

# Introduction to string indexing



UNIVERSITY OF  
MARYLAND

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# Tries

A trie (pronounced “try”) is a rooted tree representing a collection of strings with one node per common prefix

Smallest tree such that:

Each edge is labeled with a character  $c \in \Sigma$

A node has at most one outgoing edge labeled  $c$ , for  $c \in \Sigma$

Each key is “spelled out” along some path starting at the root

Natural way to represent either a *set* or a *map* where keys are strings

This structure is also known as a  $\Sigma$ -tree

# Tries: example

Represent this map with a trie:

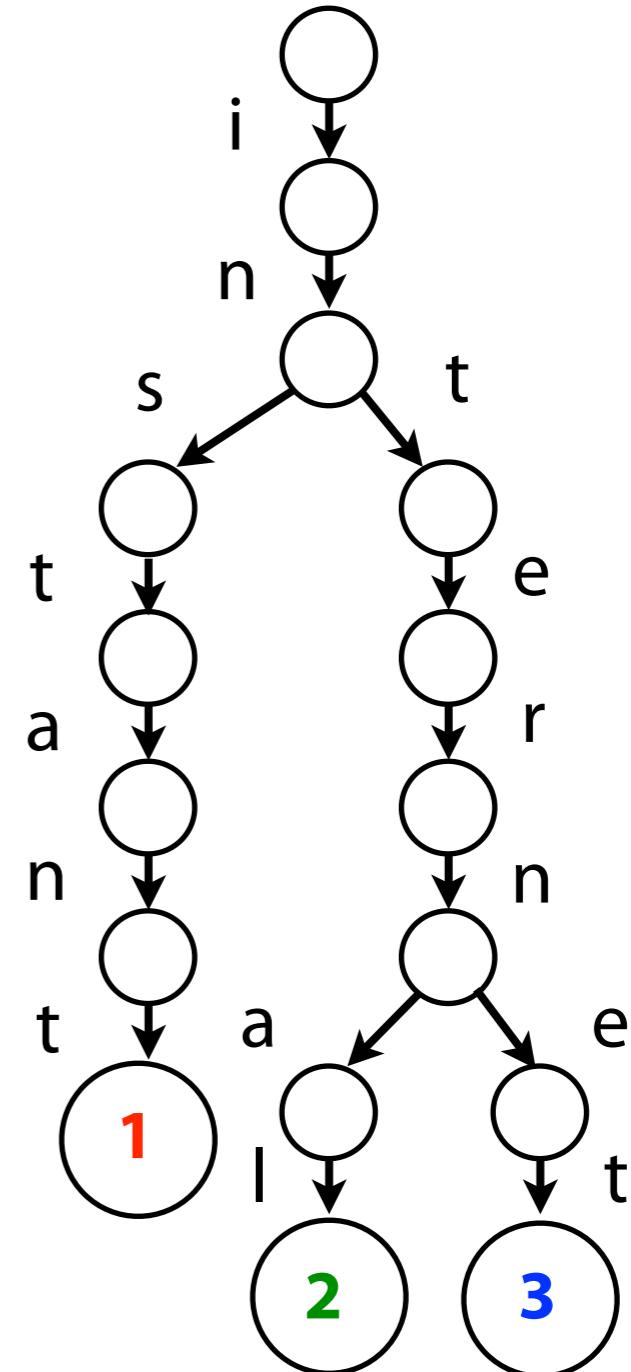
Key	Value
instant	1
internal	2
internet	3

The smallest tree such that:

Each edge is labeled with a character  $c \in \Sigma$

A node has at most one outgoing edge  
labeled  $c$ , for  $c \in \Sigma$

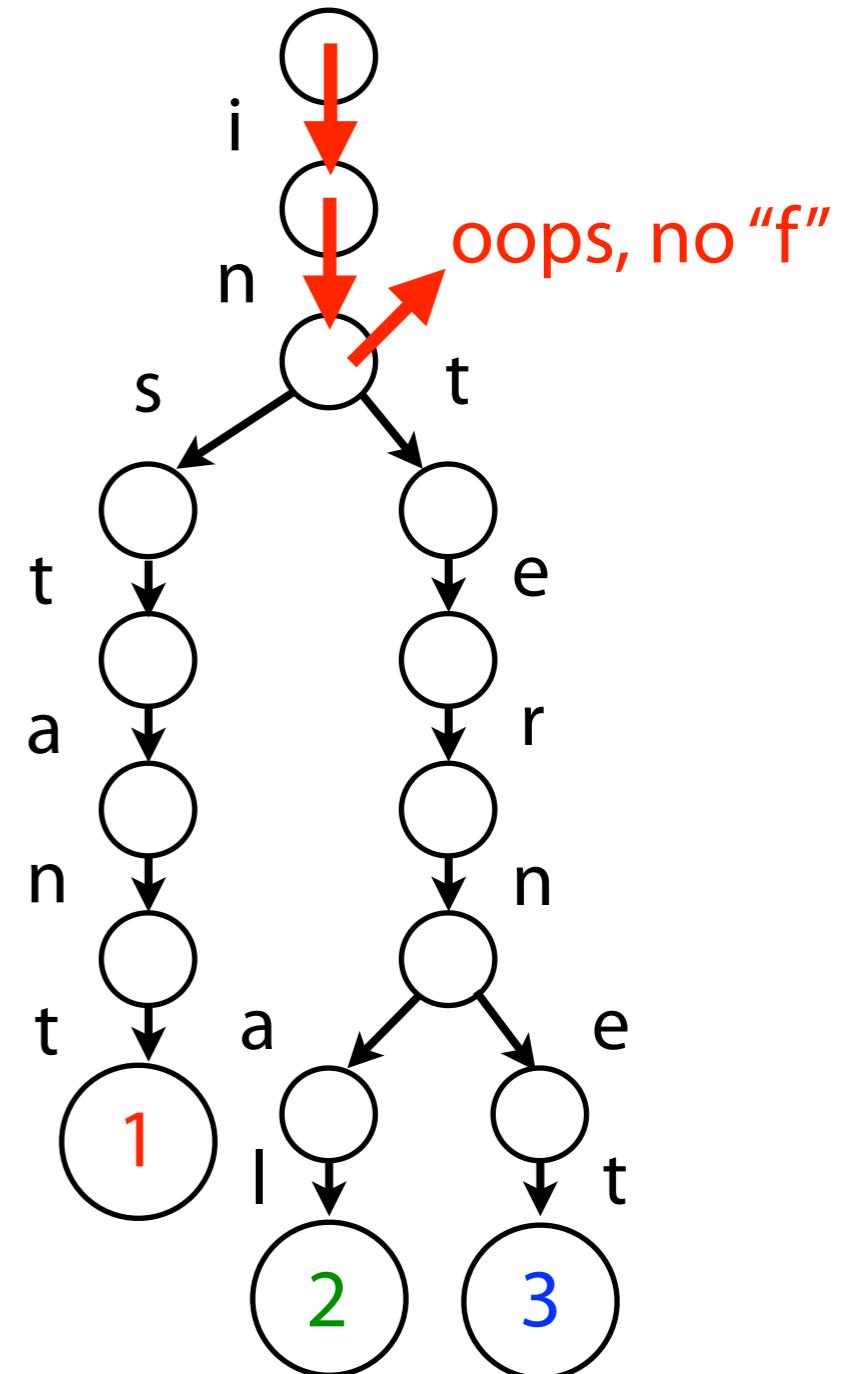
Each key is “spelled out” along some path  
starting at the root



# Tries

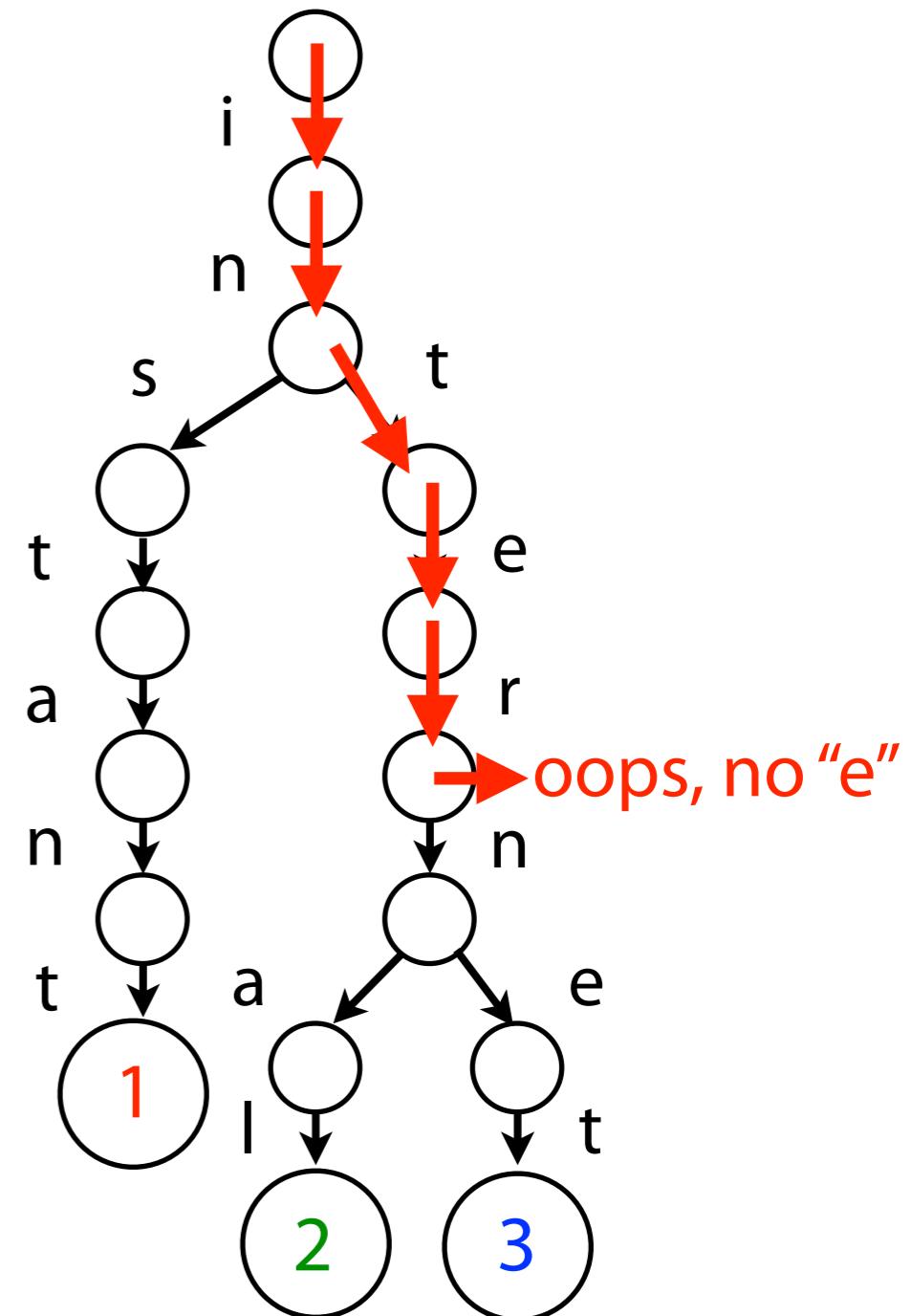
How do we check whether “infer” is in the trie?

Start at root and try to match successive characters of “infer” to edges in trie



# Tries

Matching “interesting”

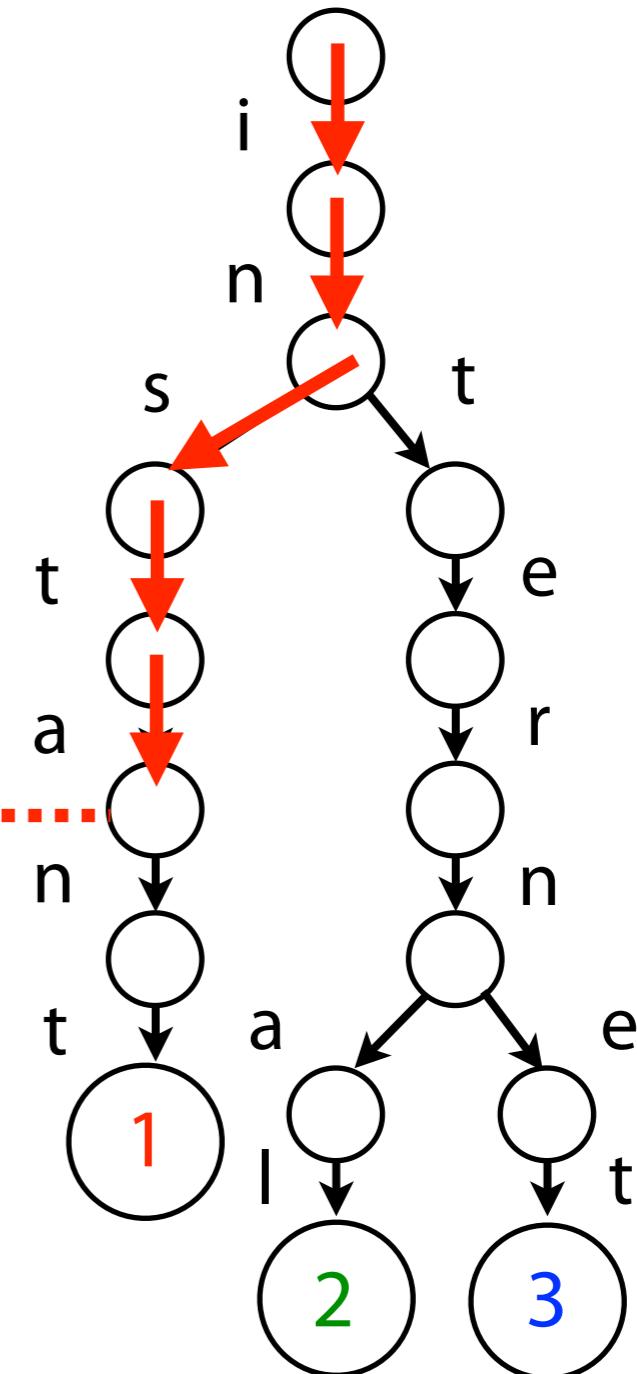


# Tries

Matching “insta”

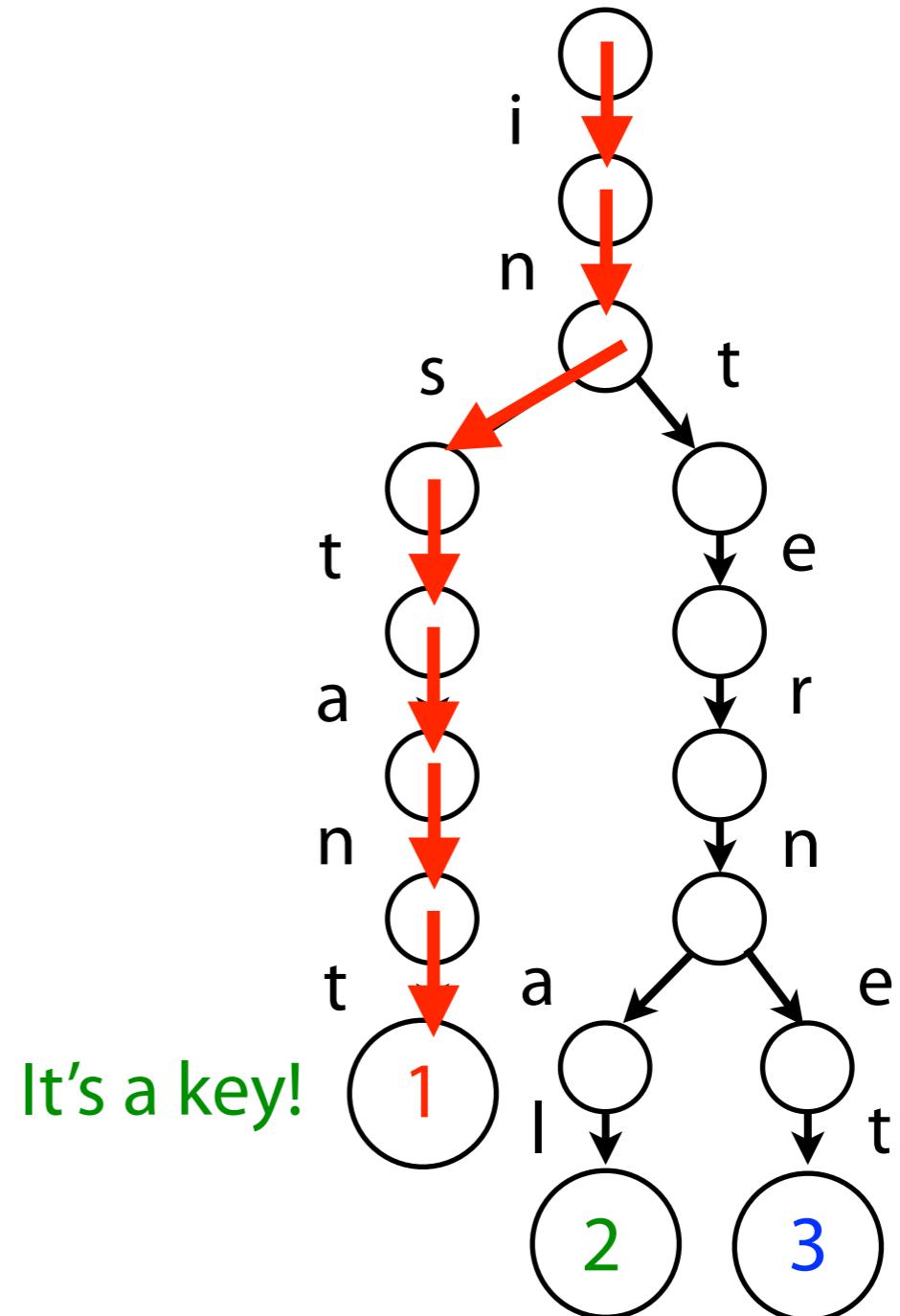
No value associated  
with node, so “insta” .....  
wasn’t a key

But it was a prefix  
of some key

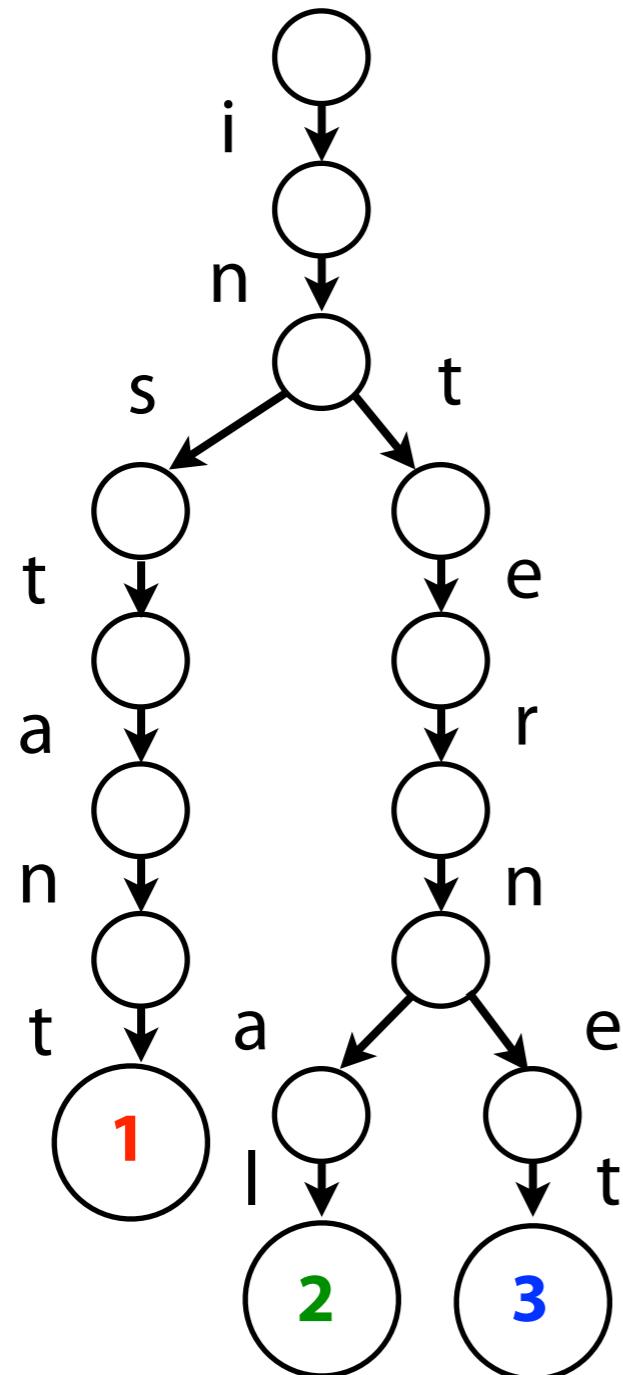


# Tries

Matching “instant”



# Tries: example



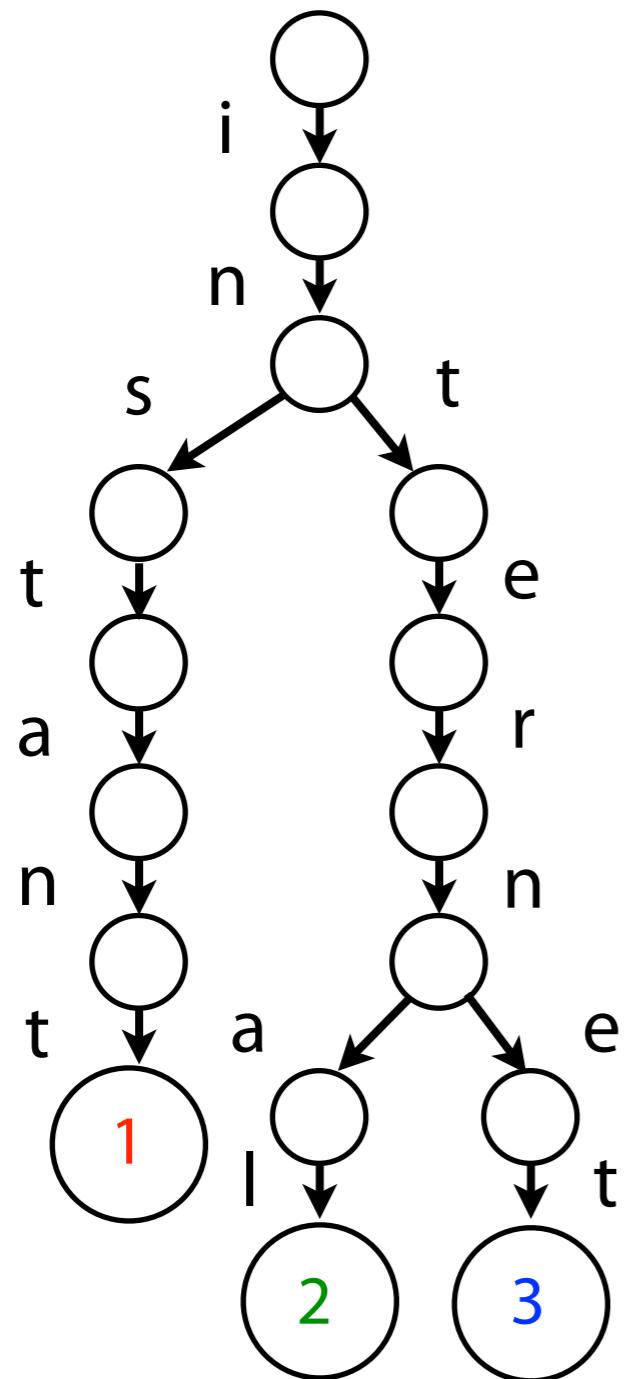
Checking for presence of a key  $P$ ,  
where  $n = |P|$ , is  **$O(n)$**  time

If total length of all keys is  $N$ , trie  
has  **$O(N)$**  nodes

What about  $|\Sigma|$ ?

