree: implementation

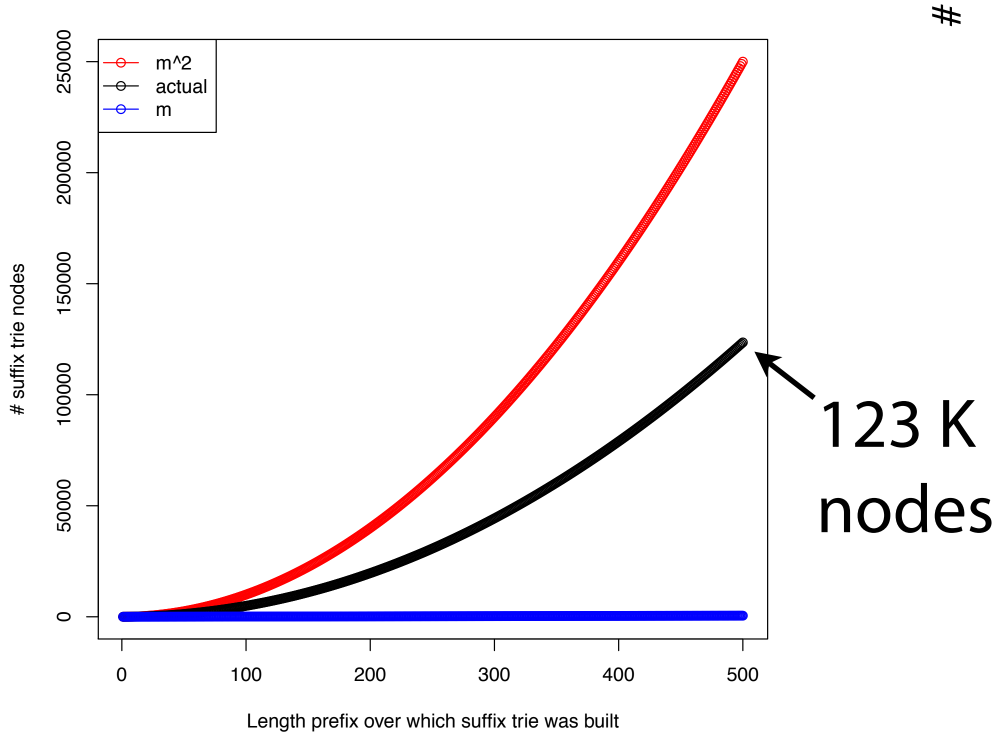
Python example here: http://nbviewer.ipython.org/6665861