Depends how we represent outgoing  
edges. If we don't assume  $|\Sigma|$  is a  
small constant, it shows up in one or  
both bounds.

# Tries



How to represent edges between a node and its children?

Map (from characters to child nodes)

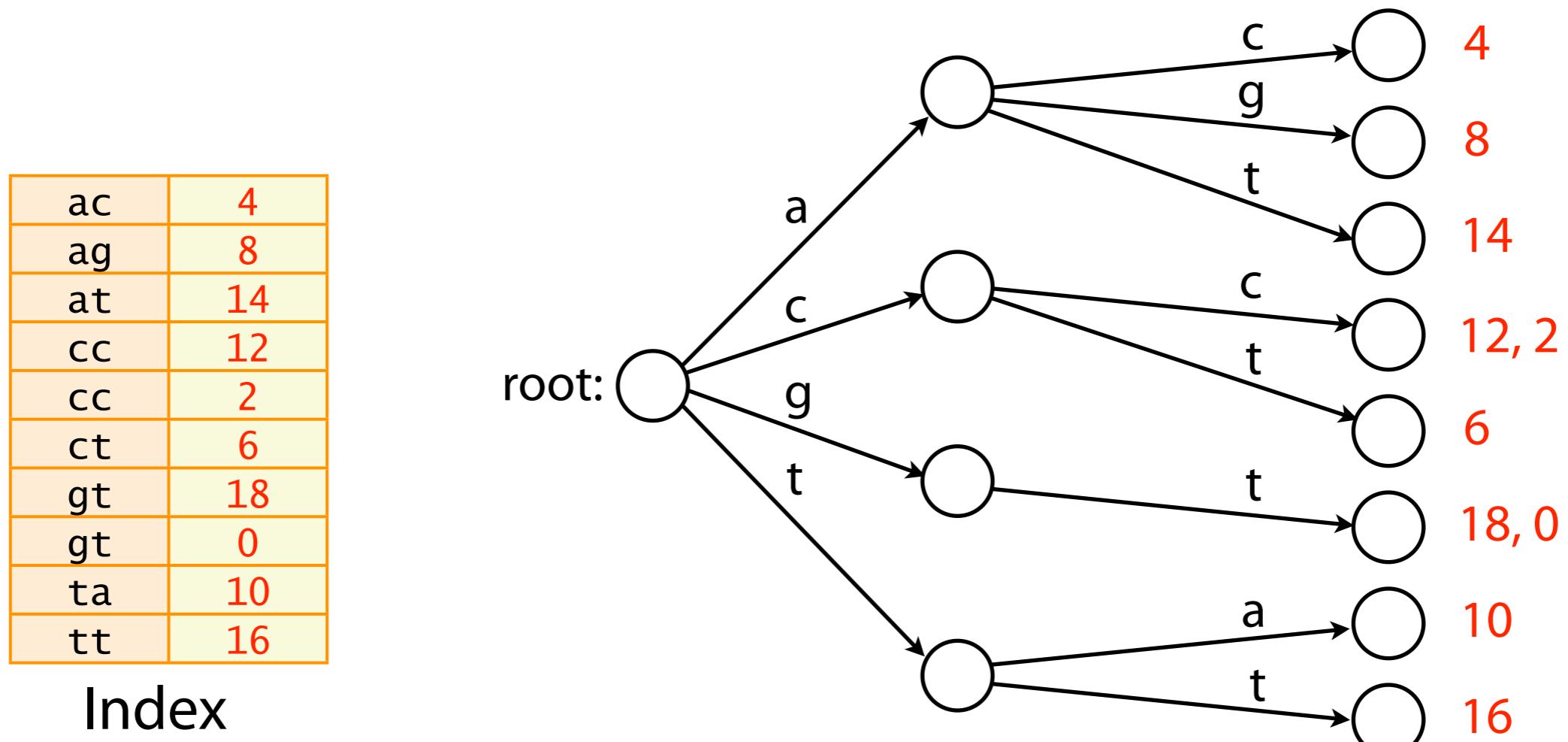
Idea 1: Hash table

Idea 2: Sorted lists

Assuming hash table, it's reasonable to say querying with  $P$ ,  $|P| = n$ , is  $O(n)$  time

# Tries: another example

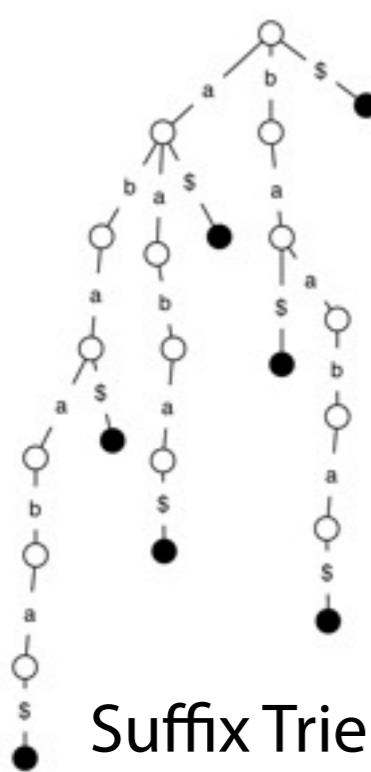
We can index  $T$  with a trie. The trie maps substrings to offsets where they occur



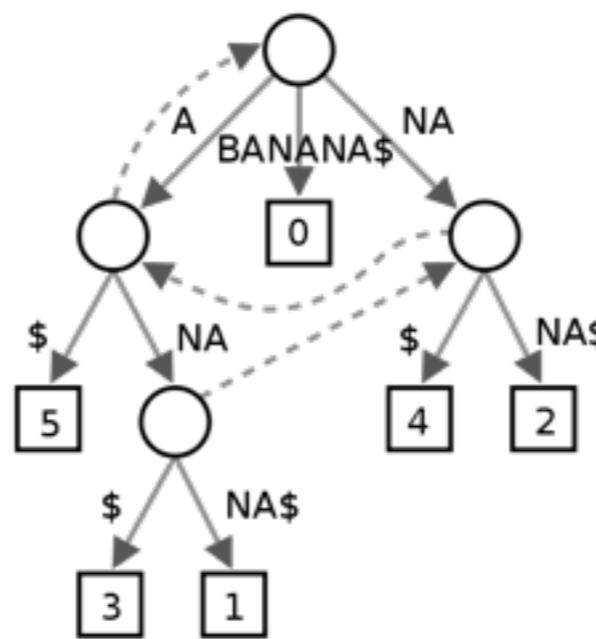
# Indexing with suffixes

Some indices (e.g. the inverted index) are based on extracting substrings from  $T$

A very different approach is to extract *suffixes* from  $T$ . This will lead us to some interesting and practical index data structures:



Suffix Trie



Suffix Tree

6	\$
5	A\$
3	ANAS\$
1	ANANAS\$
0	BANANAS\$
4	NA\$
2	NANAS\$

Suffix Array

\$ BANANA  
A \$ BANAN  
ANA \$ BAN  
ANANA \$ B  
BANANA \$  
NA \$ BANA  
NANA \$ BA

FM Index

# Trie Definitions

A  $\Sigma$ -tree (trie) is a rooted tree where each edge is labeled with a single character  $c \in \Sigma$ , such that no node has two outgoing edges labeled with the same character.

- for a node  $v$  in  $T$ , **depth**( $v$ ) or **node-depth**( $v$ ) is the distance from  $v$  to the root.
- **node-depth**( $r$ ) = 0
- **string**( $v$ ) = concatenation of all characters on the path  $r \rightsquigarrow v$
- **string-depth**( $v$ ) =  $|\text{string}(v)|$  (note: **string-depth**( $v$ )  $\geq$  **node-depth**( $v$ ))
- for a string  $x$ , if  $\exists$  node  $v$  with **string**( $v$ ) =  $x$ , we say **node**( $x$ ) =  $v$
- $T$  **displays** string  $x$  if  $\exists$  node  $v$  and string  $y$  such that  $xy = \text{string}(v)$
- **words**( $T$ ) = {  $x$  |  $T$  **displays**  $x$  }
- A **suffix trie** of string  $s$  is a  $\Sigma$ -tree such that **words**( $T$ ) = {  $s'$  |  $s'$  is a substring of  $s$  }
- An **internal/leaf** edge leads to an **internal/leaf** node

# Suffix trie

Build a **trie** containing all **suffixes** of a text  $T$

$T$ : GTTATAGCTGATCGCGGGCGTAGCGG

GT<sub>1</sub>TATAGCTGATCGCGGGCGTAGCGG

TT<sub>1</sub>ATAGCTGATCGCGGGCGTAGCGG

TATAGCTGATCGCGGGCGTAGCGG

ATAGCTGATCGCGGGCGTAGCGG

TAGCTGATCGCGGGCGTAGCGG

AGCTGATCGCGGGCGTAGCGG

GCTGATCGCGGGCGTAGCGG

CTGATCGCGGGCGTAGCGG

TGATCGCGGGCGTAGCGG

GATCGCGGGCGTAGCGG

ATCGCGGGCGTAGCGG

TCGCGGGCGTAGCGG

CGCGGGCGTAGCGG

GC CGGGCGTAGCGG

CGGGCGTAGCGG

GGCGTAGCGG

GC GTAGCGG

CG TAGCGG

GT AGCGG

TAGCGG

AGCGG

GC GG

C GG

GG

G



$m(m+1)/2$

chars

# Suffix trie

First add special *terminal character* **\$** to the end of  $T$

**\$** is a character that does not appear elsewhere in  $T$ , and we define it to be less than other characters (for DNA: **\$ < A < C < G < T**)

**\$** enforces a rule we're all used to using: e.g. "as" comes before "ash" in the dictionary. **\$ also guarantees no suffix is a prefix of any other suffix.**

$T$ : GTTATAGCTGATCGCGGGGTAGCGG \$

  GTTATAGCTGATCGCGGGGTAGCGG \$

    TTATAGCTGATCGCGGGGTAGCGG \$

      TATAGCTGATCGCGGGGTAGCGG \$

      ATAGCTGATCGCGGGGTAGCGG \$

      TAGCTGATCGCGGGGTAGCGG \$

      AGCTGATCGCGGGGTAGCGG \$

      GCTGATCGCGGGGTAGCGG \$

      CTGATCGCGGGGTAGCGG \$

      TGATCGCGGGGTAGCGG \$

      GATCGCGGGGTAGCGG \$

      ATCGCGGGGTAGCGG \$

      TCGCGGGGTAGCGG \$

      CGCGGGGTAGCGG \$

      GCGGGGTAGCGG \$

      CGGCGTAGCGG \$

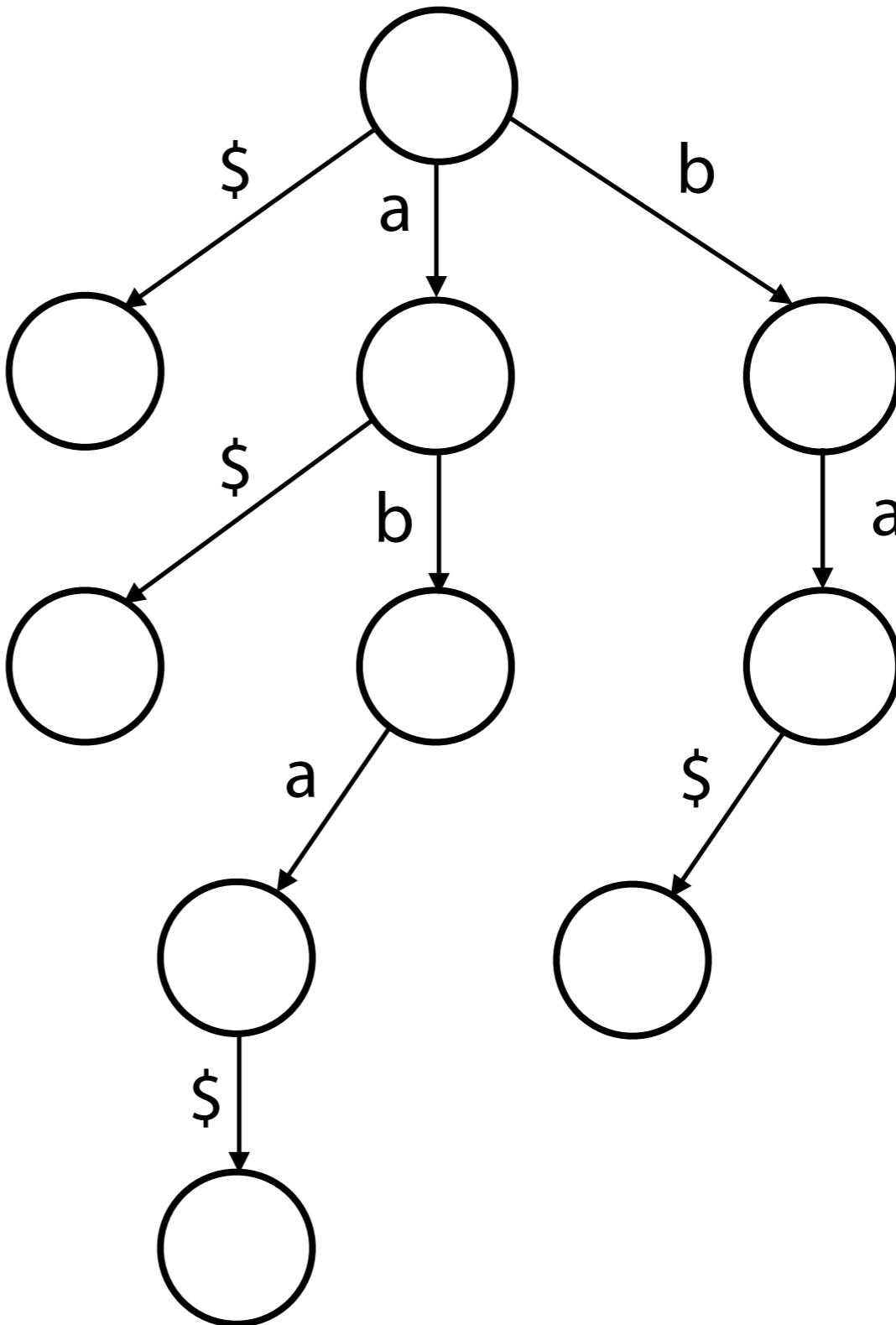
      GGCGTAGCGG \$

      GCGTAGCGG \$

# Suffix trie

T: aba \$

What's the suffix trie?

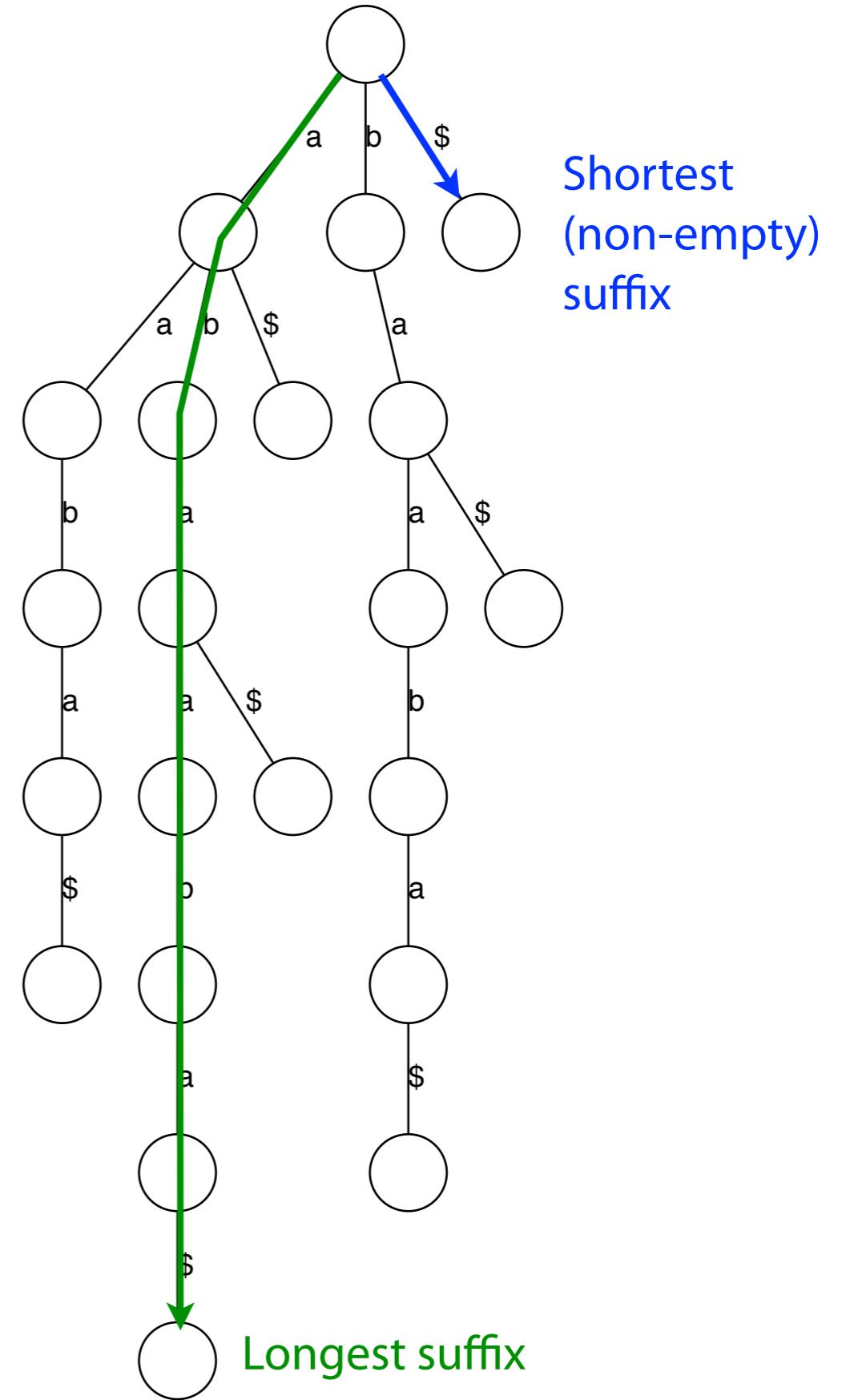


# Suffix trie

T: abaaba \$

Each path from root to leaf represents a suffix; each suffix is represented by some path from root to leaf

Would this still be the case if we hadn't added \$?