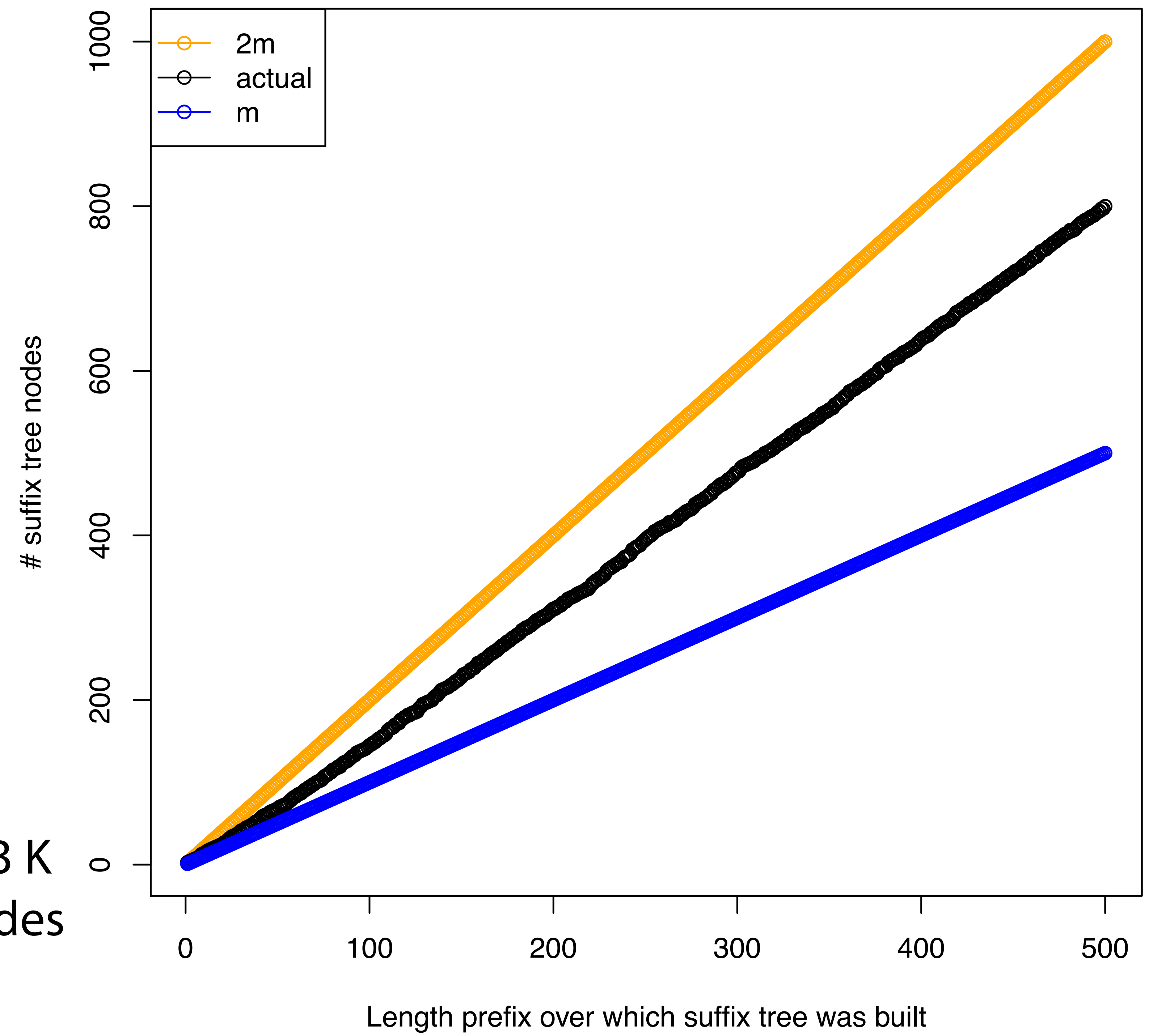
Suffix tree: actual growth

Built suffix trees for the first 500 prefixes of the lambda phage virus genome

Black curve shows # nodes increasing with prefix length

Compare with suffix trie:





Suffix tree: building

Method of choice: Ukkonen's algorithm

Ukkonen, Esko. "On-line construction of suffix trees." *Algorithmica* 14.3 (1995): 249-260.

$O(m)$ time and space

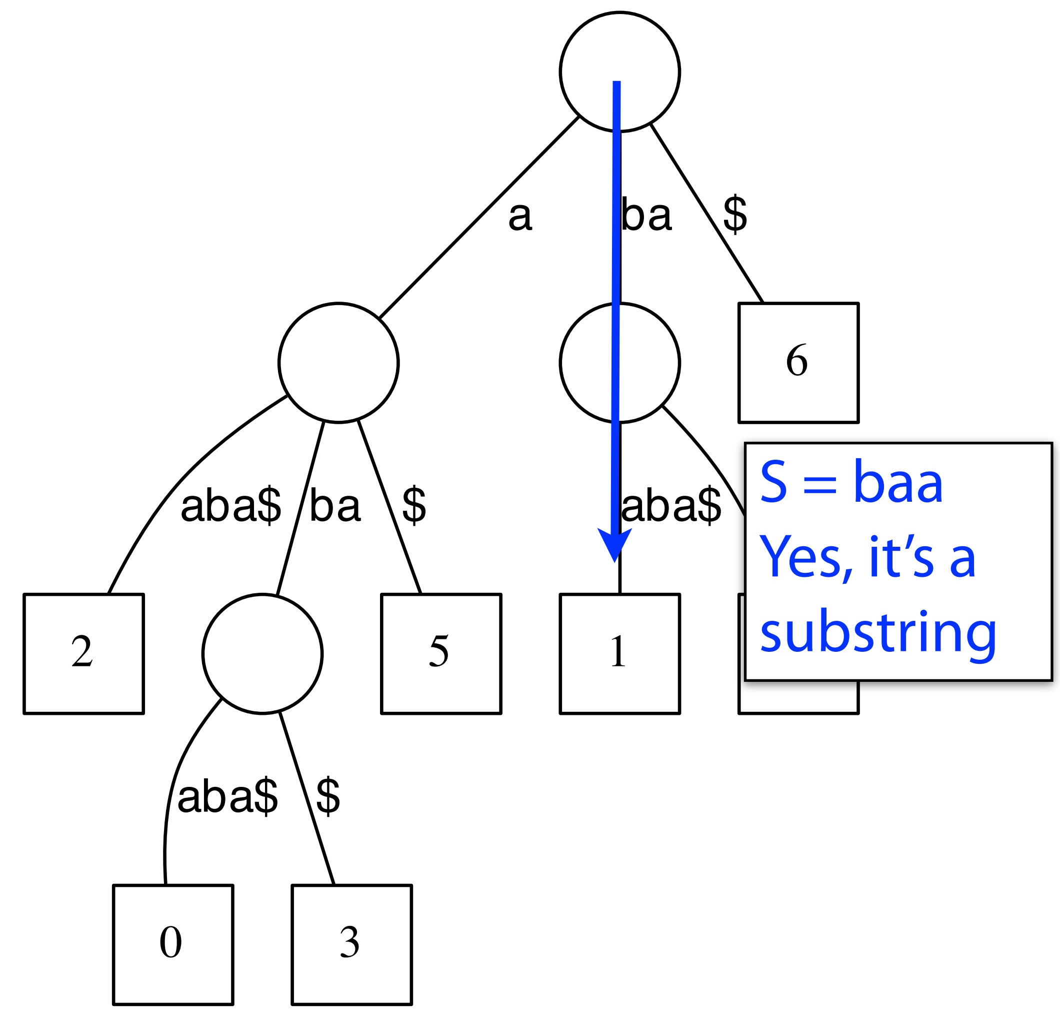
Has *online* property: if T arrives one character at a time, algorithm efficiently updates suffix tree upon each arrival

We won't cover it here; see Gusfield Ch. 6 for details

Suffix tree

How do we check whether a string *S* is a substring of *T*?

Essentially same procedure as for suffix trie, except we have to deal with coalesced edges



Suffix tree

How do we check whether a string *S* is a suffix of *T*?