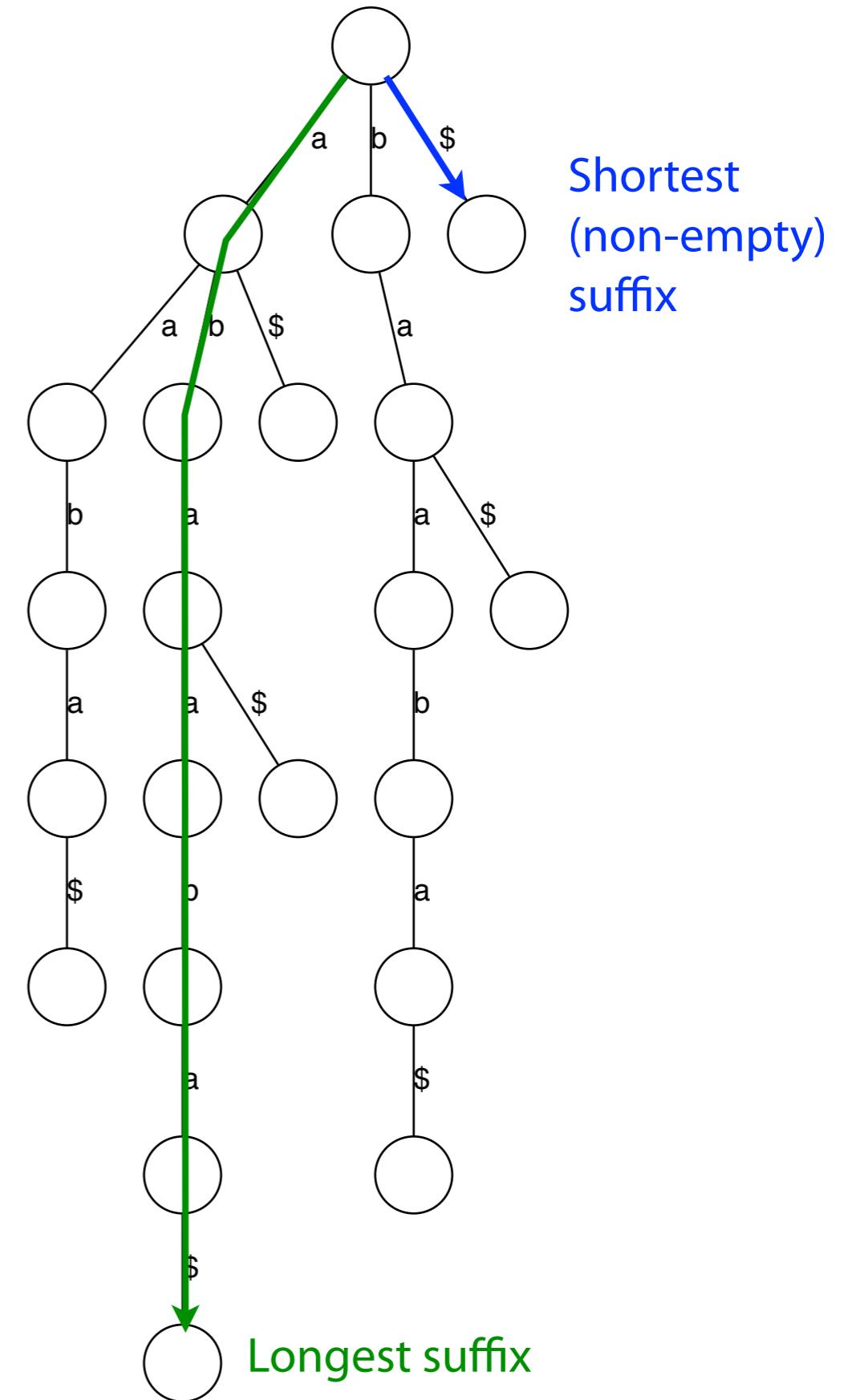
# Suffix trie

$T$ : abaaba

$T\$$ : abaaba\$

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Would this still be the case if we hadn't added \$?



# Suffix trie

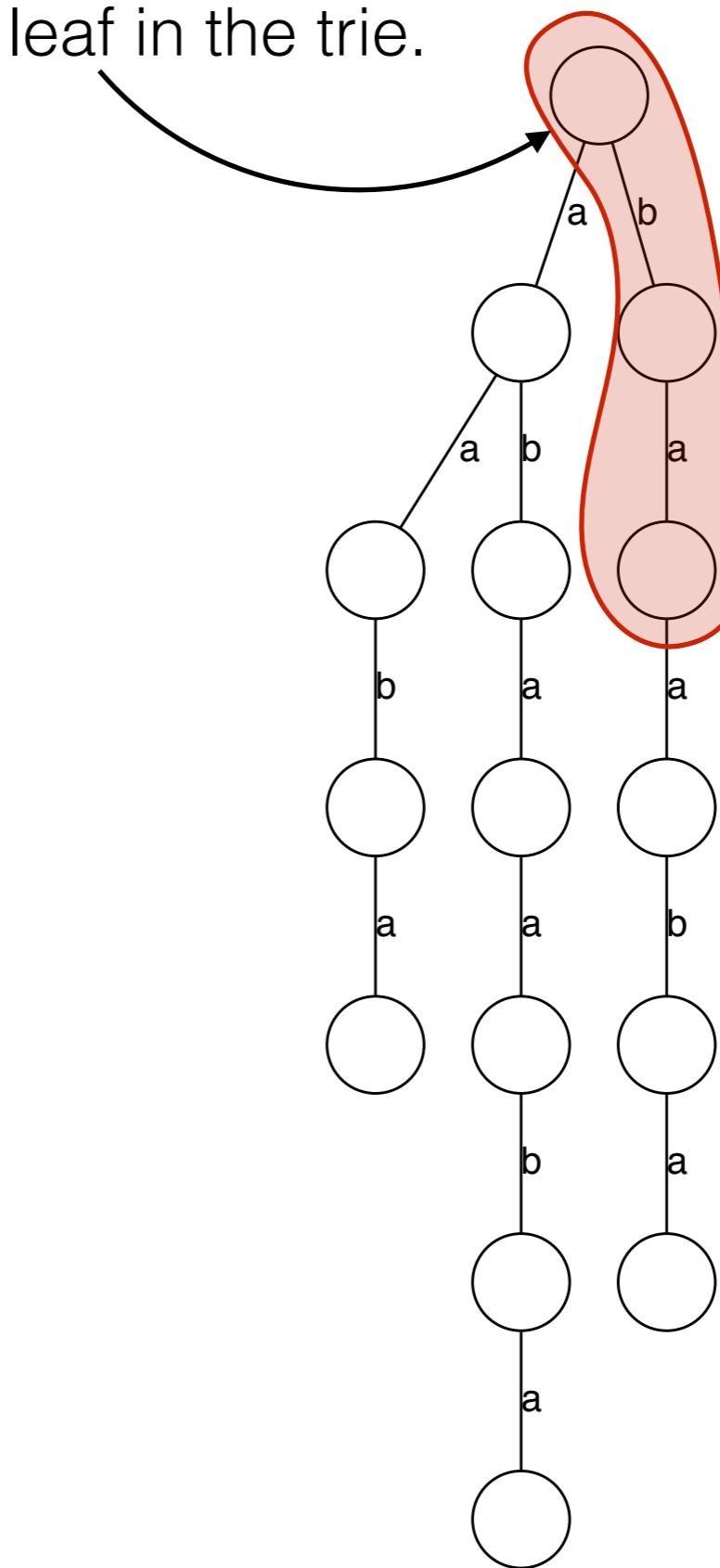
$T$ : abaaba

Each path from root to leaf represents a suffix; each suffix is represented by some path from root to leaf

Would this still be the case if we hadn't added  $\$$ ? **No**

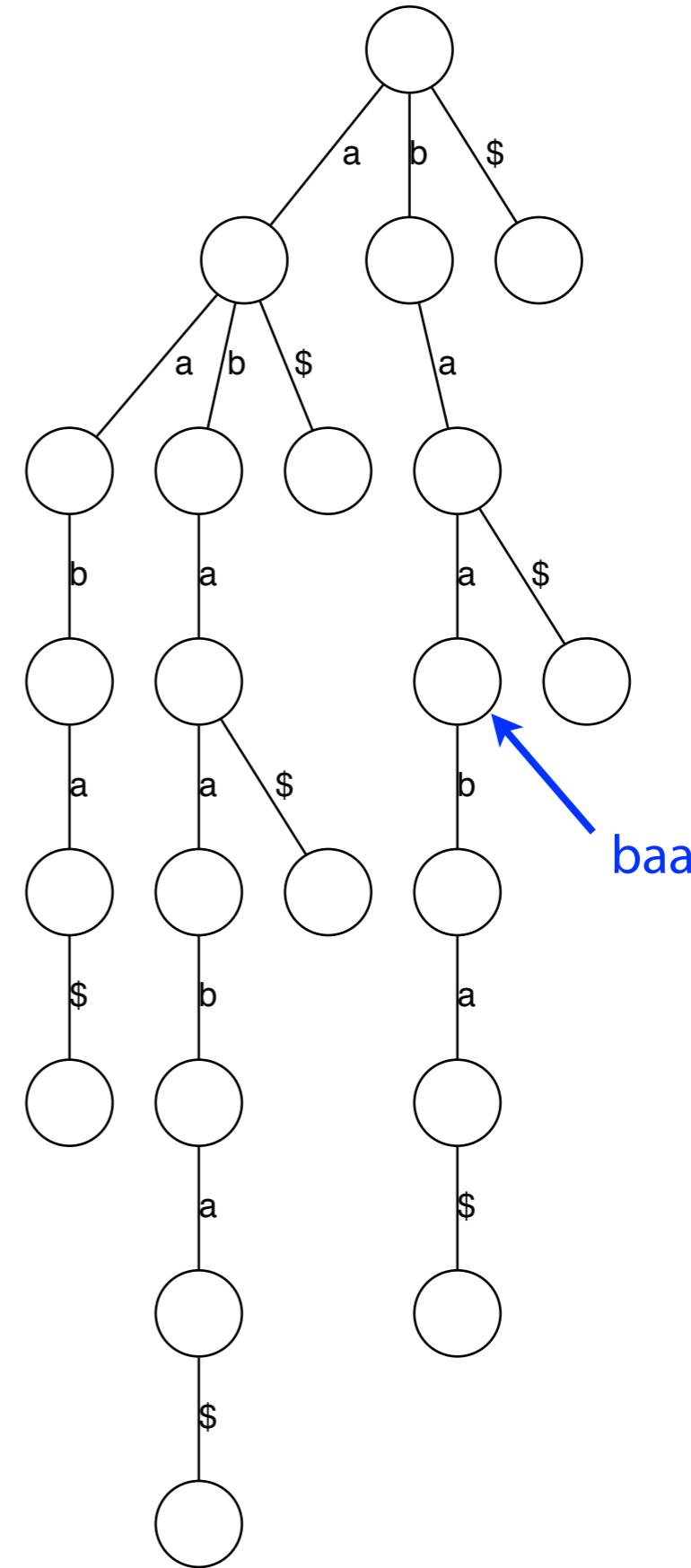
Without the  $\$$ , we have problems; e.g. here “ba” is a prefix of “baaba”

Without  $\$$ , no way to spell out this suffix & end at a leaf in the trie.



# Suffix trie

Think of each node as having a label, spelling out characters on path from root to node



# Suffix trie

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

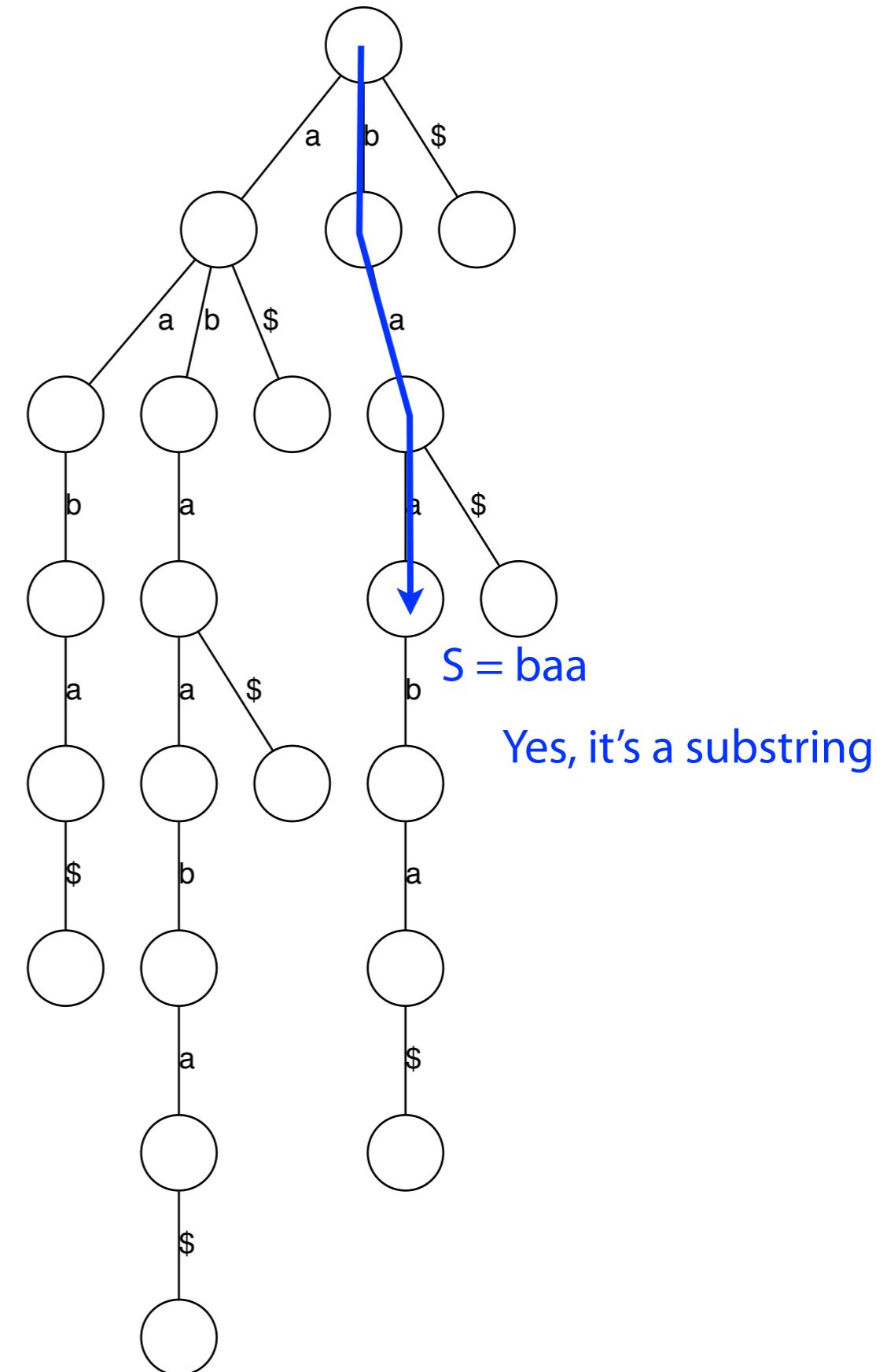
Note: Each of  $T$ 's substrings is spelled out along a path from the root.

Every substring is a prefix of some suffix of  $T$ .

Start at the root and follow the edges labeled with the characters of  $S$

If we “fall off” the trie -- i.e. there is no outgoing edge for next character of  $S$ , then  $S$  is not a substring of  $T$

If we exhaust  $S$  without falling off,  $S$  is a substring of  $T$



# Suffix trie

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

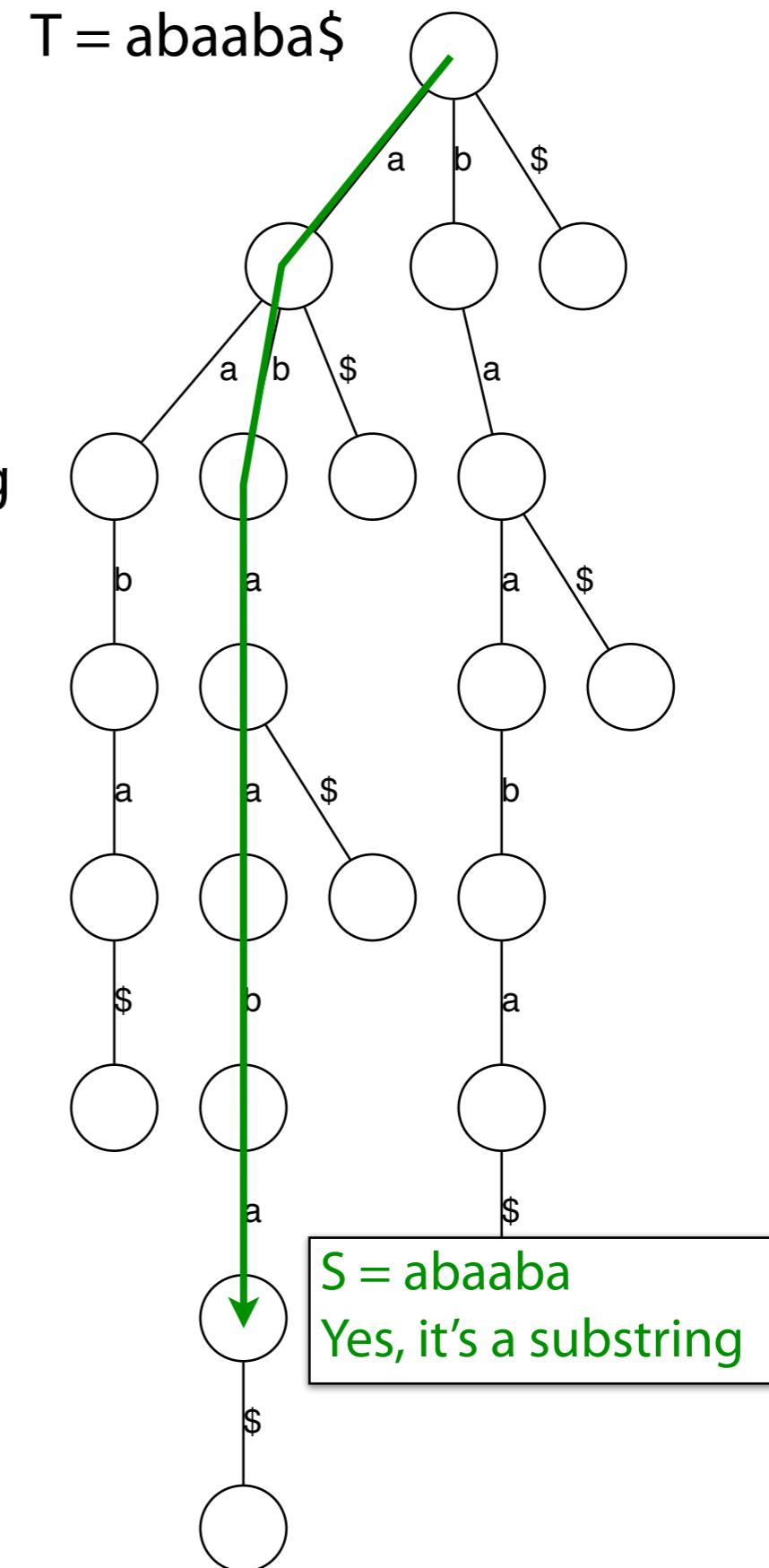
Note: Each of T's substrings is spelled out along a path from the root.

Every substring is a prefix of some suffix of T.