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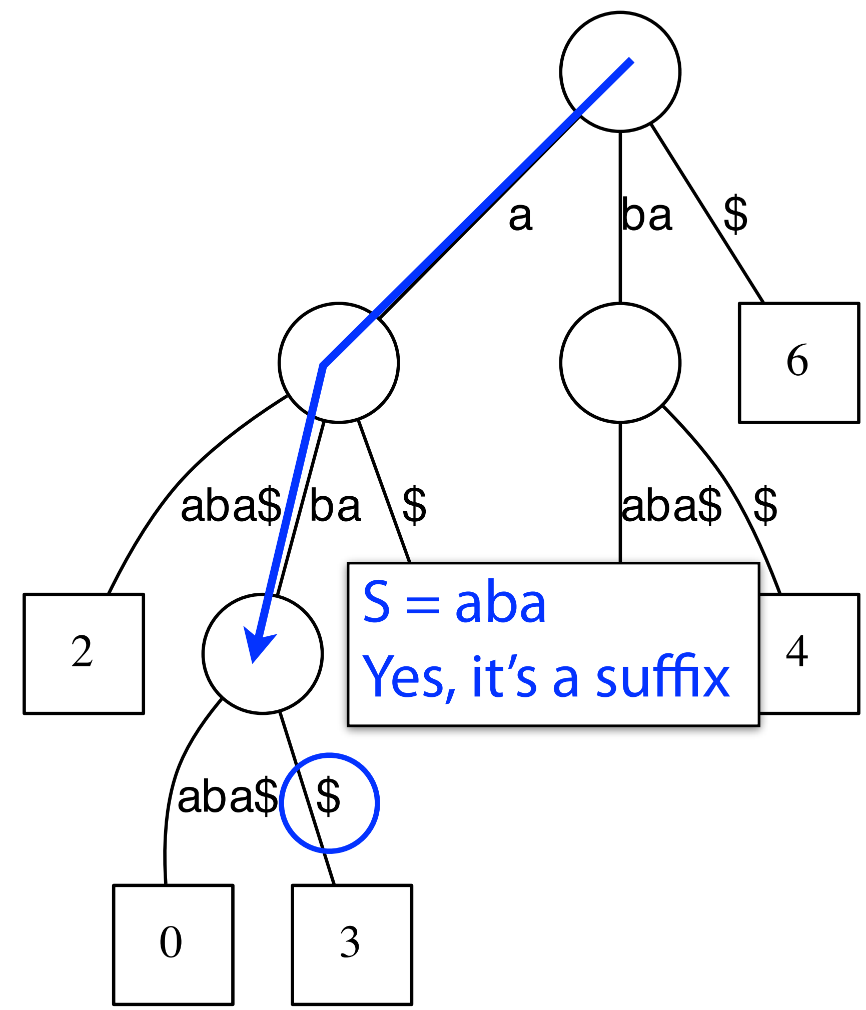
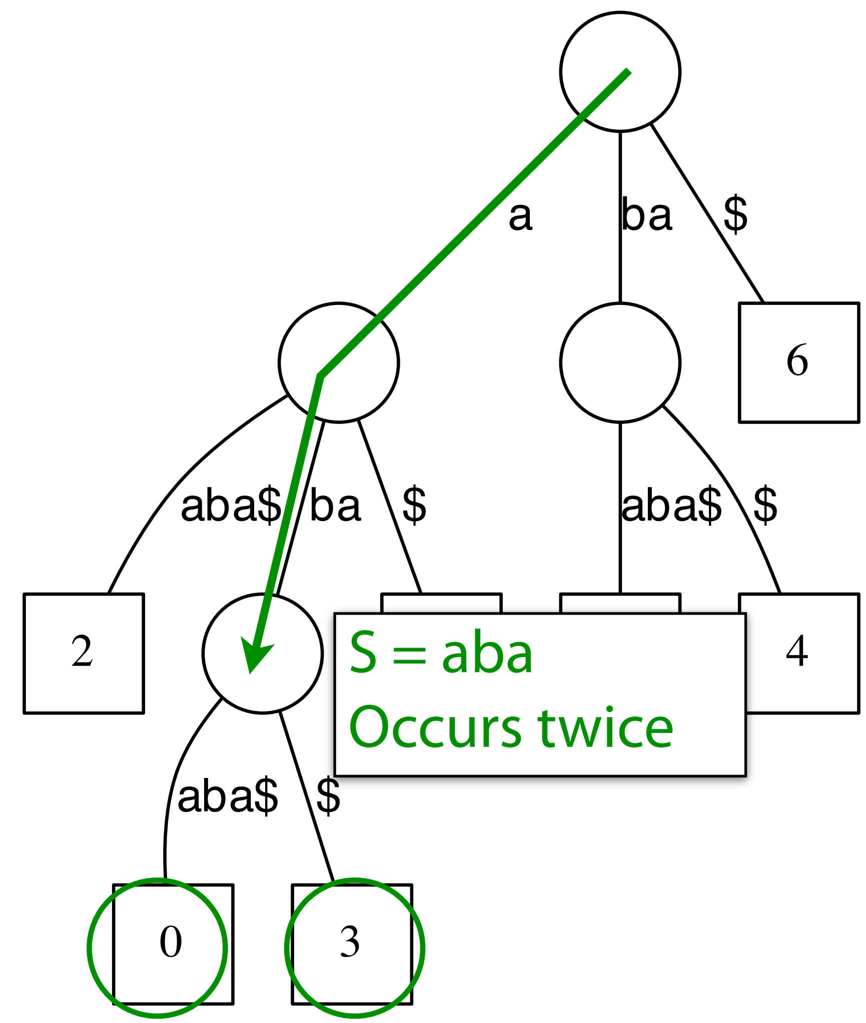


Suffix tree

How do we count the **number of times** a string *S* occurs as a substring of *T*?

Same procedure as for suffix trie



Suffix tree: applications

With suffix tree of T, we can find all matches of P to T. Let k = # matches.

E.g., P = ab, T = abaaba$

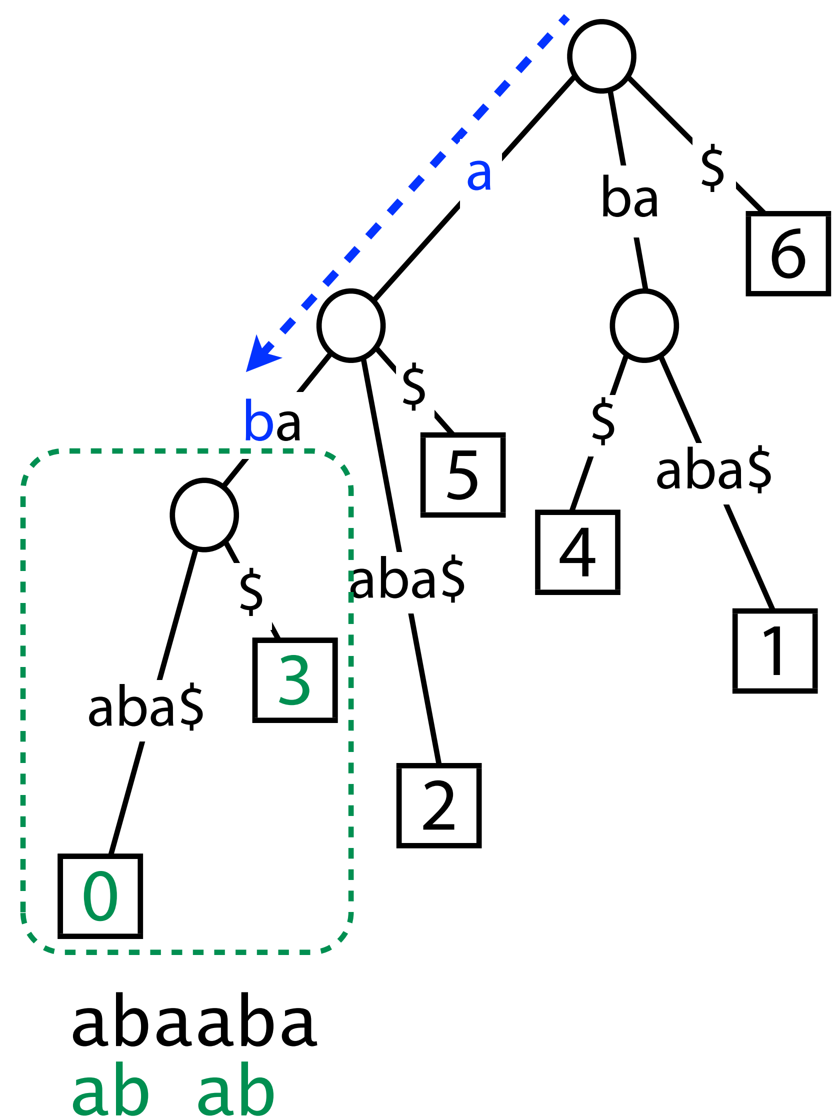
$O(n)$ Step 1: walk down ab path

If we "fall off" there are no matches

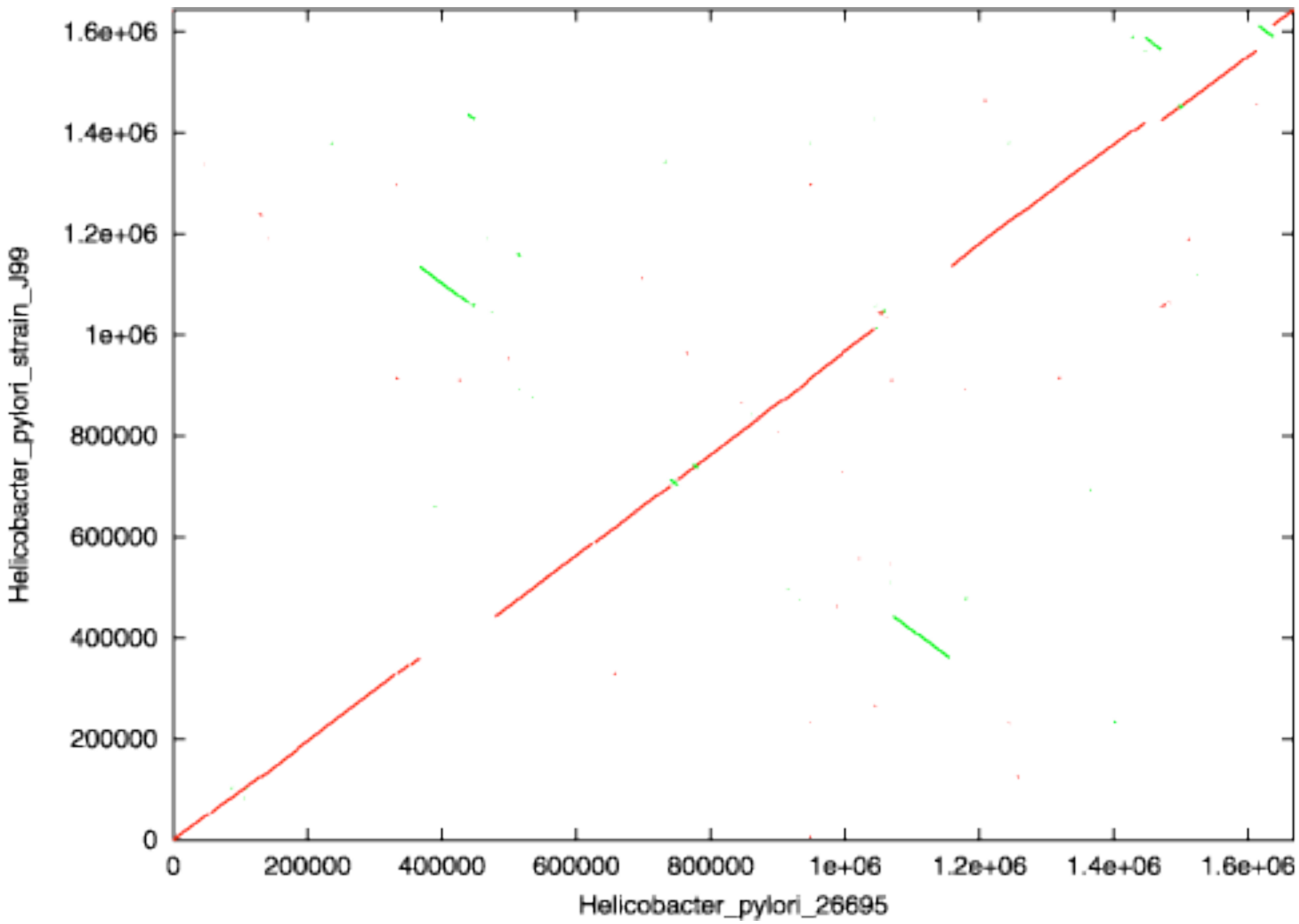