Start at the root and follow the edges labeled with the characters of S

If we “fall off” the trie -- i.e. there is no outgoing edge for next character of S, then S is not a substring of T

If we exhaust S without falling off, S is a substring of T



# Suffix trie

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

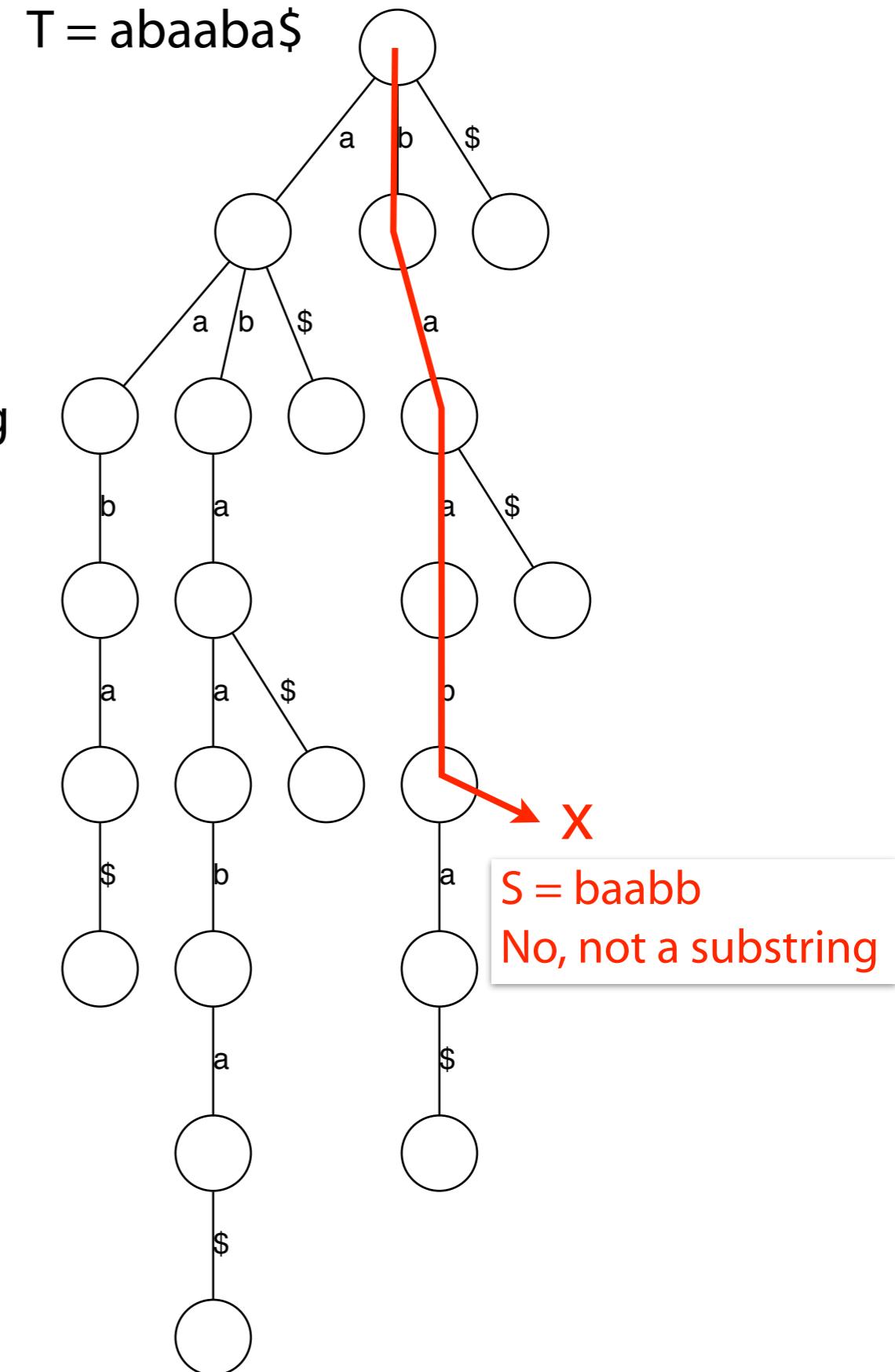
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Start at the root and follow the edges labeled with the characters of S

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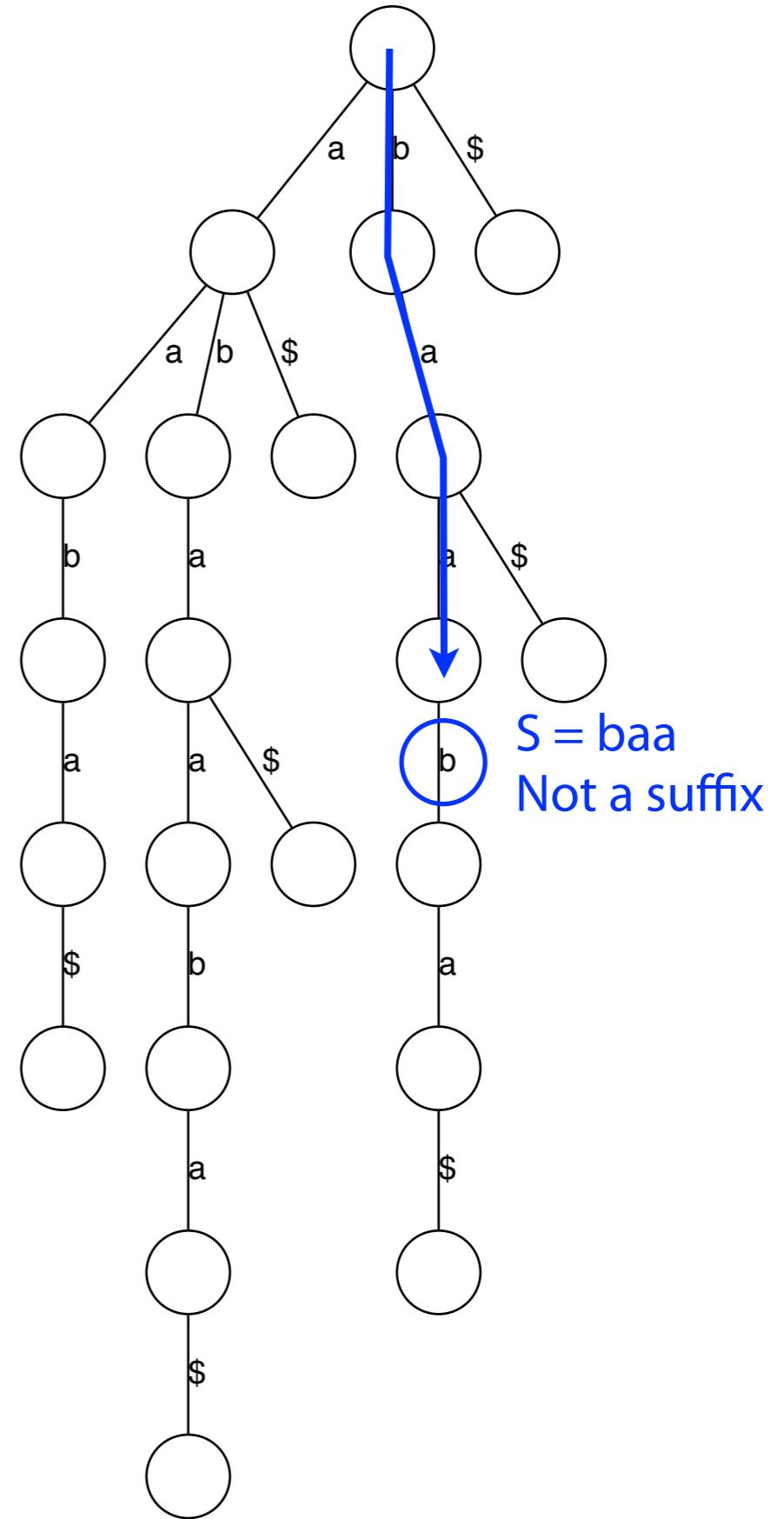
If we exhaust S without falling off, S is a substring of T



# Suffix trie

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

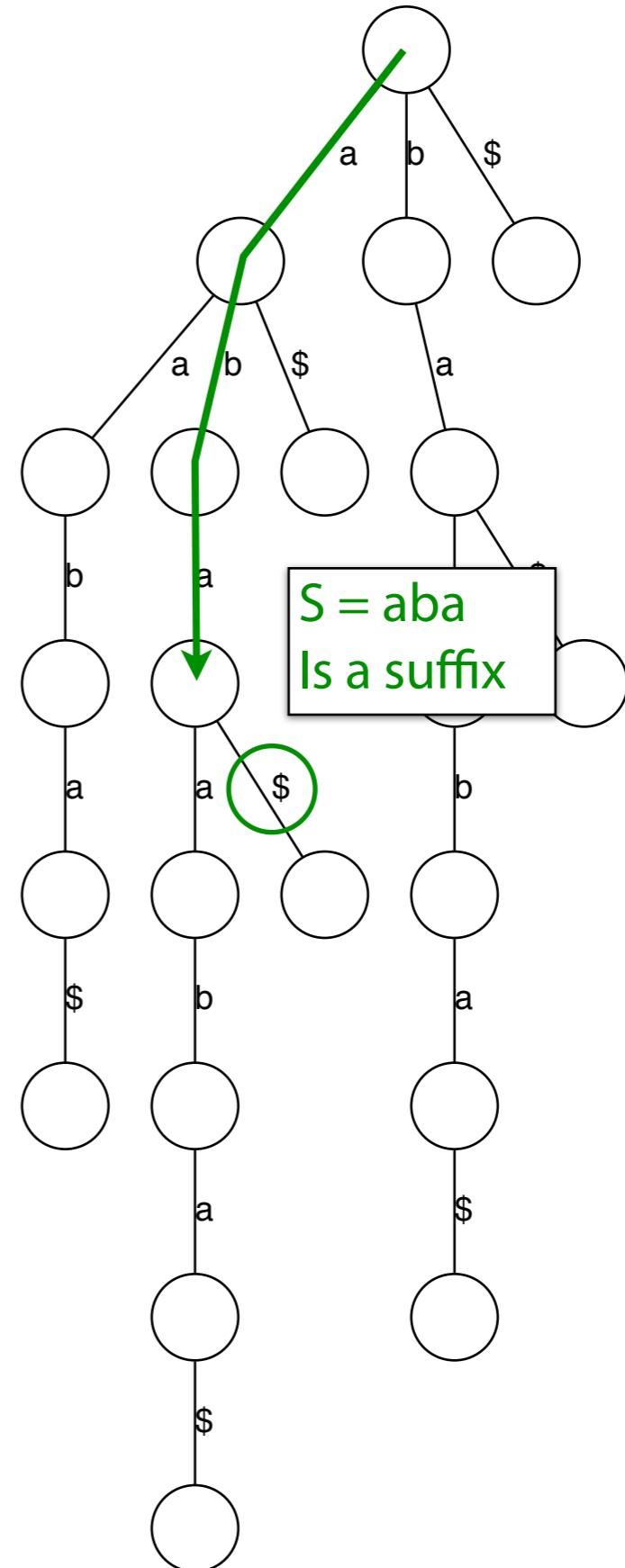
Same procedure as for substring, but additionally check terminal node for \$ child



# Suffix trie

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

Same procedure as for substring, but additionally check terminal node for \$ child

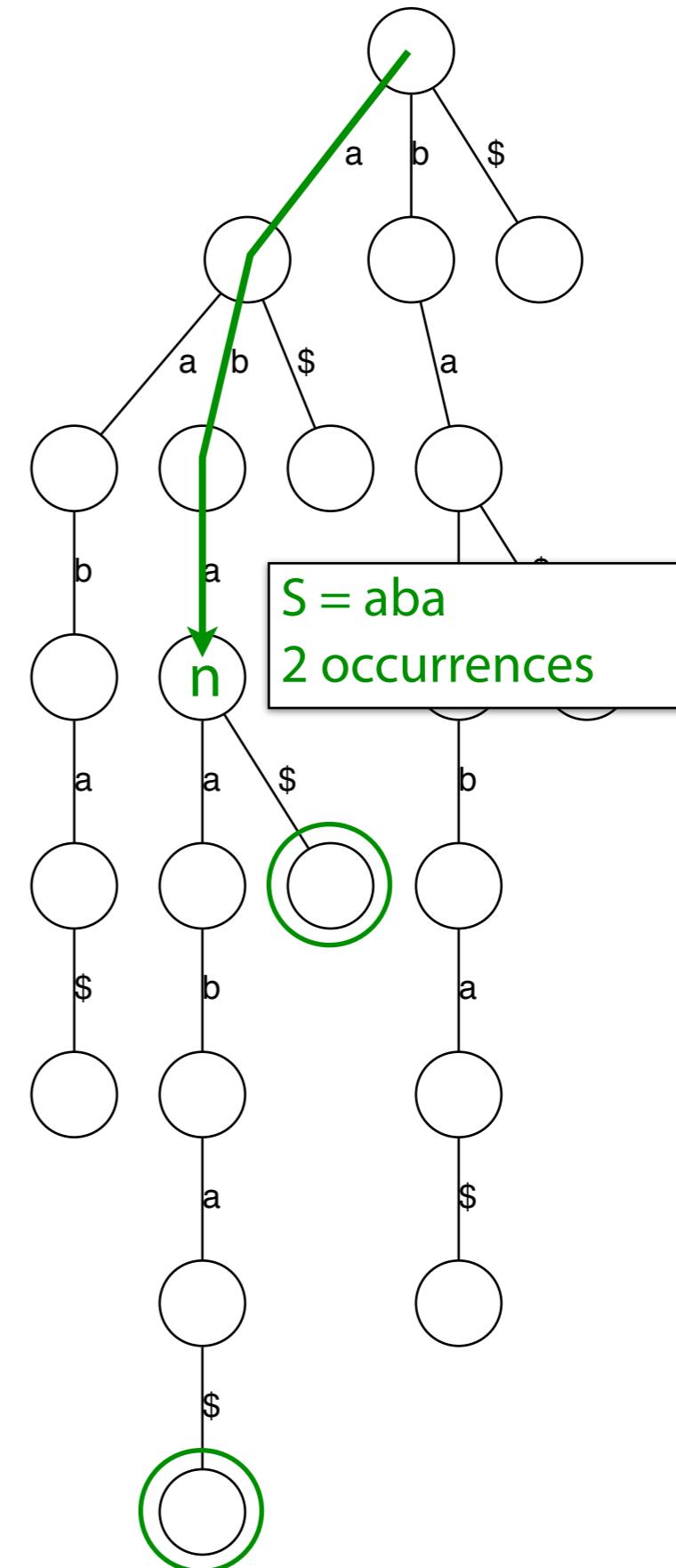


# Suffix trie

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

Follow path labeled with  $S$ . If we fall off, answer is 0. If we end up at node  $n$ , answer equals # of leaves in subtree rooted at  $n$ .

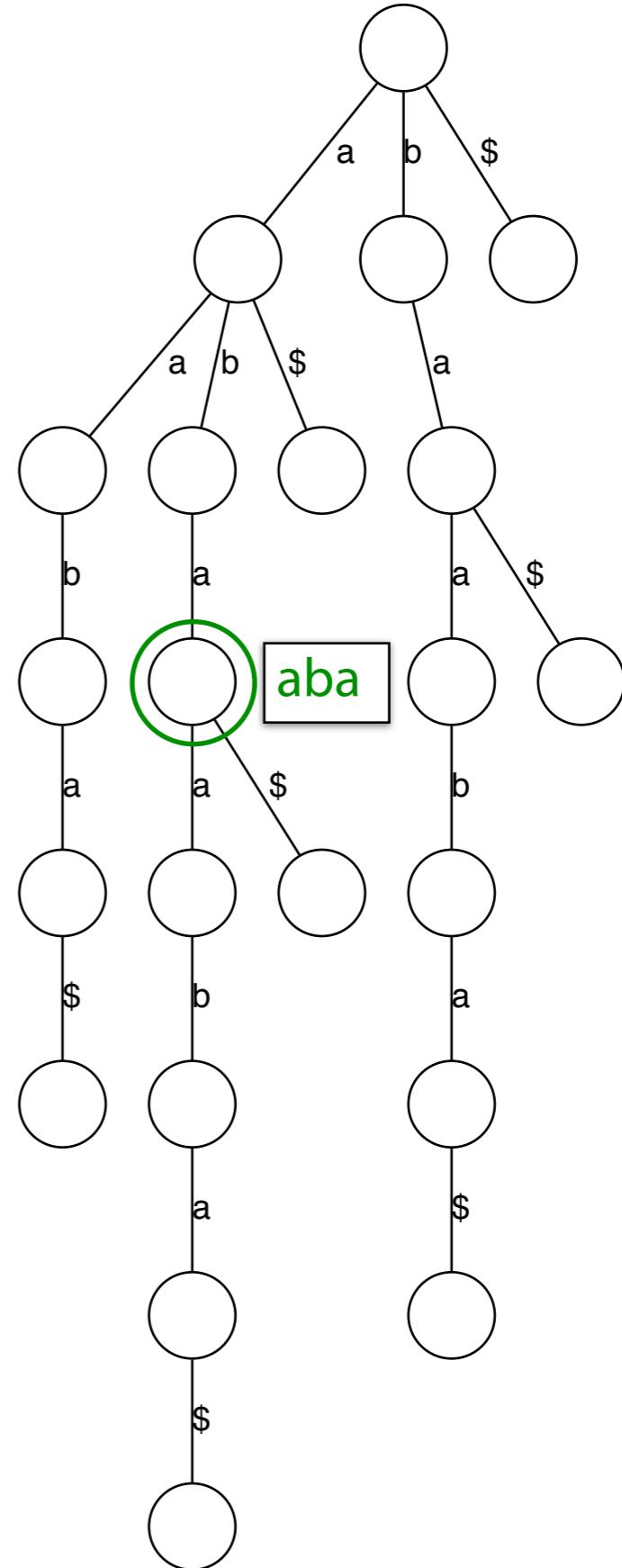
Leaves can be counted with depth-first traversal.



# Suffix trie

How do we find the longest repeated substring of T?

Find the deepest node with more than one child



# Suffix trie

How many nodes does the suffix trie have?

Is there a class of string where the number of suffix trie nodes grows linearly with  $m$ ?

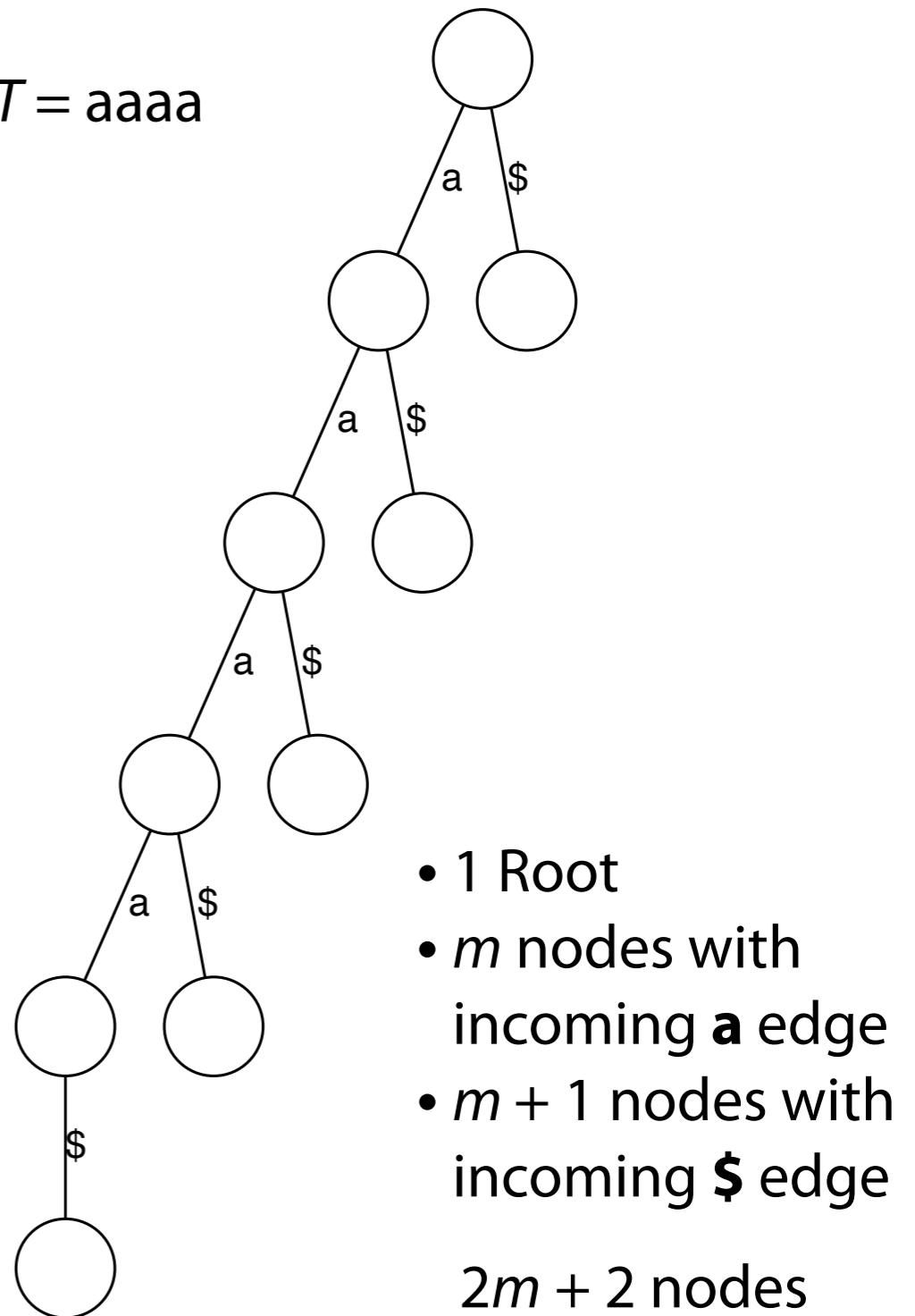
# Suffix trie

How many nodes does the suffix trie have?

Is there a class of string where the number of suffix trie nodes grows linearly with  $m$ ?

Yes: e.g. a string of  $m$  a's in a row ( $a^m$ )

$T = \text{aaaa}$



# Suffix trie

Is there a class of string where the number of suffix trie nodes grows with  $m^2$ ?