$O(k)$ Step 2: visit all leaf nodes below

Report each leaf offset as match offset

$O(n + k)$ time



Suffix tree application: find long common substrings



Dots are *maximal unique matches* (*MUMs*), a kind of long substring shared by two sequences

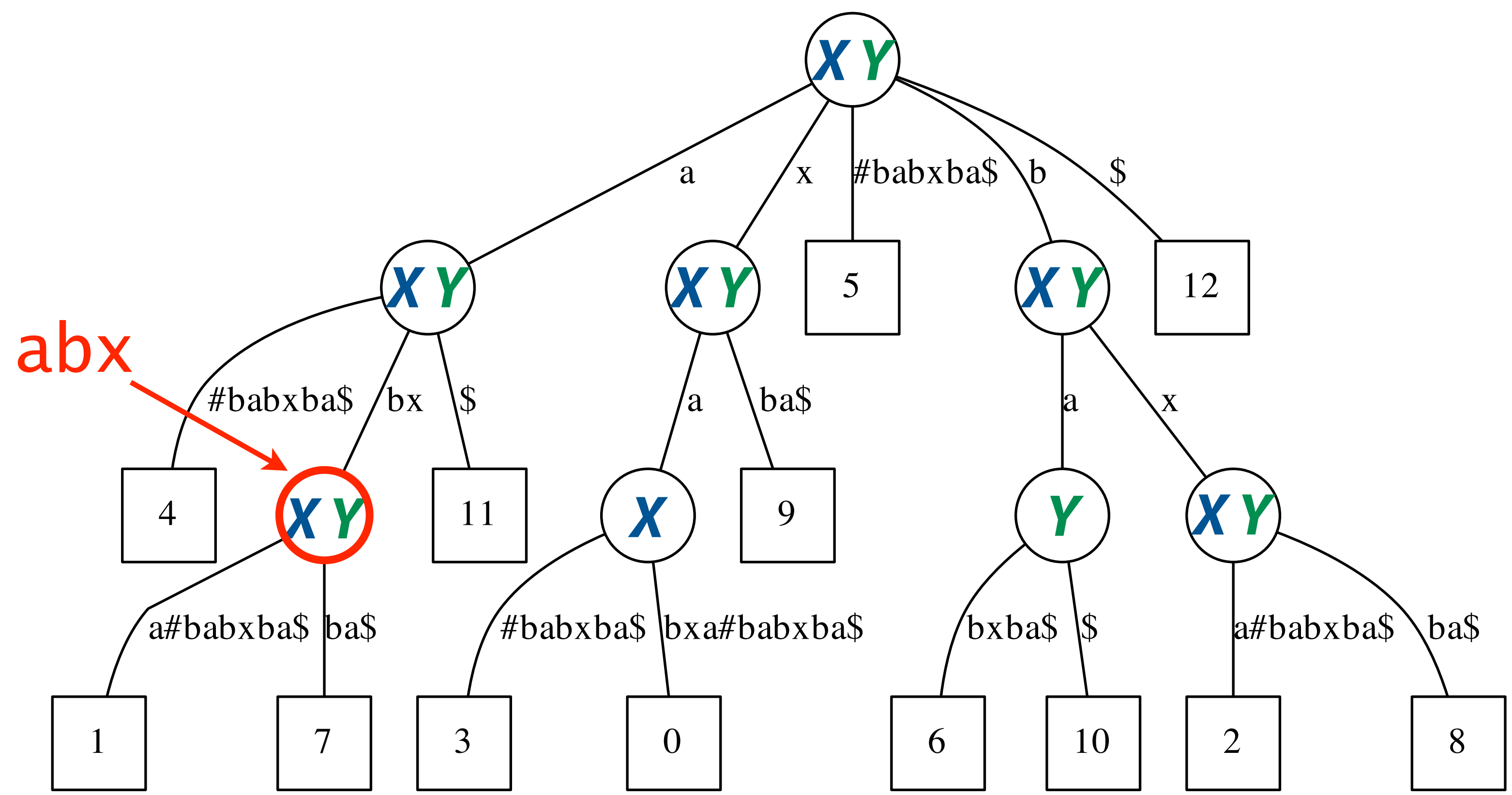
Red = match was between like strands, green = different strands

Axes show different strains of Helicobacter pylori, a bacterium found in the stomach and associated with gastric ulcers

Suffix tree application: find longest common substring

To find the longest common substring (LCS) of *X* and *Y*, make a new string $X\#Y\$$ where $\#$ and $\$$ are both terminal symbols. Build a suffix tree for $X\#Y\$$.

X = xabxa
Y = babxba
***X*#*Y*$** = xabxa#babxba$



Consider leaves:
offsets in [0, 4] are suffixes of ***X***, offsets in [6, 11] are suffixes of ***Y***

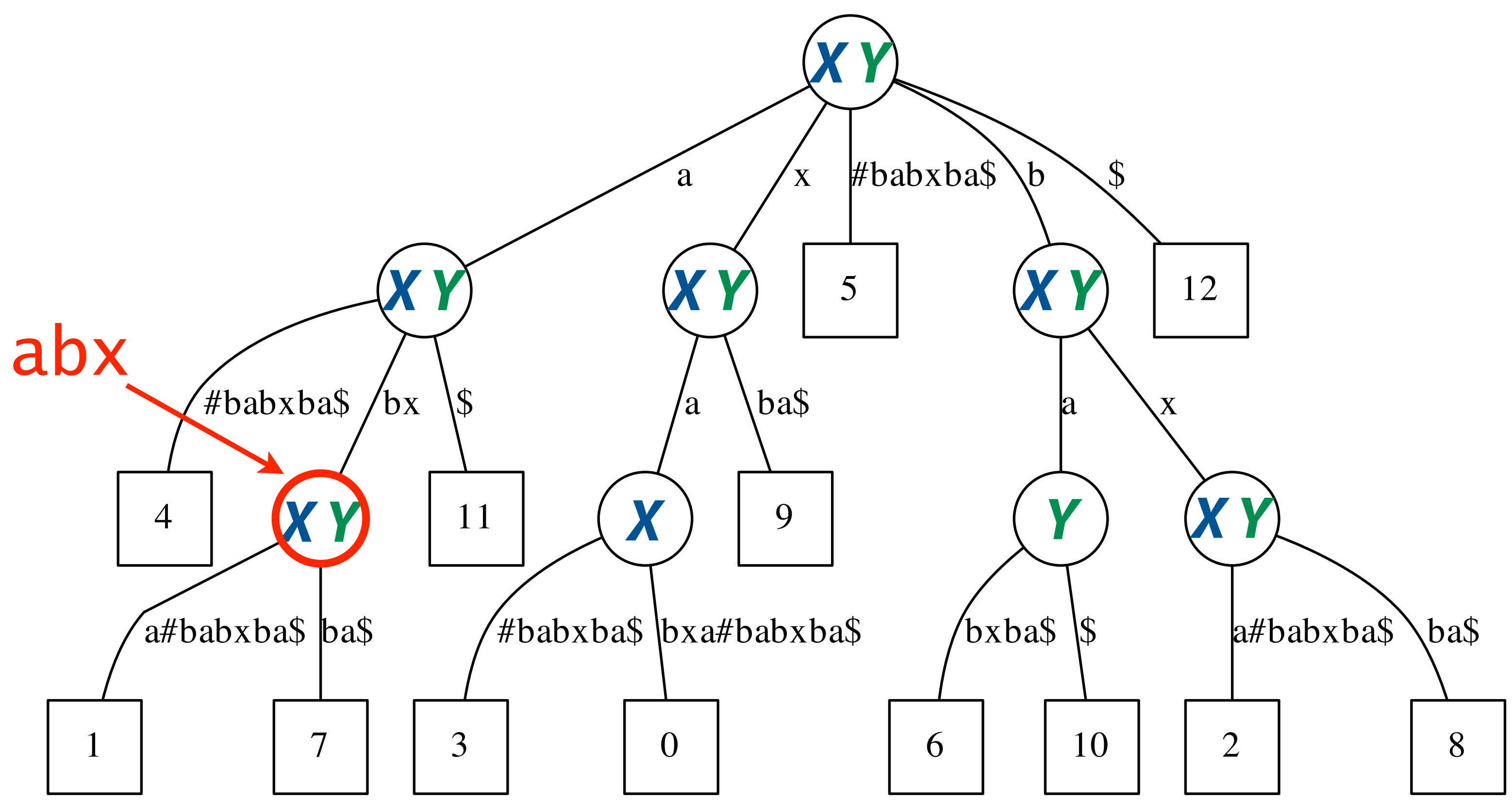
Traverse the tree and annotate each node according to whether leaves below it include suffixes of ***X***, ***Y*** or both

The deepest node annotated with both ***X*** and ***Y*** has LCS as its label.
$O(|X|+|Y|)$ time and space.