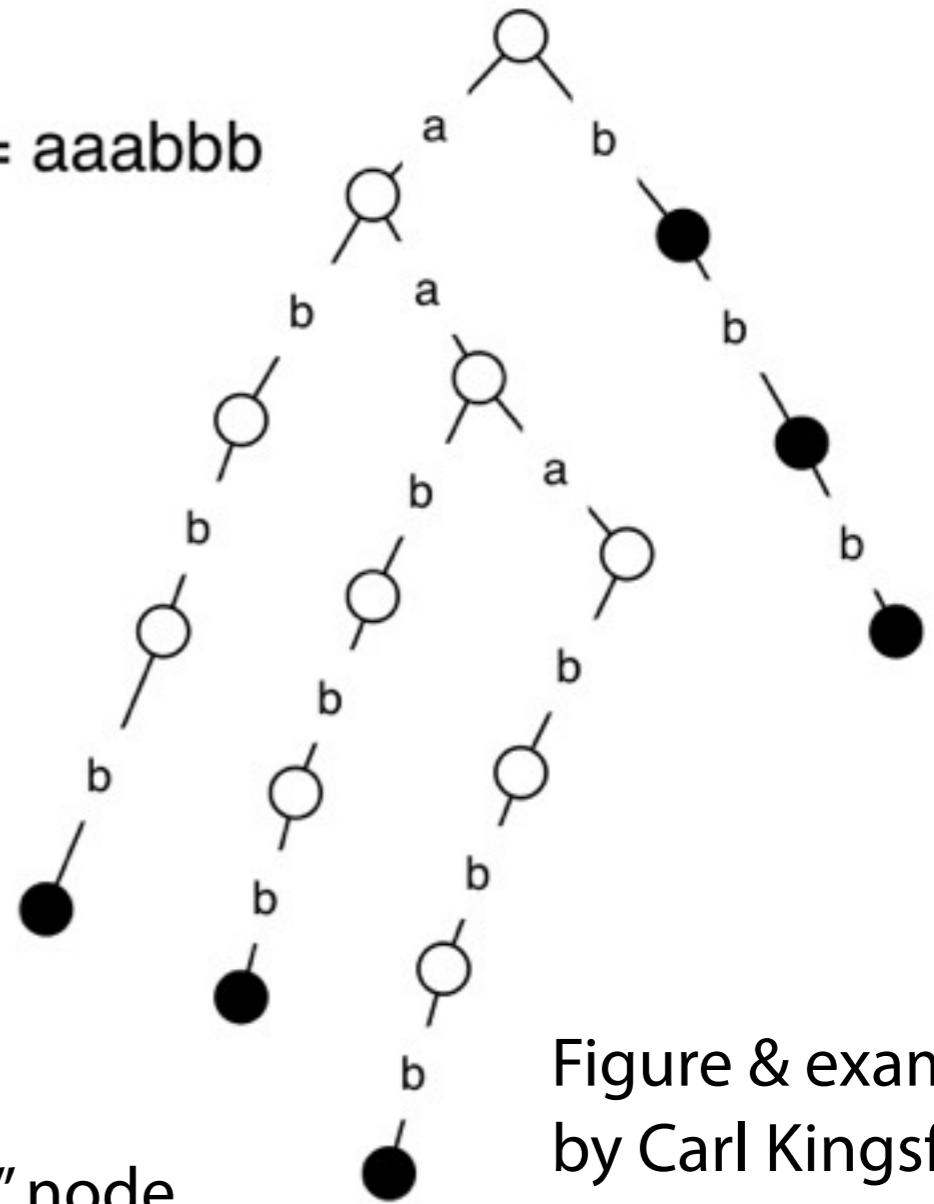
# Suffix trie

Is there a class of string where the number of suffix trie nodes grows with  $m^2$ ?

Yes:  $a^n b^n$

- 1 root
  - $n$  nodes along “b chain,” right
  - $n$  nodes along “a chain,” middle
  - $n$  chains of  $n$  “b” nodes hanging off each “a chain” node
  - $2n + 1$  leaves (not shown)

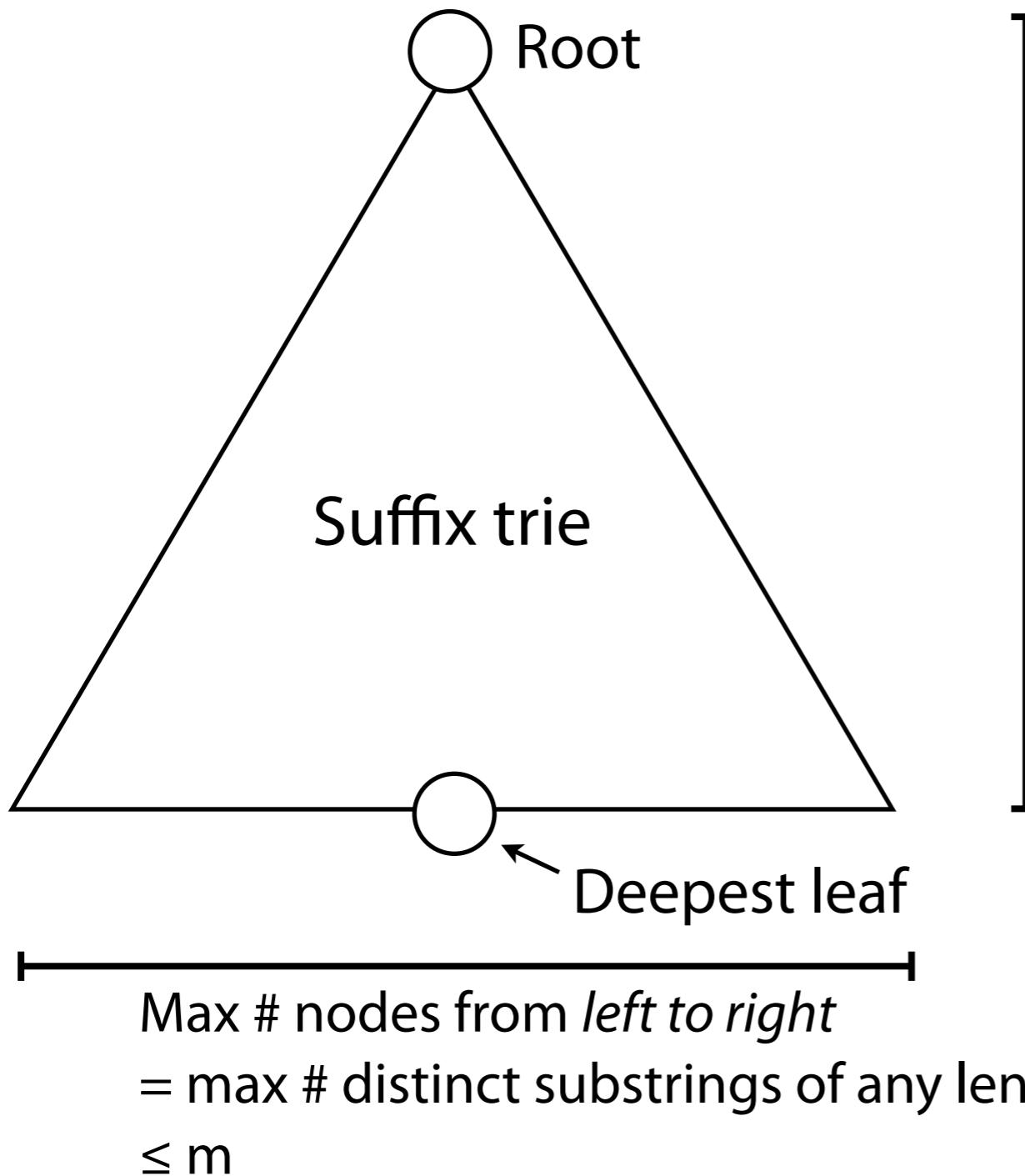
$$T = \text{aaabb}$$



# Figure & example by Carl Kingsford

# Suffix trie: upper bound on size

Could worst-case # nodes be worse than  $O(m^2)$ ?



Max # nodes from *top to bottom*  
= length of longest suffix + 1  
=  $m + 1$

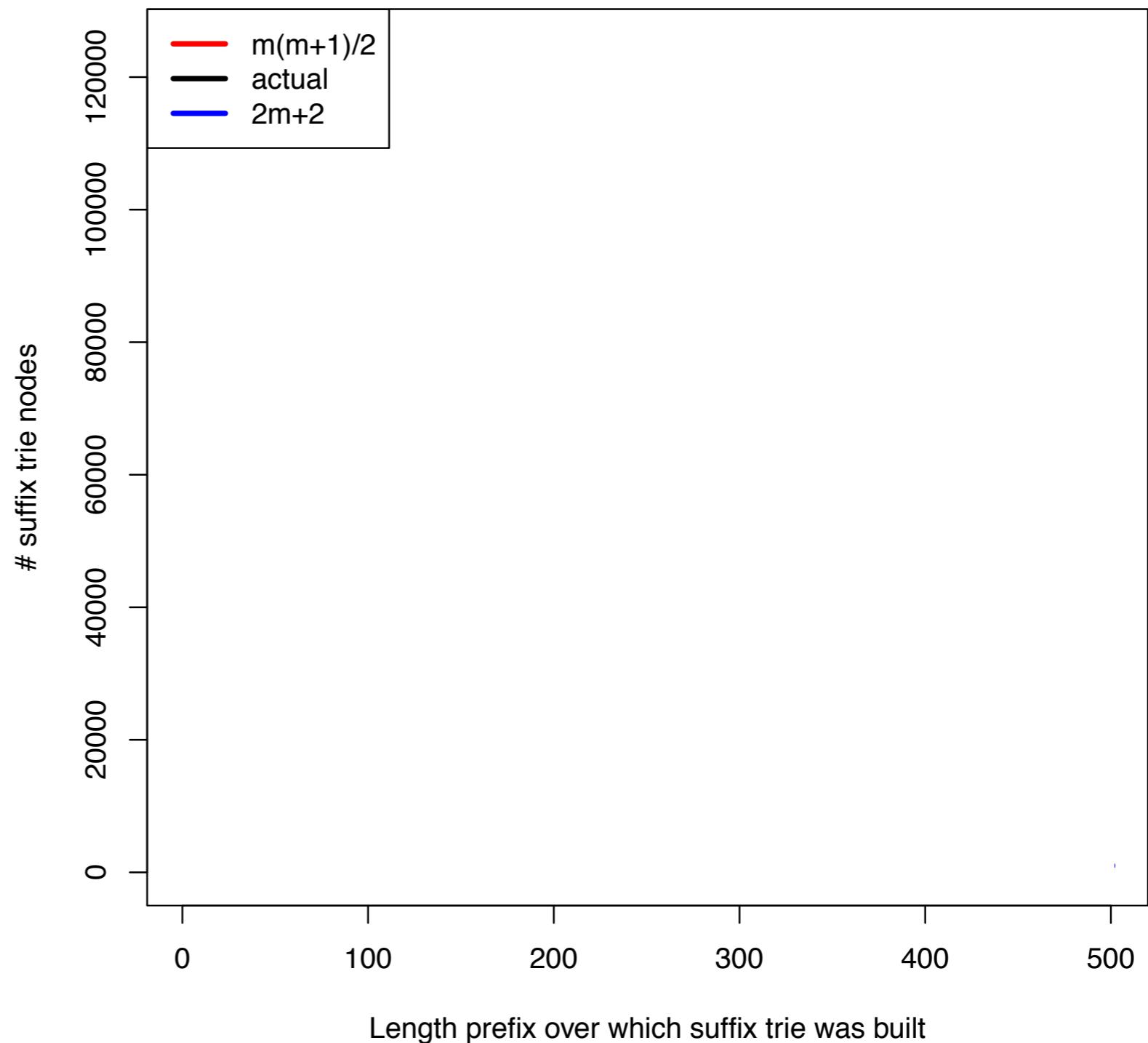
Max # nodes from *left to right*  
= max # distinct substrings of any length  
 $\leq m$

$O(m^2)$  is worst case

# Suffix trie: actual growth

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

Black curve shows how # nodes increases with prefix length

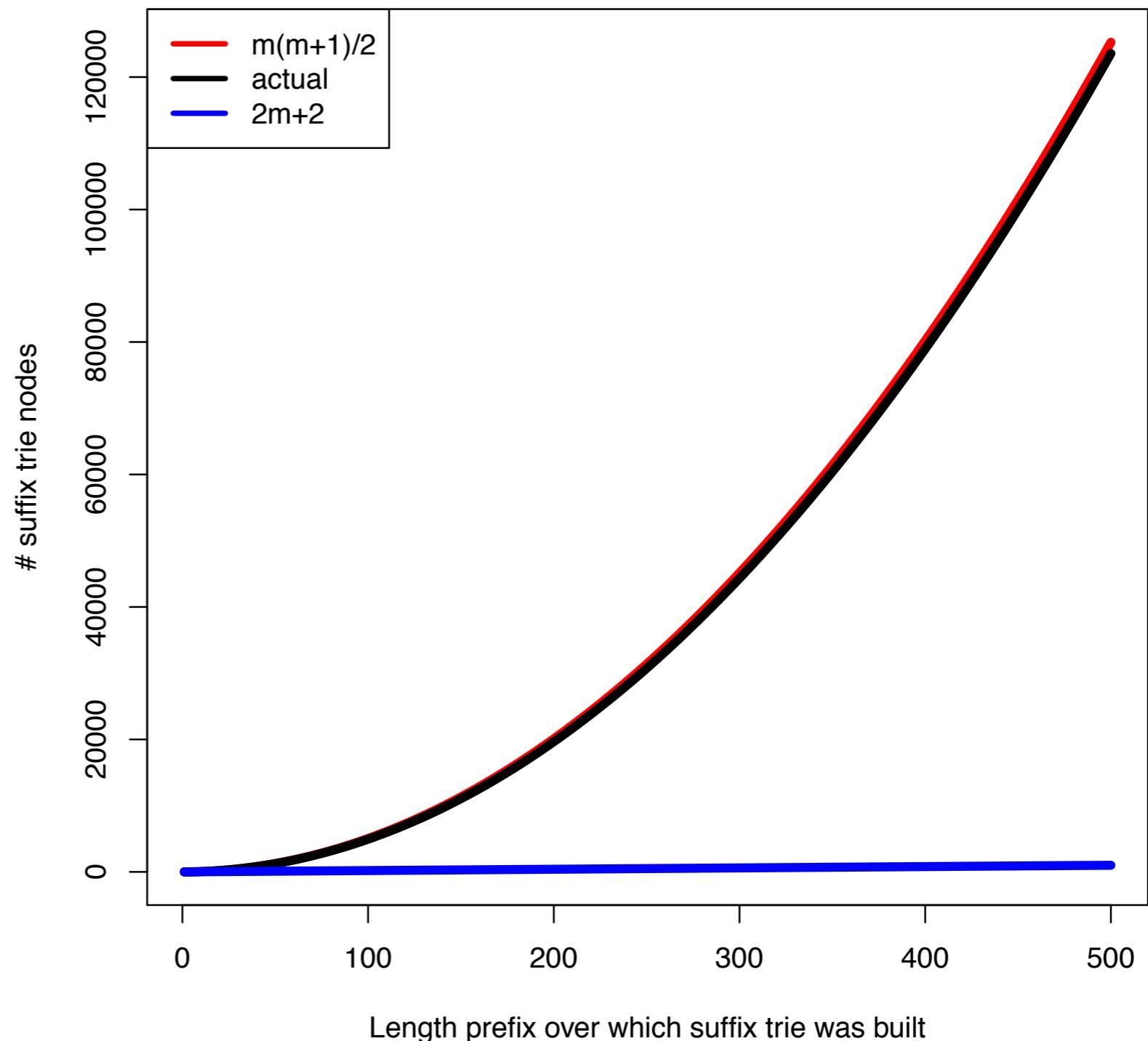


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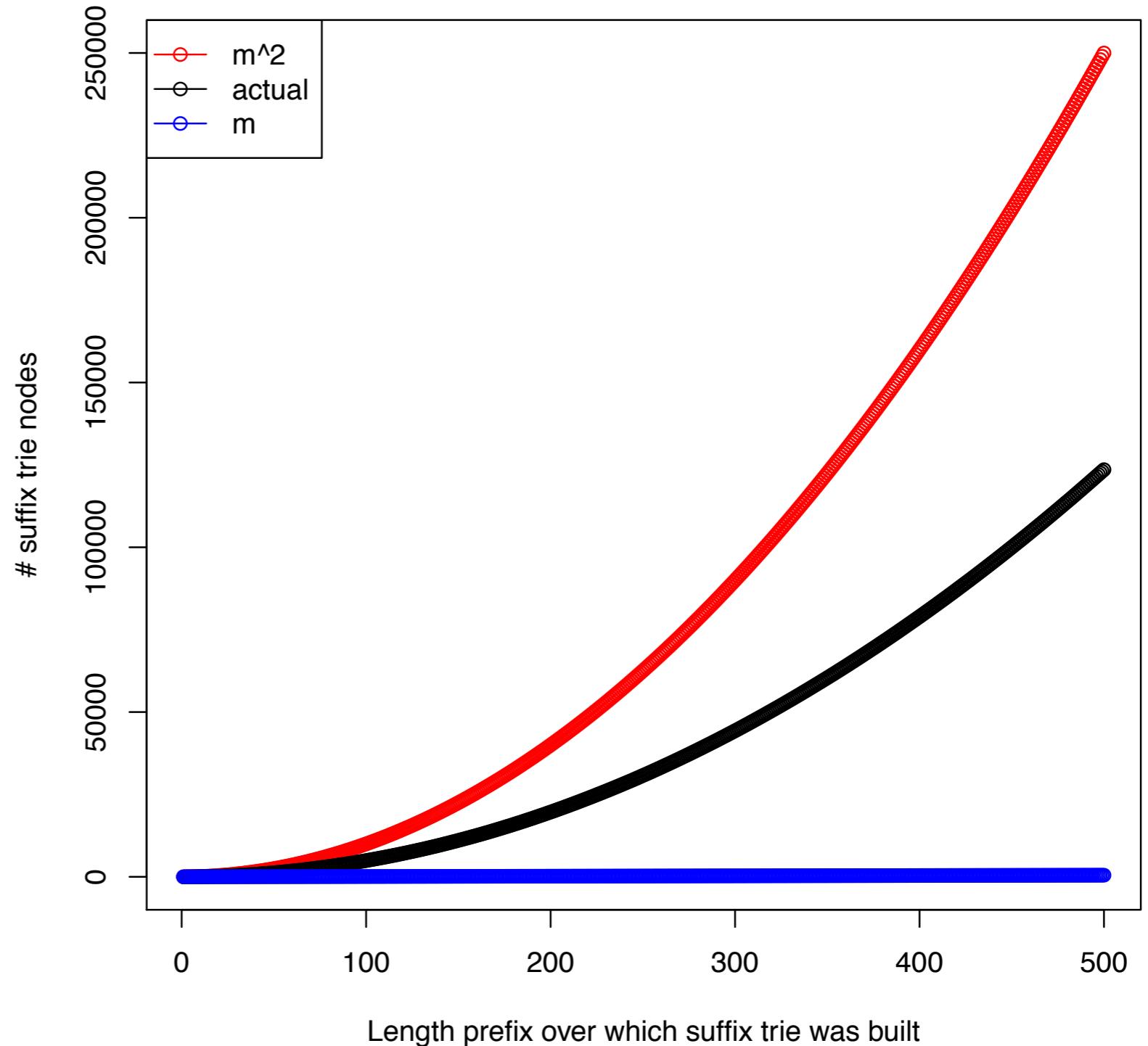
Actual growth much closer to worst case than to best!



# Suffix trie: actual growth

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Black curve shows how # nodes increases with prefix length



Suffix tries  $\Rightarrow$  Suffix trees

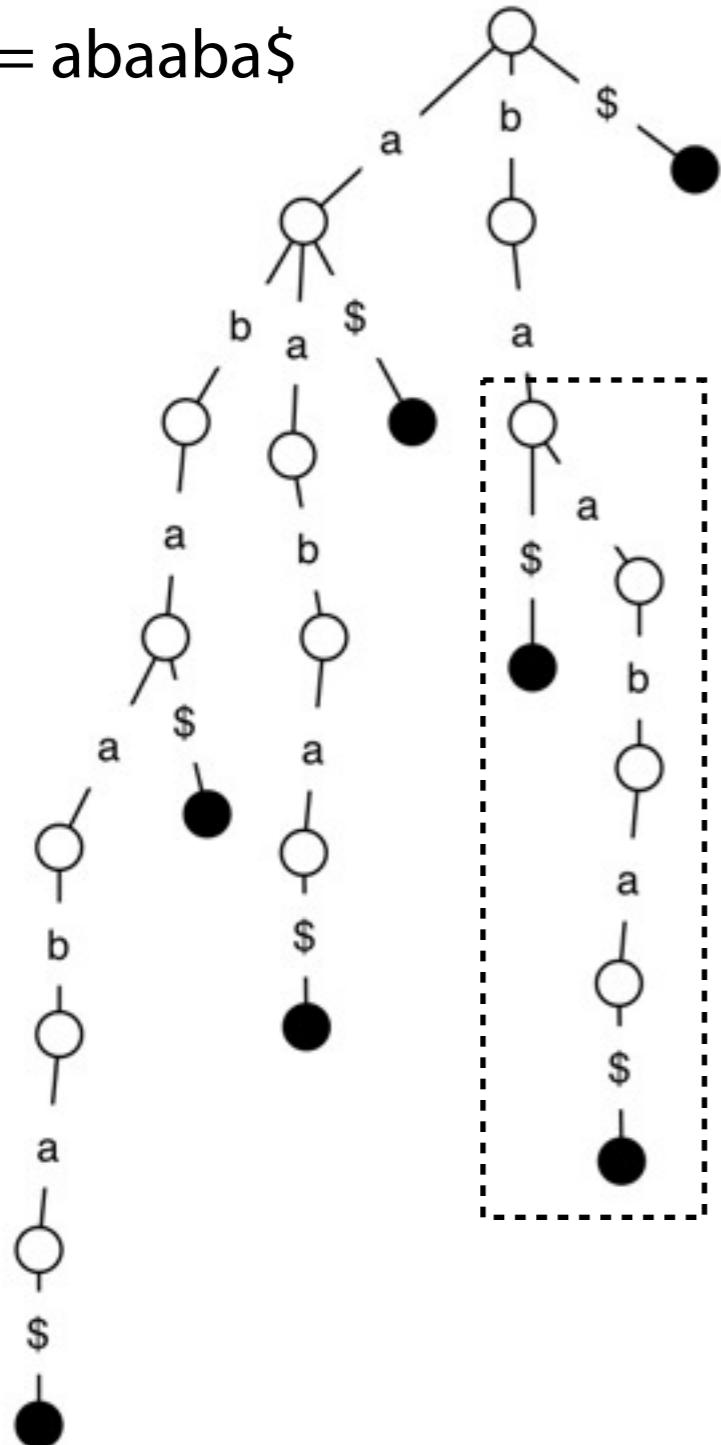
# Suffix Tree Definitions

A  $\Sigma^+$ -tree is a rooted tree,  $T$ , where each edge is labeled with *non-empty strings*, where no node has two outgoing edges labeled with strings having the same *first* character.  $T$  is **compact** if all internal nodes have  $\geq 2$  children.

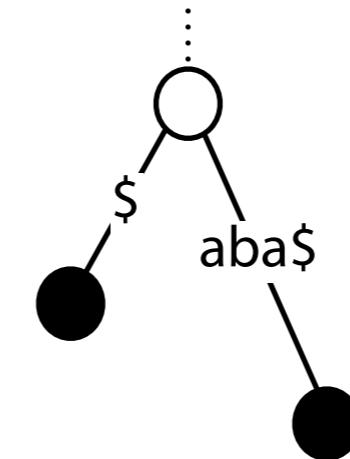
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- $T$  **displays** string  $x$  if  $\exists$  node  $v$  and string  $y$  such that  $xy = \text{string}(v)$
- **words**( $T$ ) = {  $x$  |  $T$  **displays**  $x$  }
- A **suffix tree** of string  $s$  is a compact  $\Sigma^+$ -tree such that **words**( $T$ ) = { $s'$  |  $s'$  is a substring of  $s$ }

# Suffix trie: making it smaller

$T = \text{abaaba\$}$



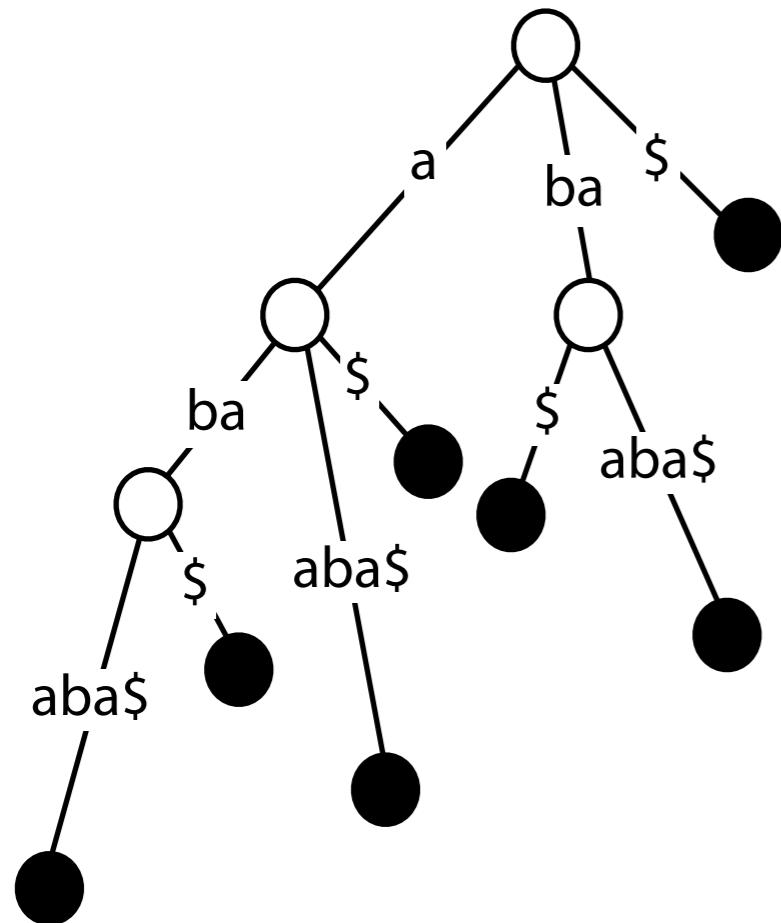
Idea 1: Coalesce non-branching paths  
into a *single edge* with a *string label*



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

# Suffix tree

$T = abaaba\$$



$L$  leaves,  $I$  internal nodes,  $E$  edges

$$E = L + I - 1$$

$E \geq 2I$  (each internal node branches)

$$L + I - 1 \geq 2I \Rightarrow I \leq L - 1$$

*but*

$L \leq m$  (at most  $m$  suffixes)

$$I \leq m - 1$$

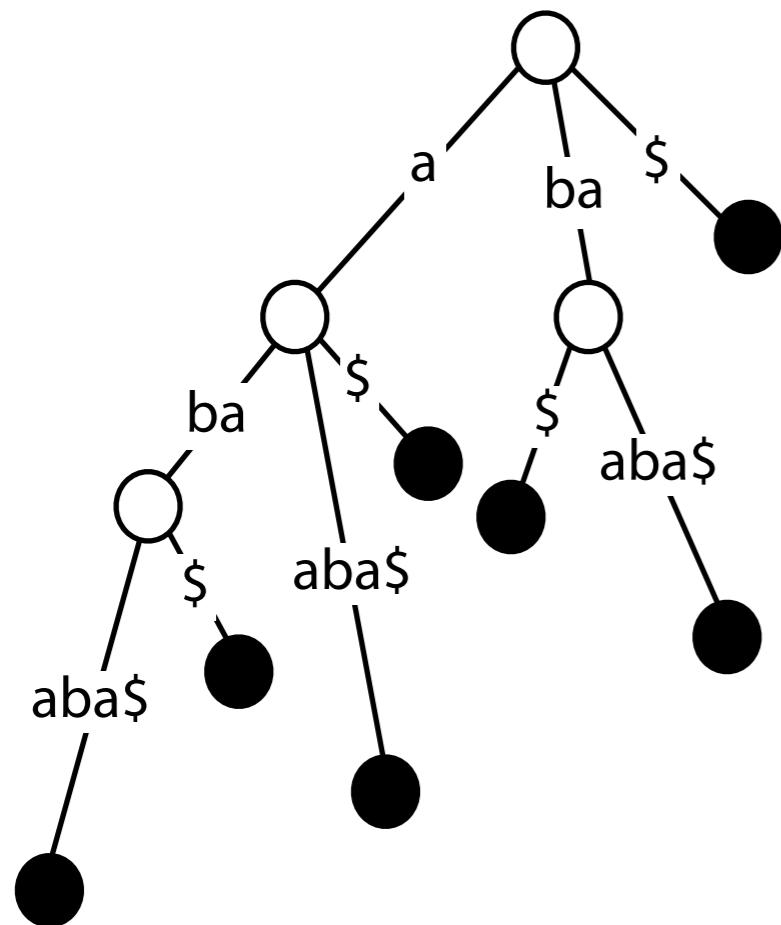
$$E = L + I - 1 \leq 2m - 2$$

$$E + L + I \leq 4m - 3 \in O(m)$$

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

# Suffix tree

$T = abaaba\$$



$L$  leaves,  $I$  internal nodes,  $E$  edges

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$L \leq m$  (at most  $m$  suffixes)

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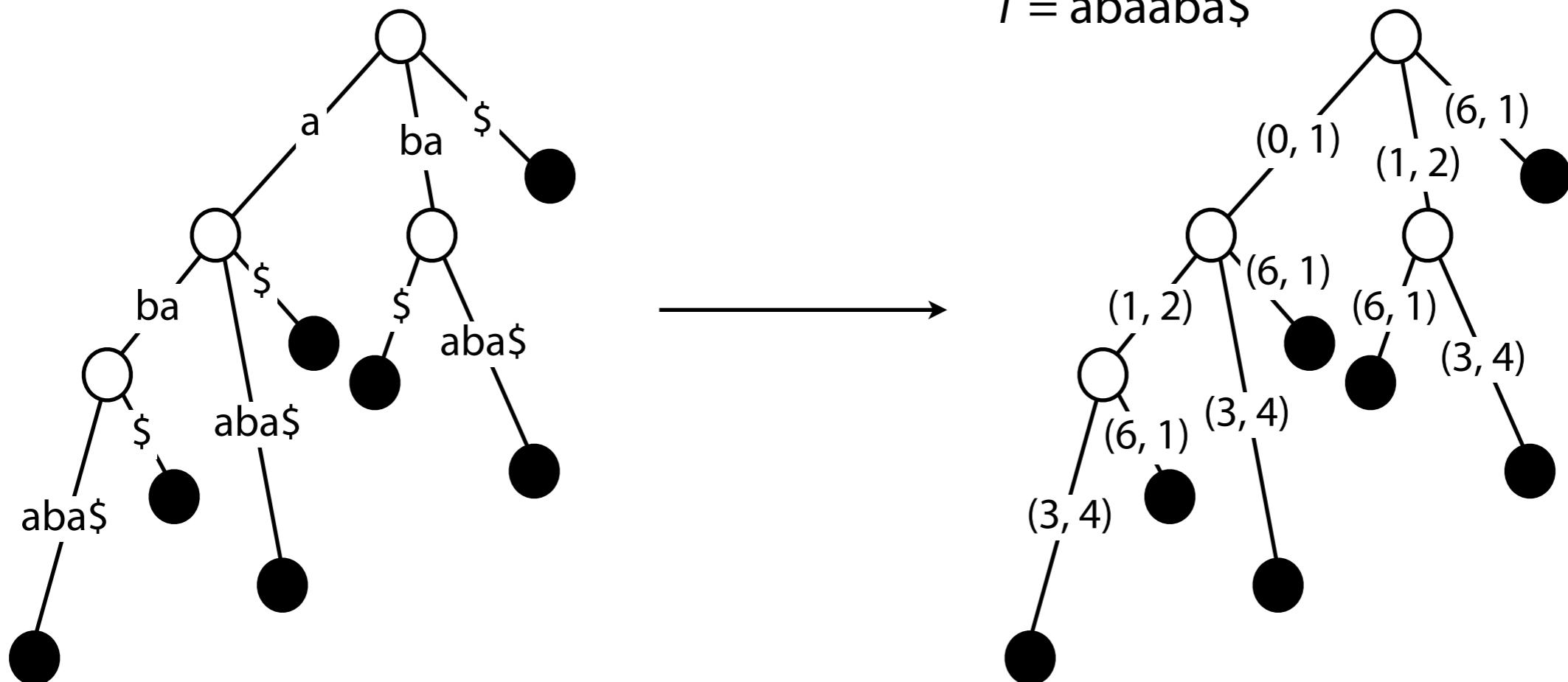
Is the total size  $O(m)$  now?

**NO:** The total length of edge labels is quadratic in  $m$ .

# Suffix tree

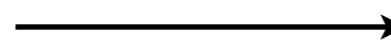
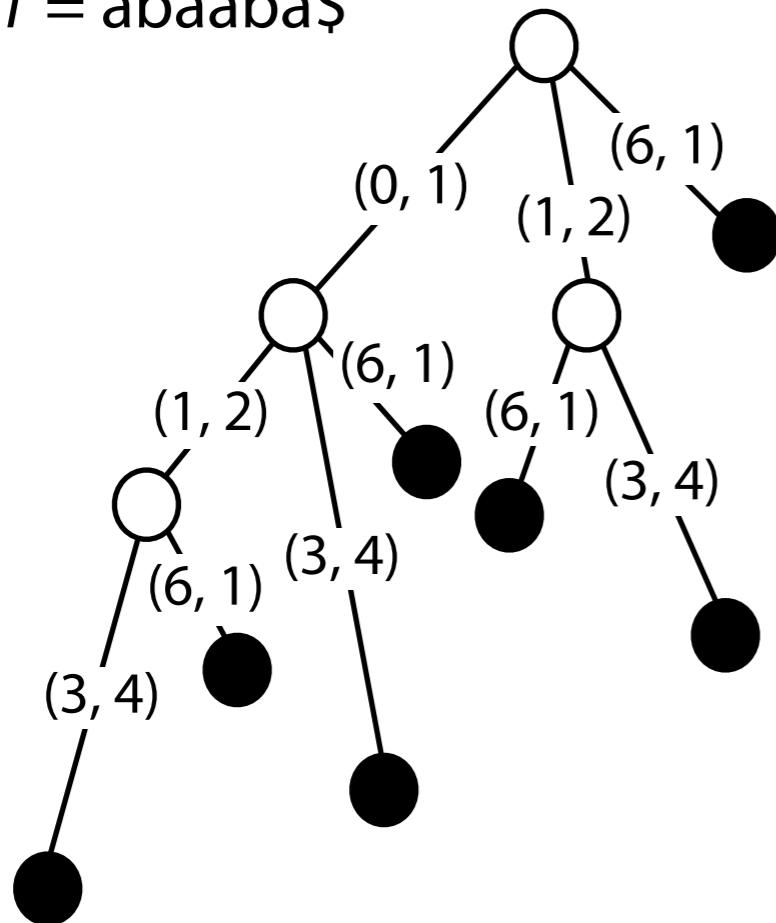
$T = abaaba\$$

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

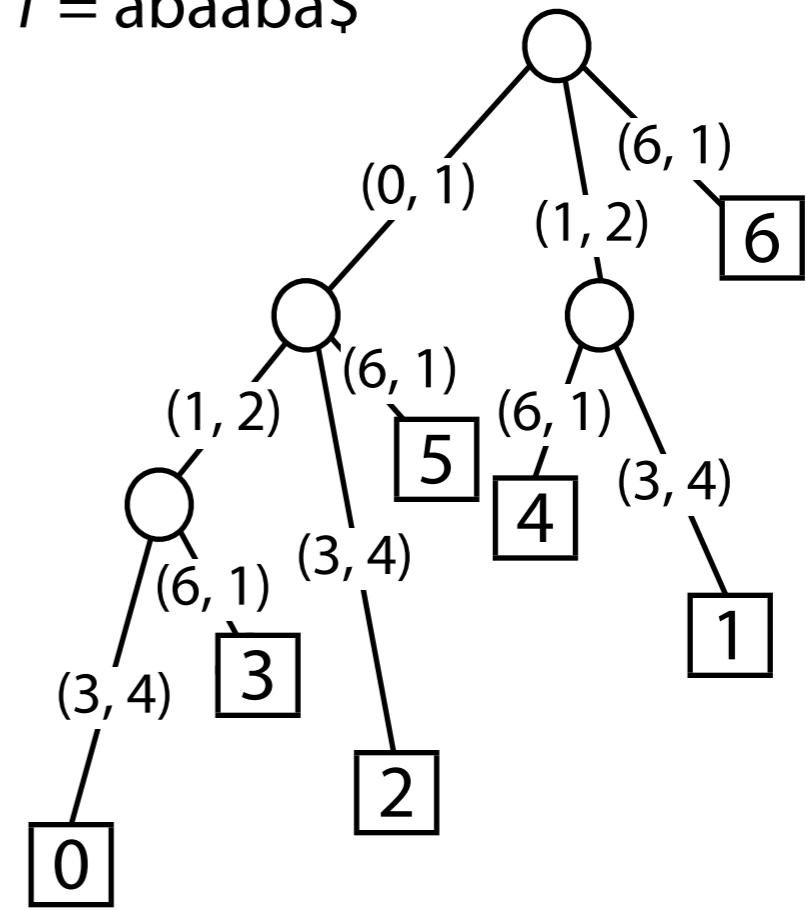


# Suffix tree: leaves hold offsets where suffixes begin

$T = abaaba\$$

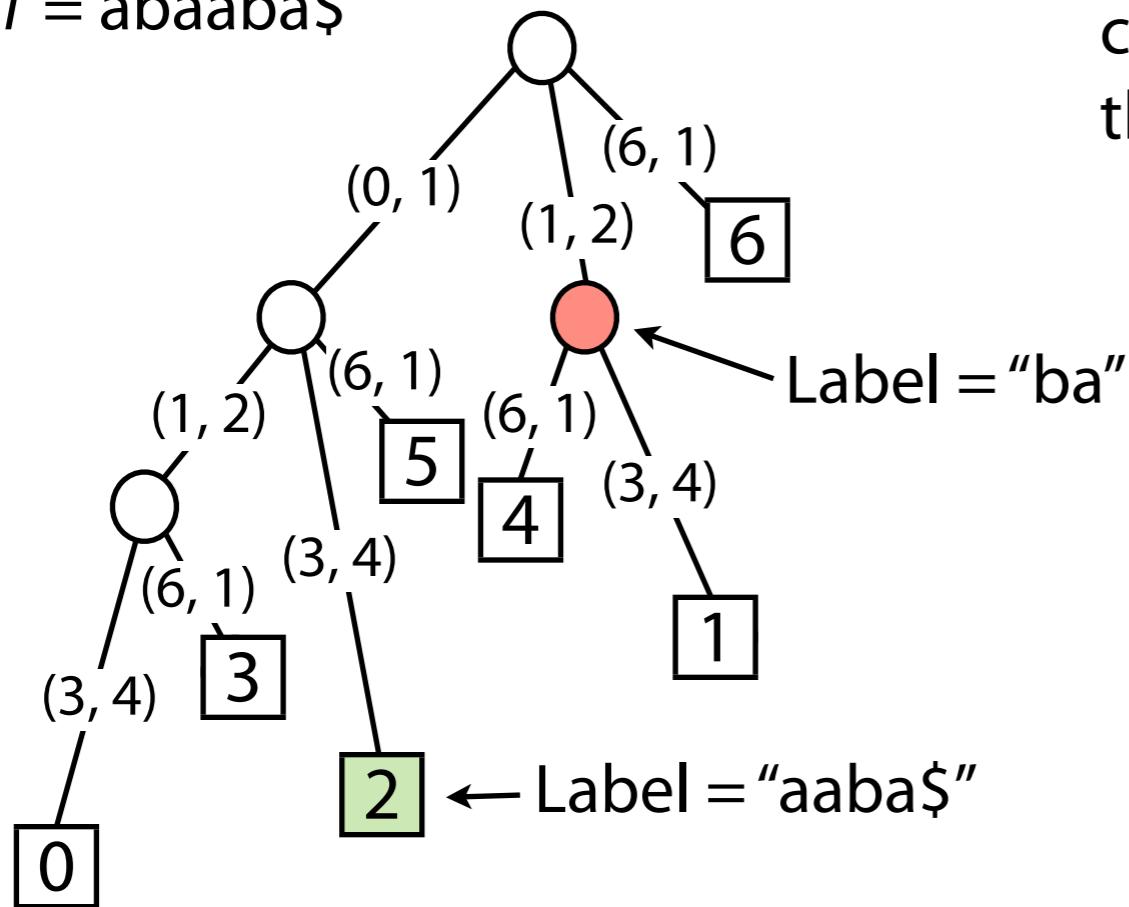


$T = abaaba\$$



# Suffix tree: labels

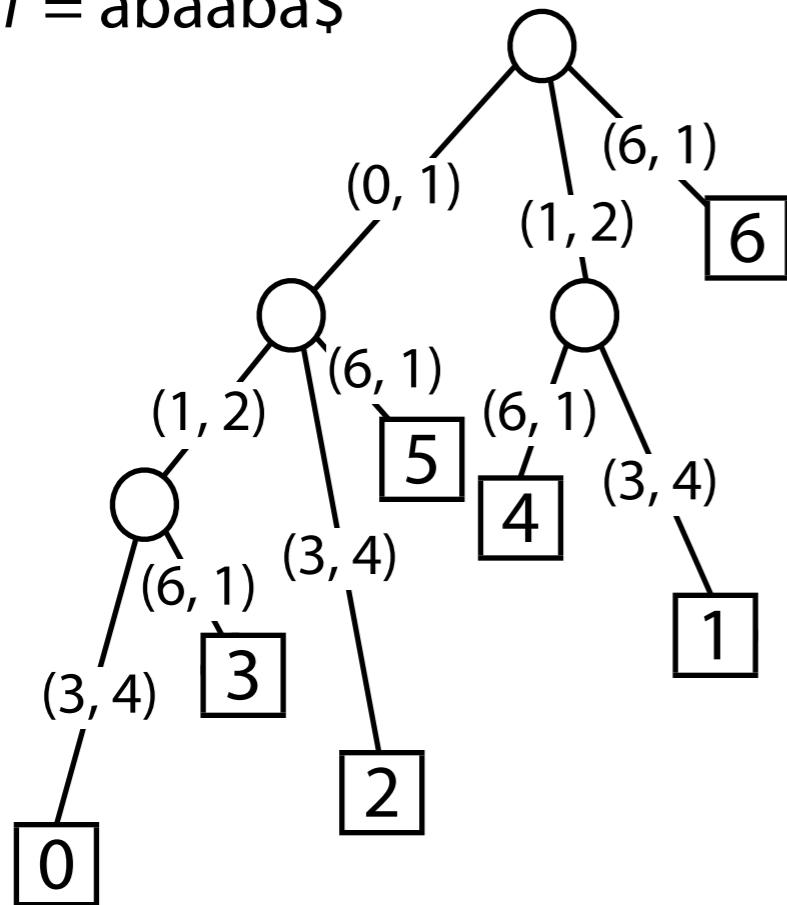
$T = \text{abaaba\$}$



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

# Suffix tree: labels

$T = \text{abaaba\$}$

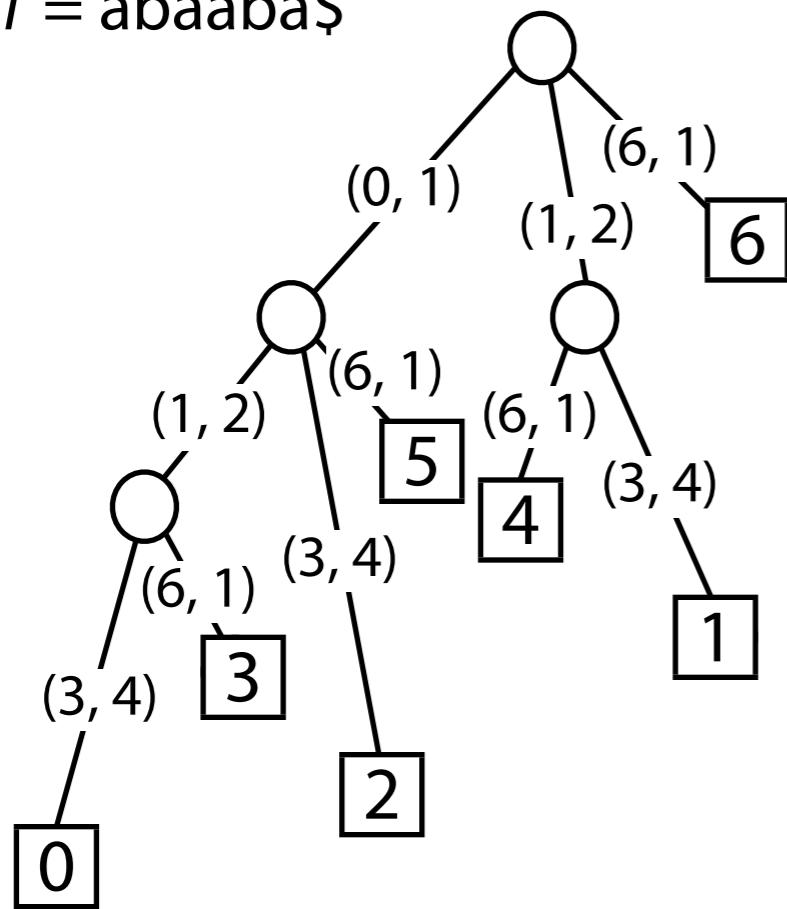


Because edges can have string labels, we must distinguish two notions of “depth”

- **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

$T = \text{abaaba\$}$



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.  $\text{ceil}(\log_2 m)$  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.