Suffix tree application: generalized suffix trees

This is one example of many applications where it is useful to build a suffix tree over many strings at once

Such a tree is called a *generalized suffix tree.* These are introduced in *Gusfield* 6.4.



Suffix trees in the real world: MUMmer

FASTA file containing "reference" ("text")

FASTA file containing ALU string

mummer — langmead@igm1:~ — bash — 120×31

```
Bens-MacBook-Pro:mummer langmead$ cat alu50.fa
>Alu
GCGCGGTGGCTCACGCCTGTAATCCCAGCACTTTGGGAGGCCGAGGCGGG
Bens-MacBook-Pro:mummer langmead$ $HOME/software/MUMmer3.23/mummer -maxmatch $HOME/fasta/hg19/chr1.fa alu50.fa
# reading input file "/Users/langmead/fasta/hg19/chr1.fa" of length 249250621
# construct suffix tree for sequence of length 249250621
# (maximum reference length is 536870908)
# (maximum query length is 4294967295)
# process 2492506 characters per dot
#....................................................................................................
# CONSTRUCTIONTIME /Users/langmead/software/MUMmer3.23/mummer /Users/langmead/fasta/hg19/chr1.fa 125.30
# reading input file "alu50.fa" of length 50
# matching query-file "alu50.fa"
# against subject-file "/Users/langmead/fasta/hg19/chr1.fa"
> Alu
61769671         1        22
219929011         1        22
162396657         1        22
109737840         1        22
82615090         1        22
32983678         1        22
84730371         1        22
248036256         1        22
150558745         1        22
11127213         1        22
236885661         1        22
31639677         1        22
16027333         1        22
21577225         1        22
26327837         1        22
243352583         1        22
```

Indexing phase: ~2 minutes

Matching phase: very fast

Columns:

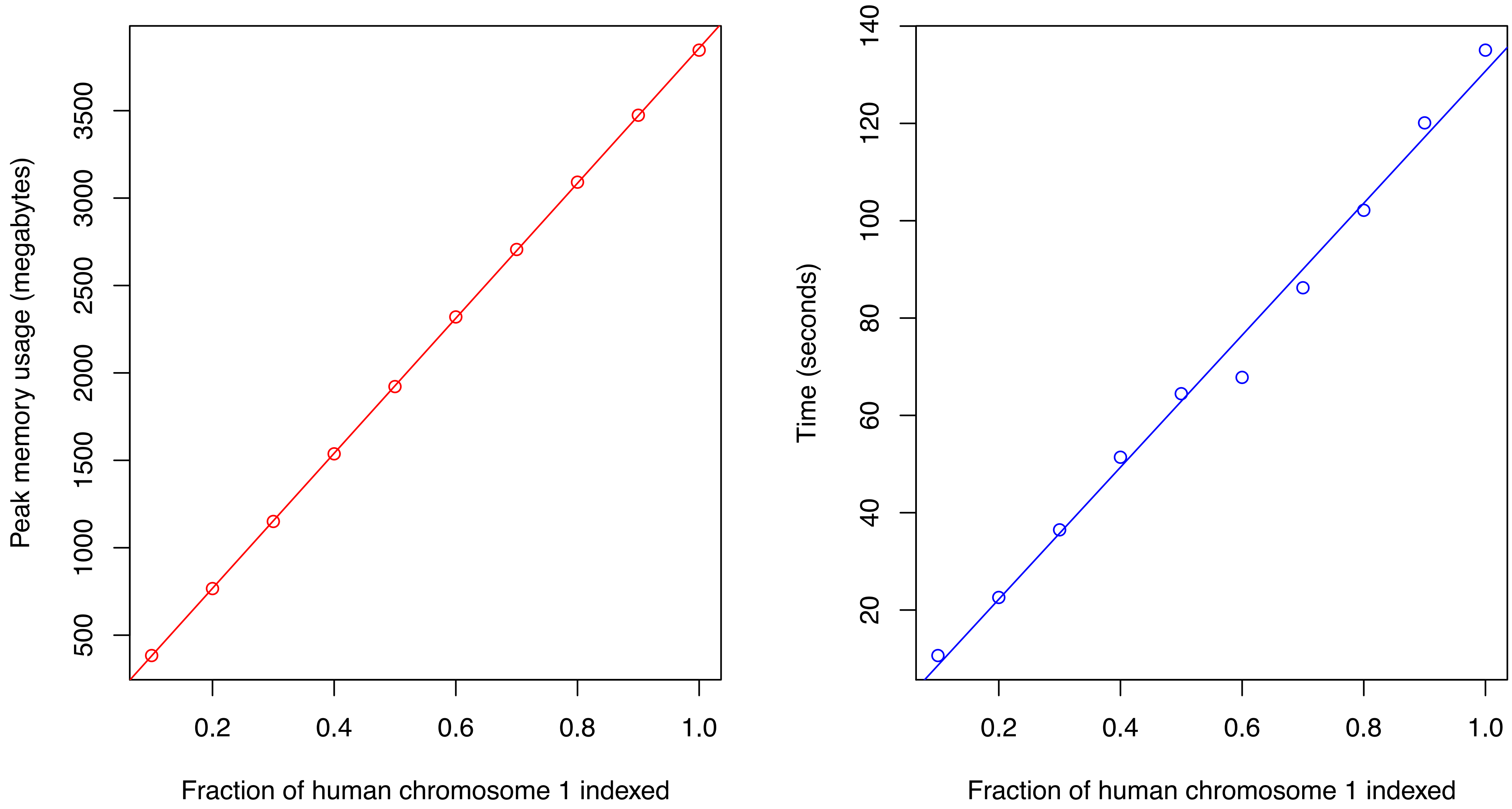
1. Match offset in T

2. Match offset in P

3. Length of exact match

Suffix trees in the real world: MUMmer

MUMmer v3.32 time and memory scaling when indexing increasingly larger fractions of human chromosome 1



For whole chromosome 1, took 2m:14s and used 3.94 GB memory

Suffix trees in the real world: MUMmer

Attempt to build index for whole human genome reference:

```
mummer: suffix tree construction failed: textlen=3101804822
larger than maximal textlen=536870908
```

We can predict it would have taken about 47 GB of memory

Suffix trees in the real world: the constant factor

While $O(m)$ is desirable, the constant in front of the m limits wider use of suffix trees in practice

Constant factor varies depending on implementation:

Estimate of MUMmer's constant factor = 3.94 GB / 250 million nt ≈ **15.75 bytes per node**

Literature reports implementations achieving as little as 8.5 bytes per node, but no implementation used in practice that I know of is better than ≈ **12.5 bytes per node**

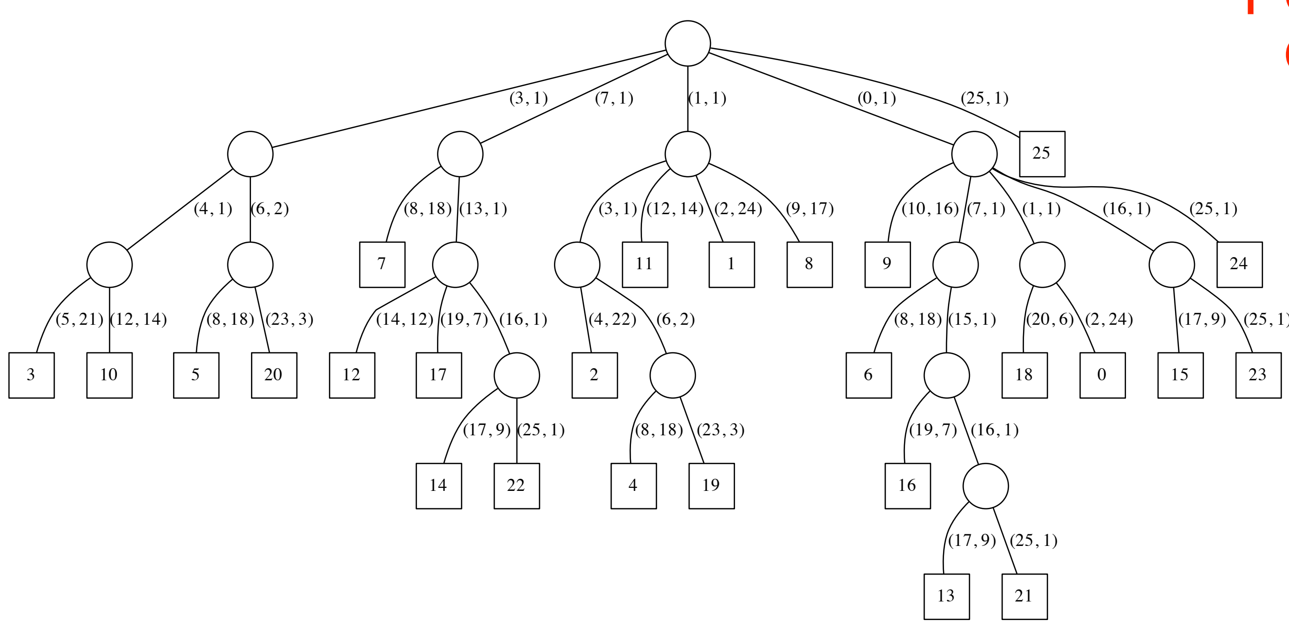
Kurtz, Stefan. "Reducing the space requirement of suffix trees." *Software Practice and Experience* 29.13 (1999): 1149-1171.

Suffix tree: summary

Organizes all suffixes into an incredibly useful, flexible data structure, in $O(m)$ time and space

A naive method (e.g. suffix trie) could easily be quadratic or worse

Used in practice for whole genome alignment, repeat identification, etc



Actual memory footprint (bytes per node) is quite high, limiting usefulness

G T T A T A G C T G A T C G C G G C G T A G C G G $ *m* chars

G T T A T A G C T G A T C G C G G C G T A G C G G $
T T A T A G C T G A T C G C G G C G T A G C G G $
T A T A G C T G A T C G C G G C G T A G C G G $
A T A G C T G A T C G C G G C G T A G C G G $
T A G C T G A T C G C G G C G T A G C G G $
A G C T G A T C G C G G C G T A G C G G $
G C T G A T C G C G G C G T A G C G G $
C T G A T C G C G G C G T A G C G G $
T G A T C G C G G C G T A G C G G $
G A T C G C G G C G T A G C G G $
A T C G C G G C G T A G C G G $
T C G C G G C G T A G C G G $
C G C G G C G T A G C G G $
G C G G C G T A G C G G $
C G G C G T A G C G G $
G G C G T A G C G G $
G C G T A G C G G $
C G T A G C G G $
G T A G C G G $
T A G C G G $
A G C G G $
G C G G $
C G G $
G G $
G $
$

m(m+1)/2 chars