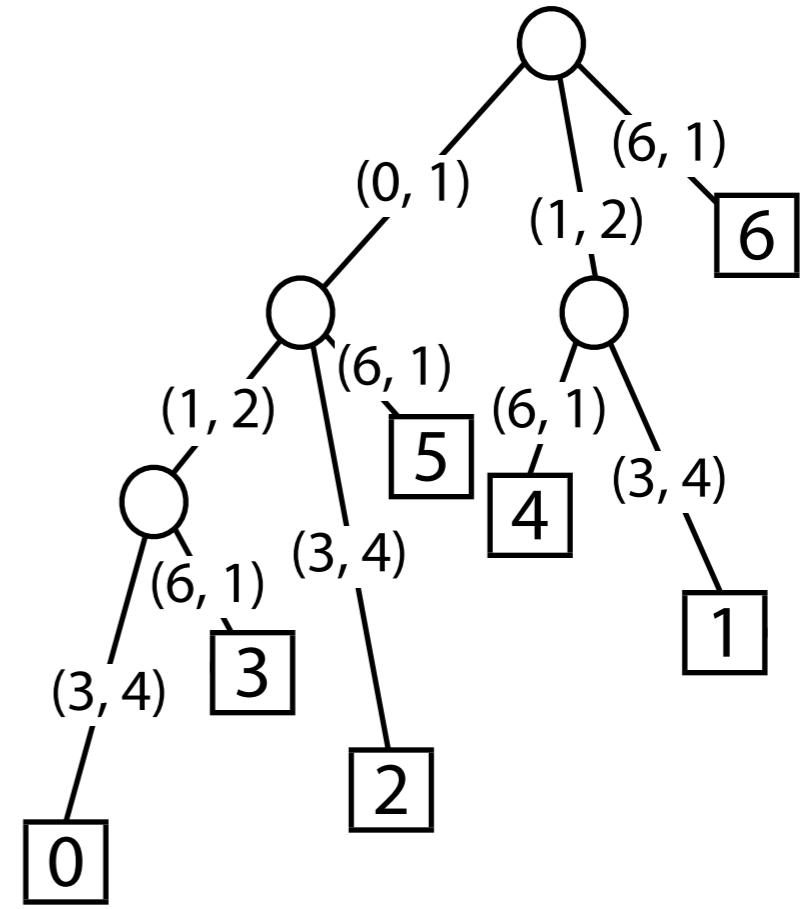
# Suffix tree: building

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 2<sup>nd</sup>-longest, then augment to include 3<sup>rd</sup>-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: building

Other methods for construction:

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

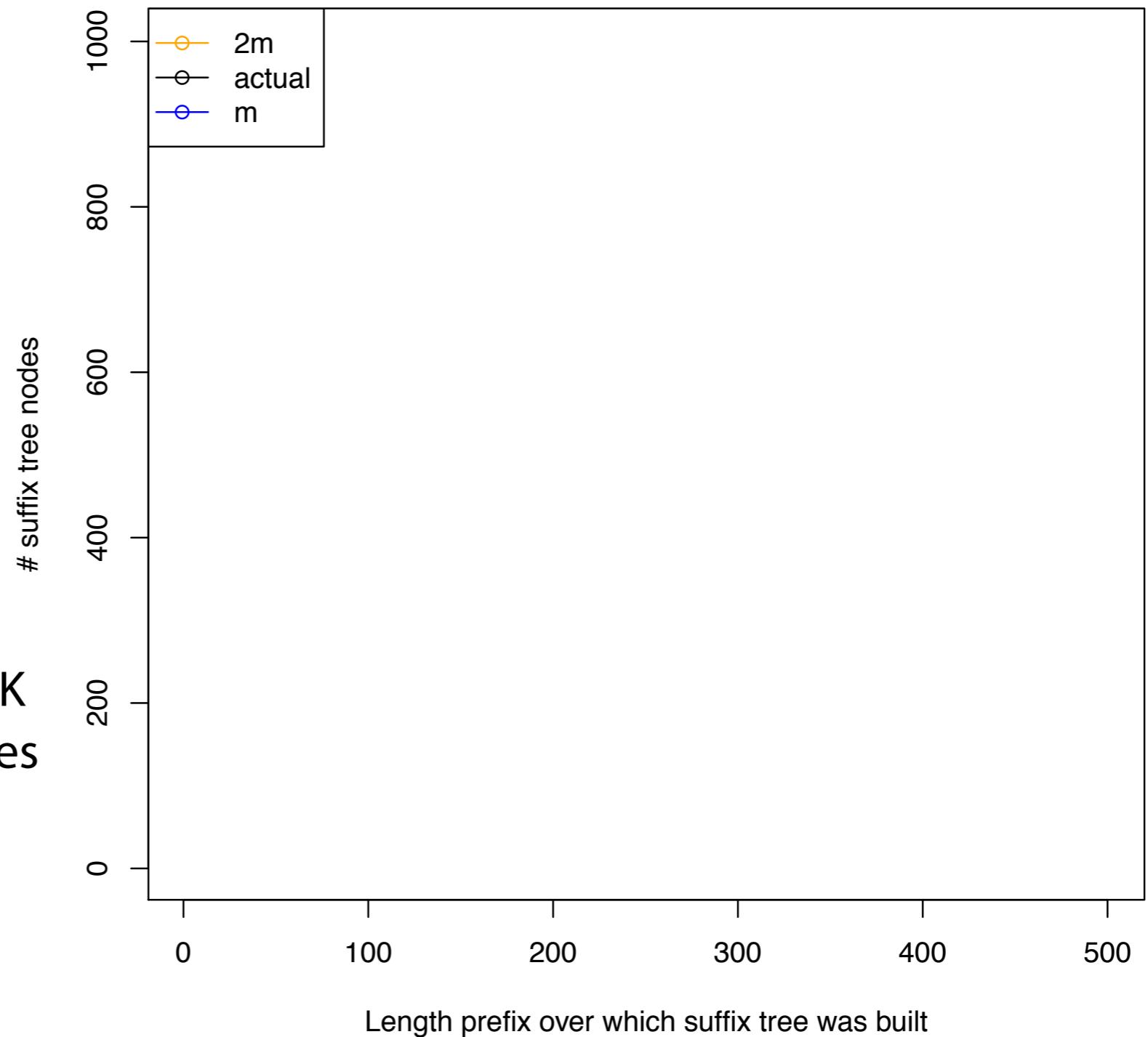
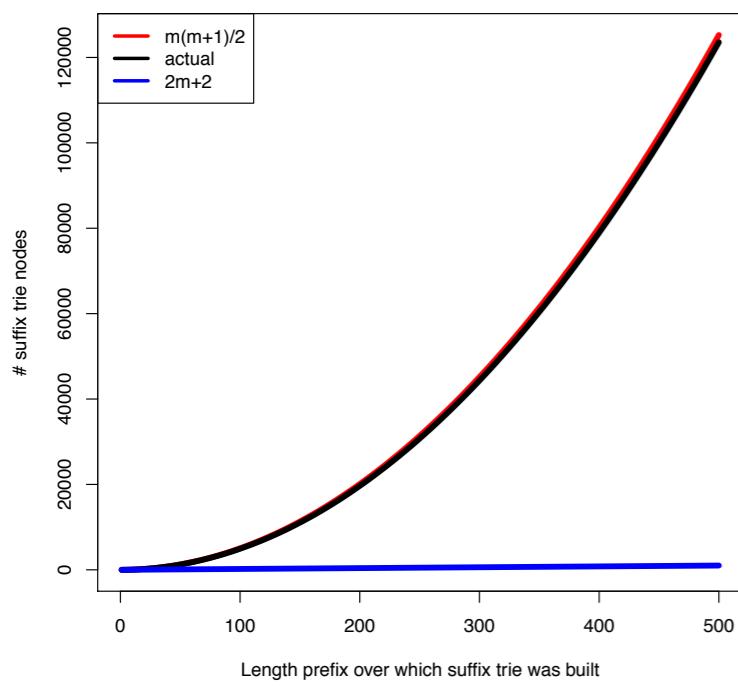
Or just Google “Ukkonen’s algorithm”

# 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

Remember suffix trie plot:

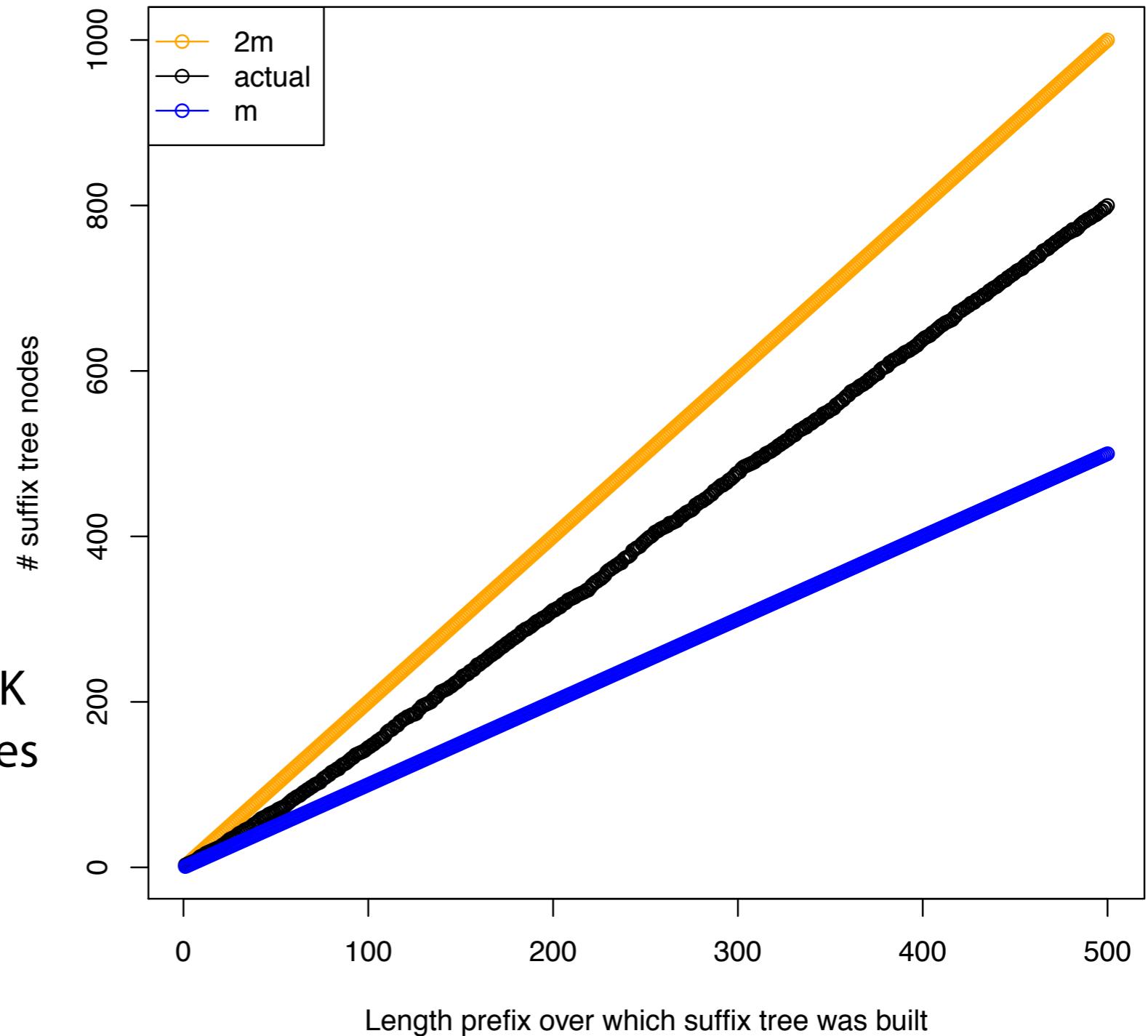
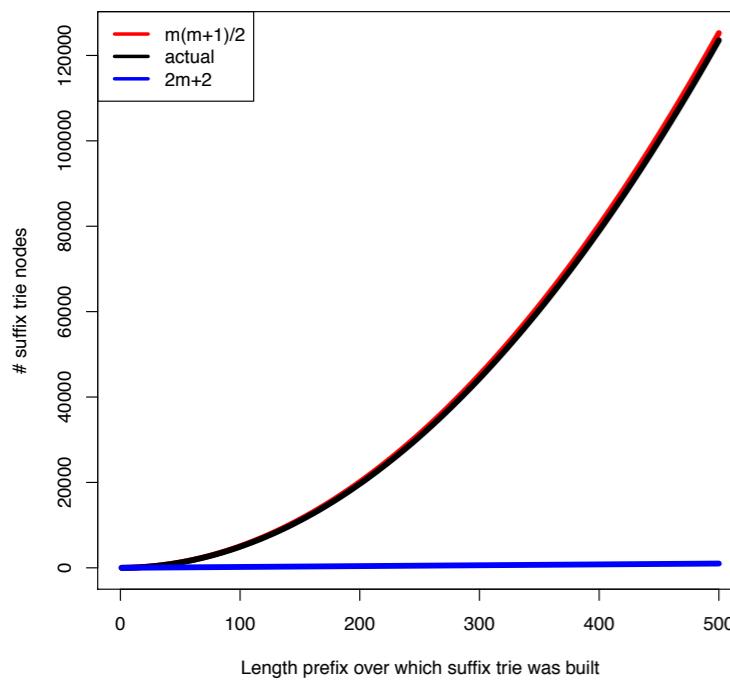


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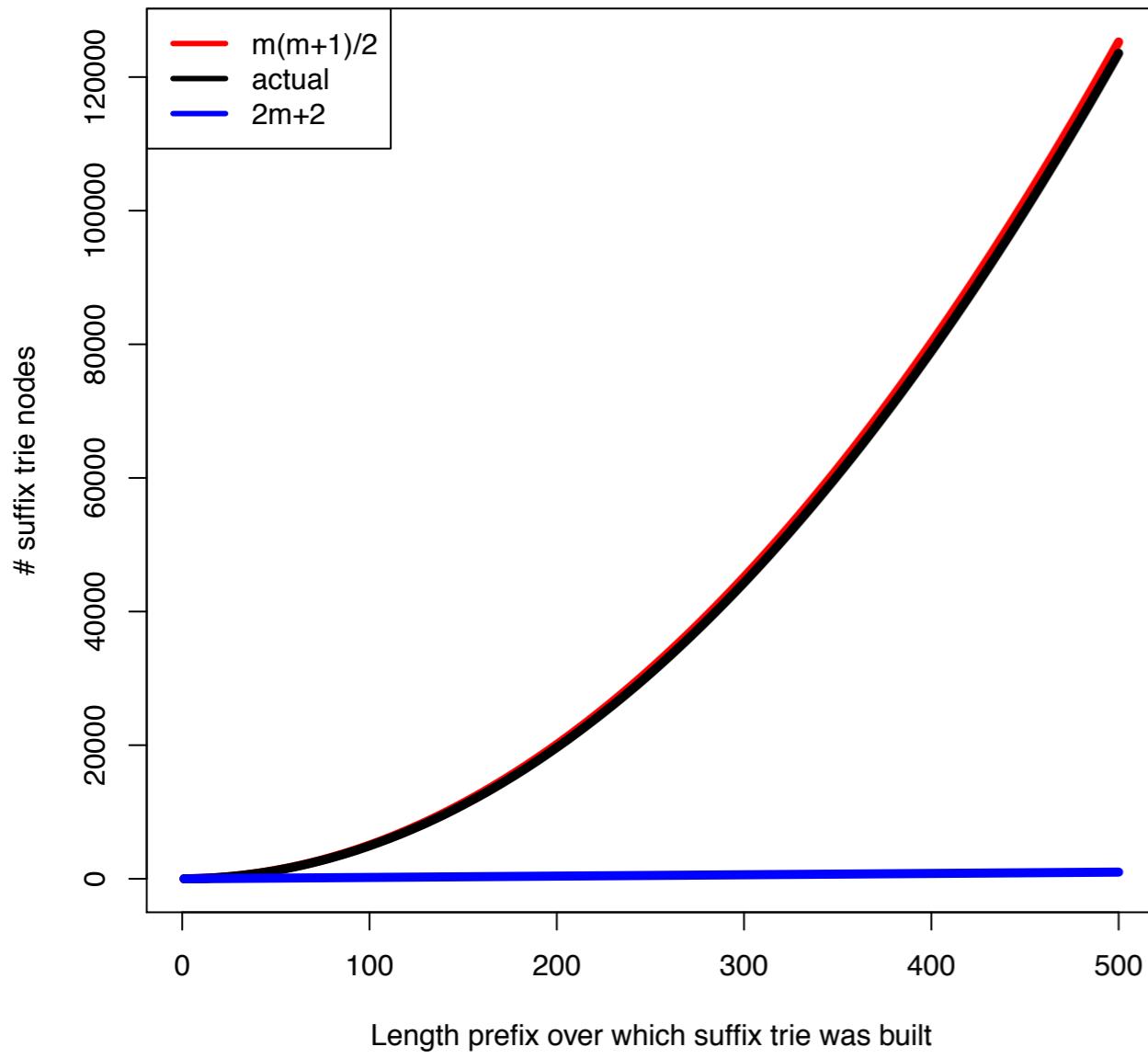
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Remember suffix trie plot:



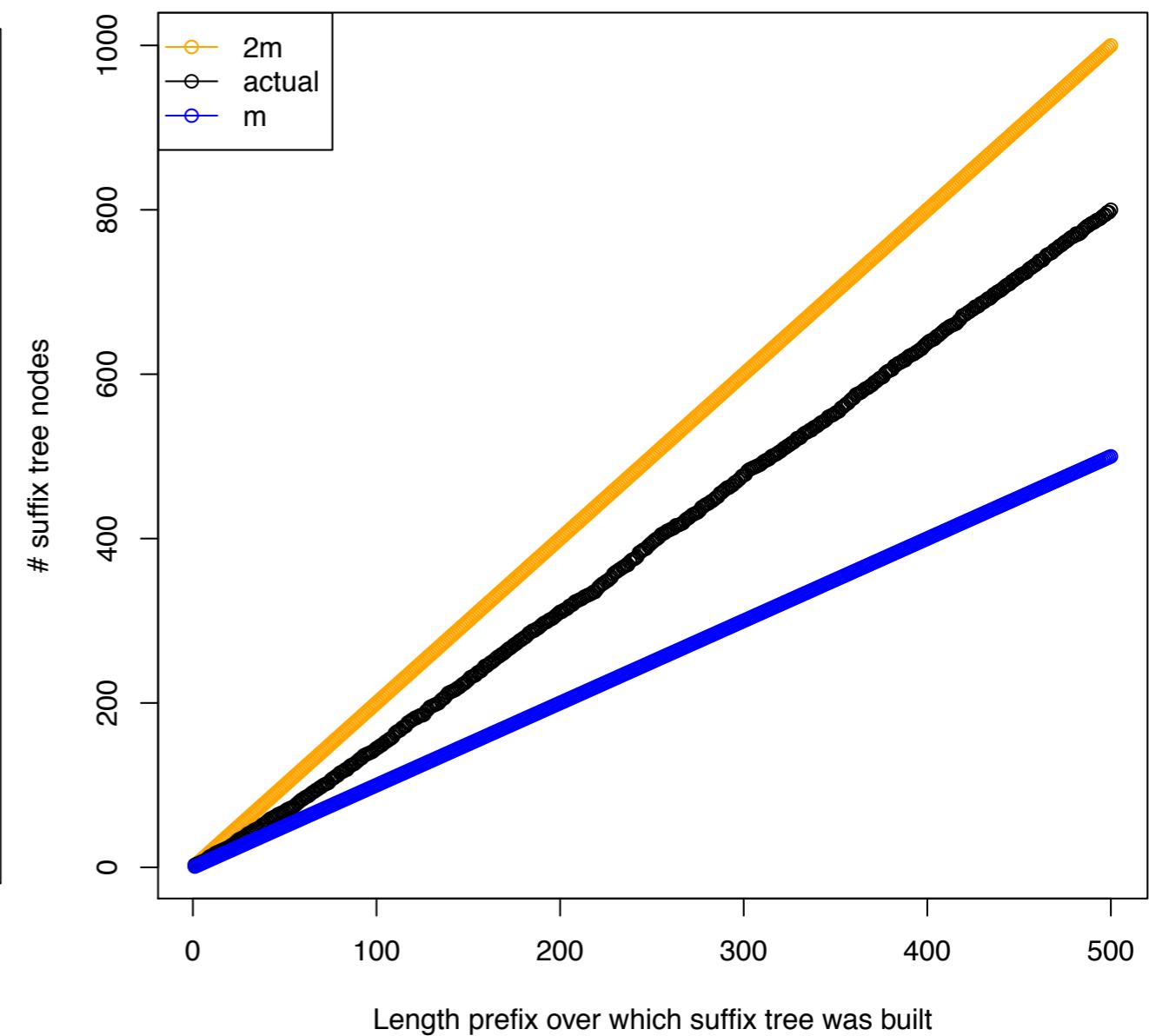
# Suffix trie

>100K nodes



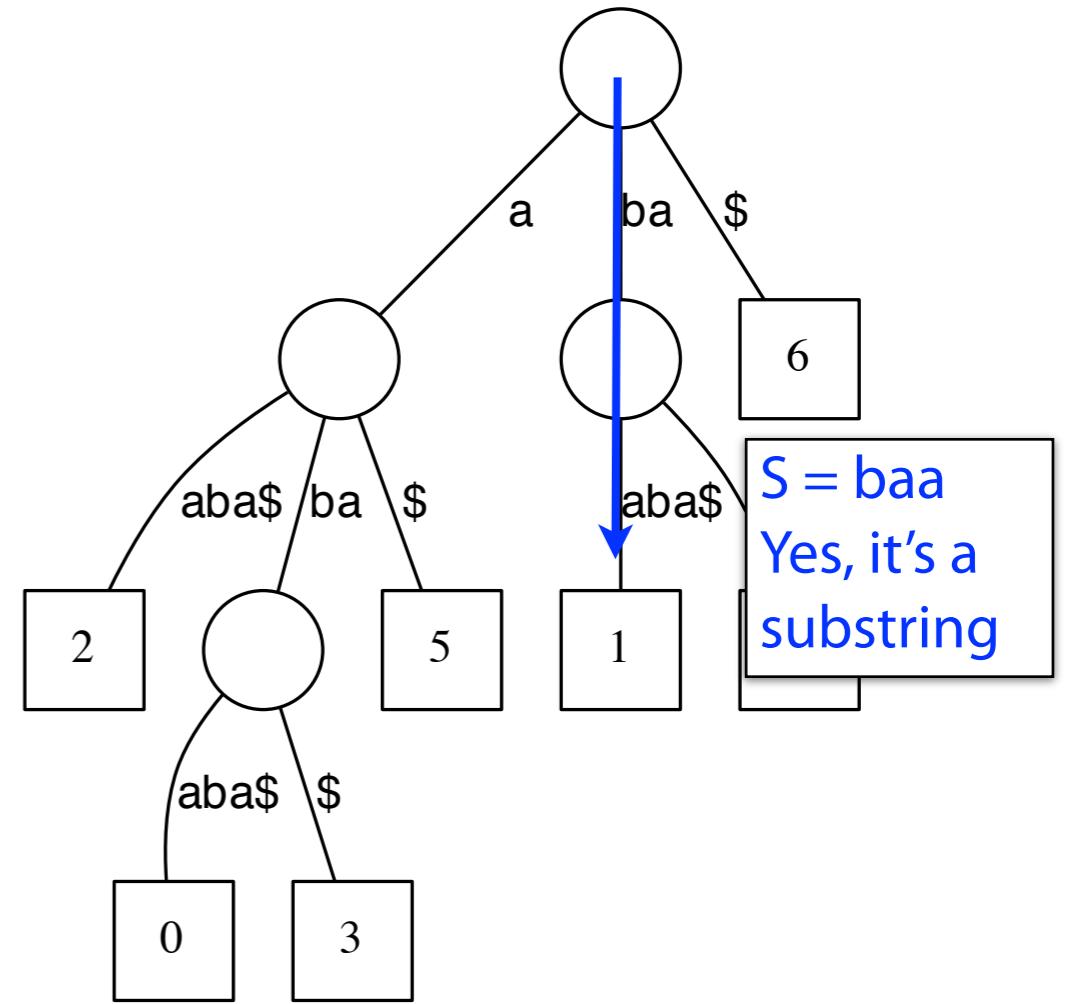
# Suffix tree

<1K nodes



# Suffix tree

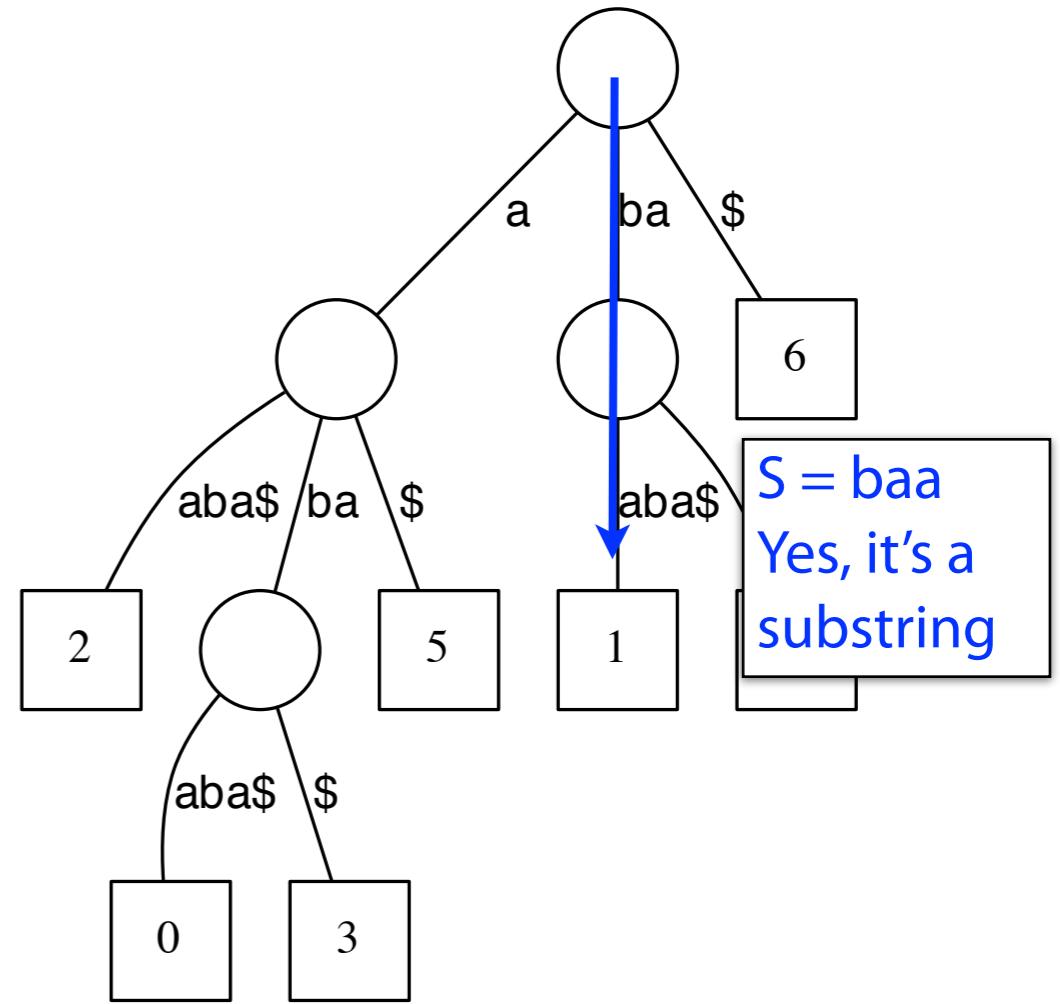
How do we check whether a string  $S$  is a substring of  $T$ ?



# Suffix tree

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

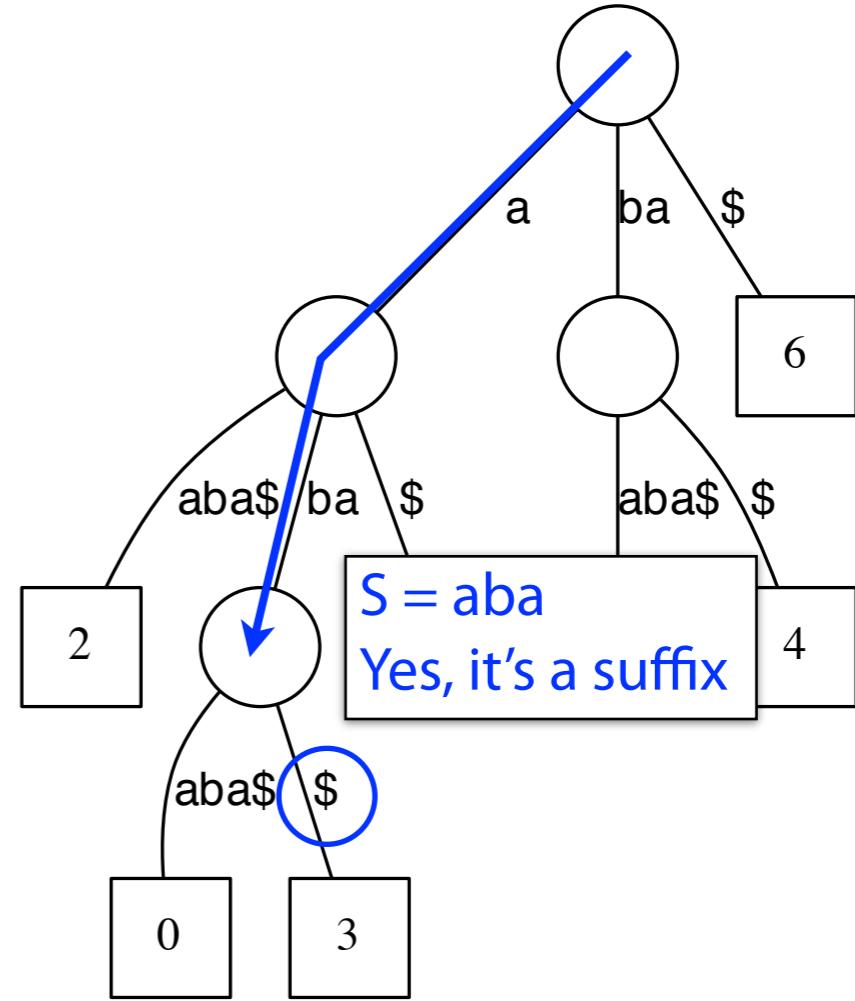
Essentially same procedure as for suffix trie, except we have to deal with coalesced edges



# Suffix tree

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

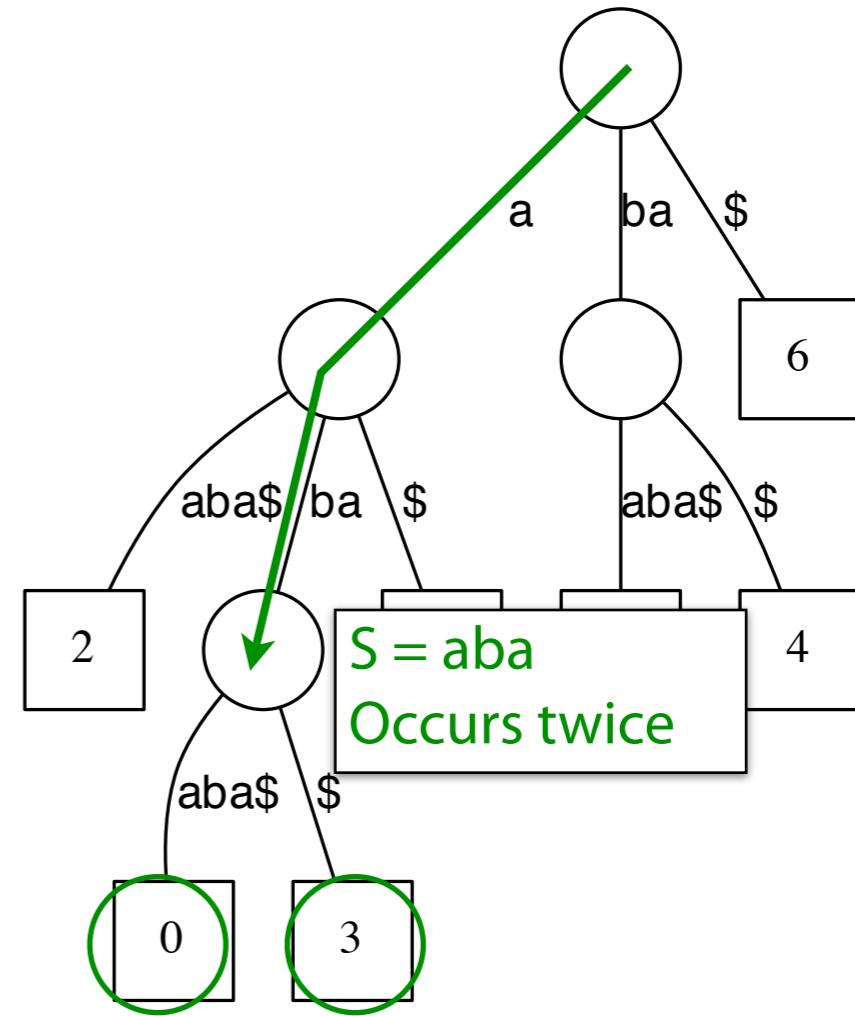
Essentially same procedure as for suffix trie, except we have to deal with coalesced edges



# 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.,  $P = ab, T = abaaba\$$

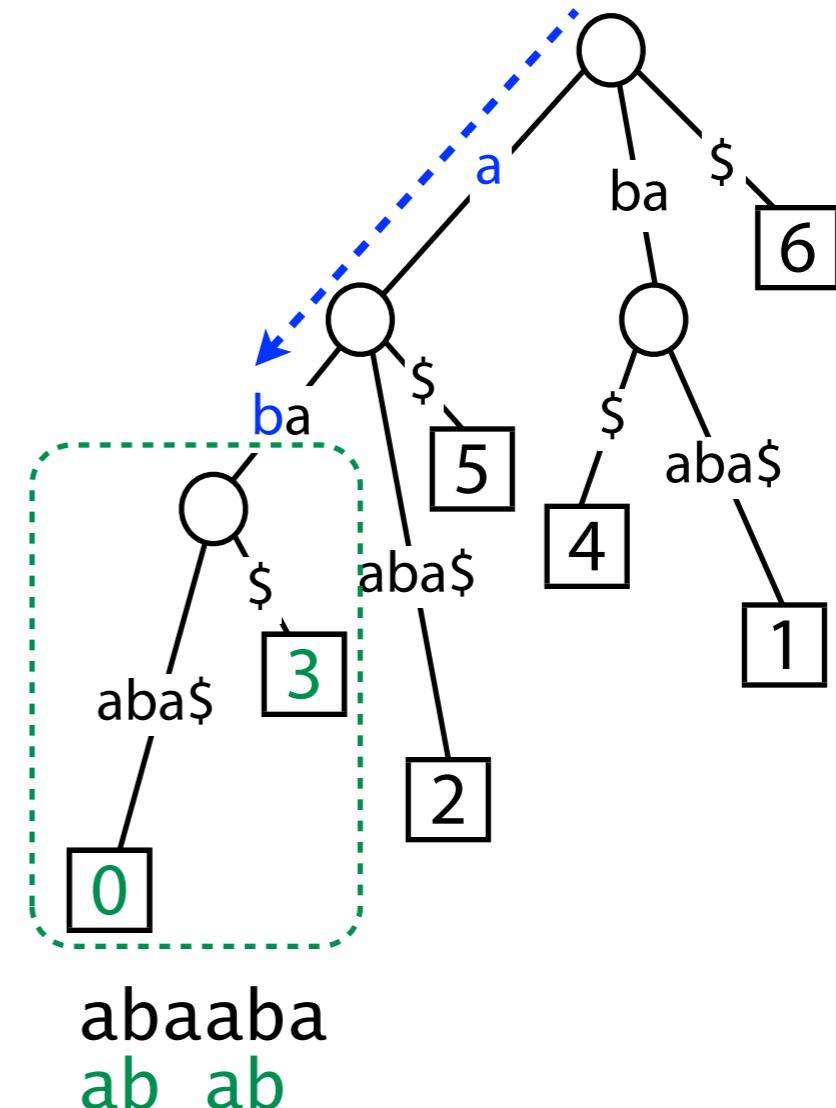
$O(n)$  Step 1: walk down ab path

If we “fall off” there are no matches

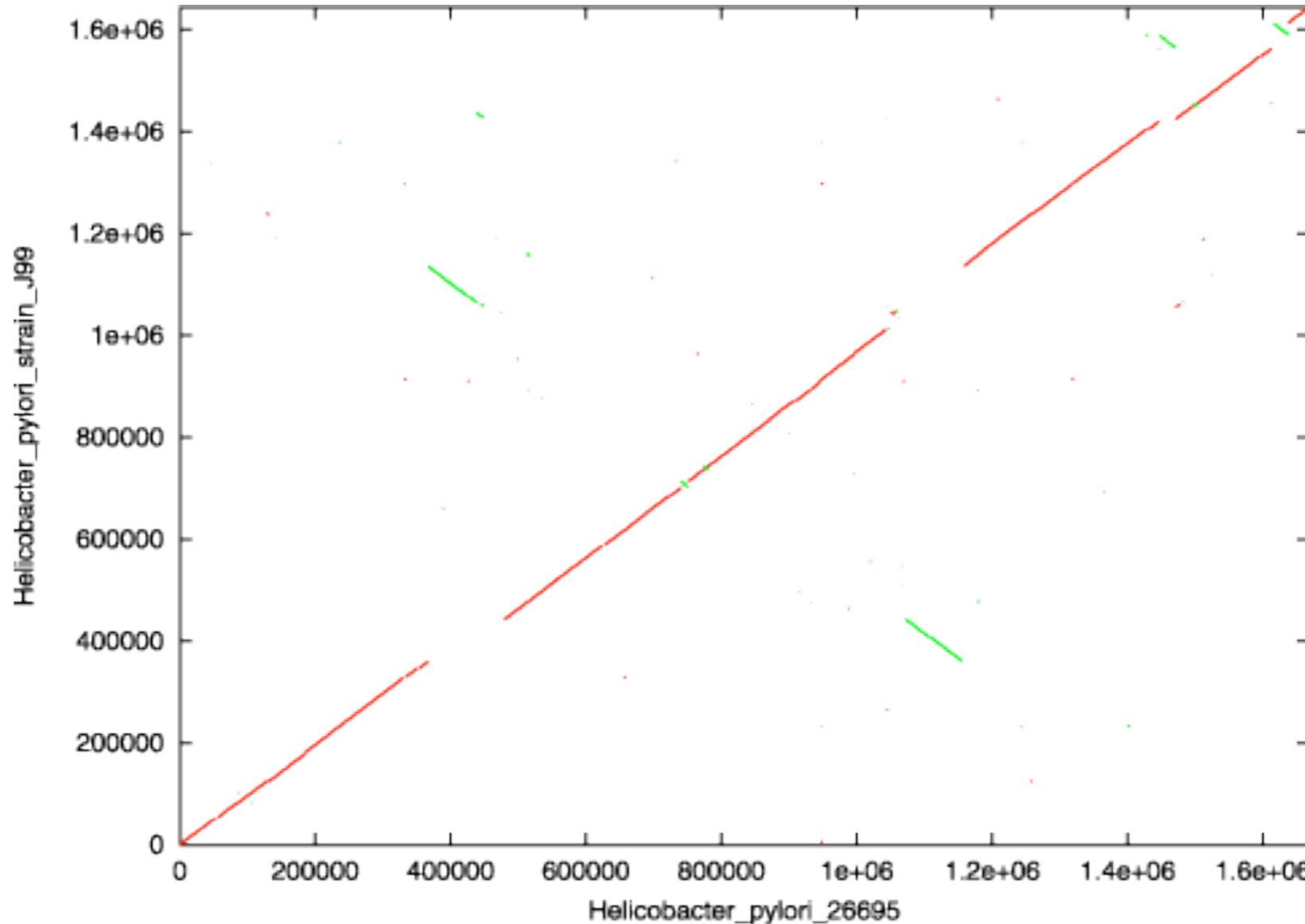
$O(k)$  Step 2: visit all leaf nodes below

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

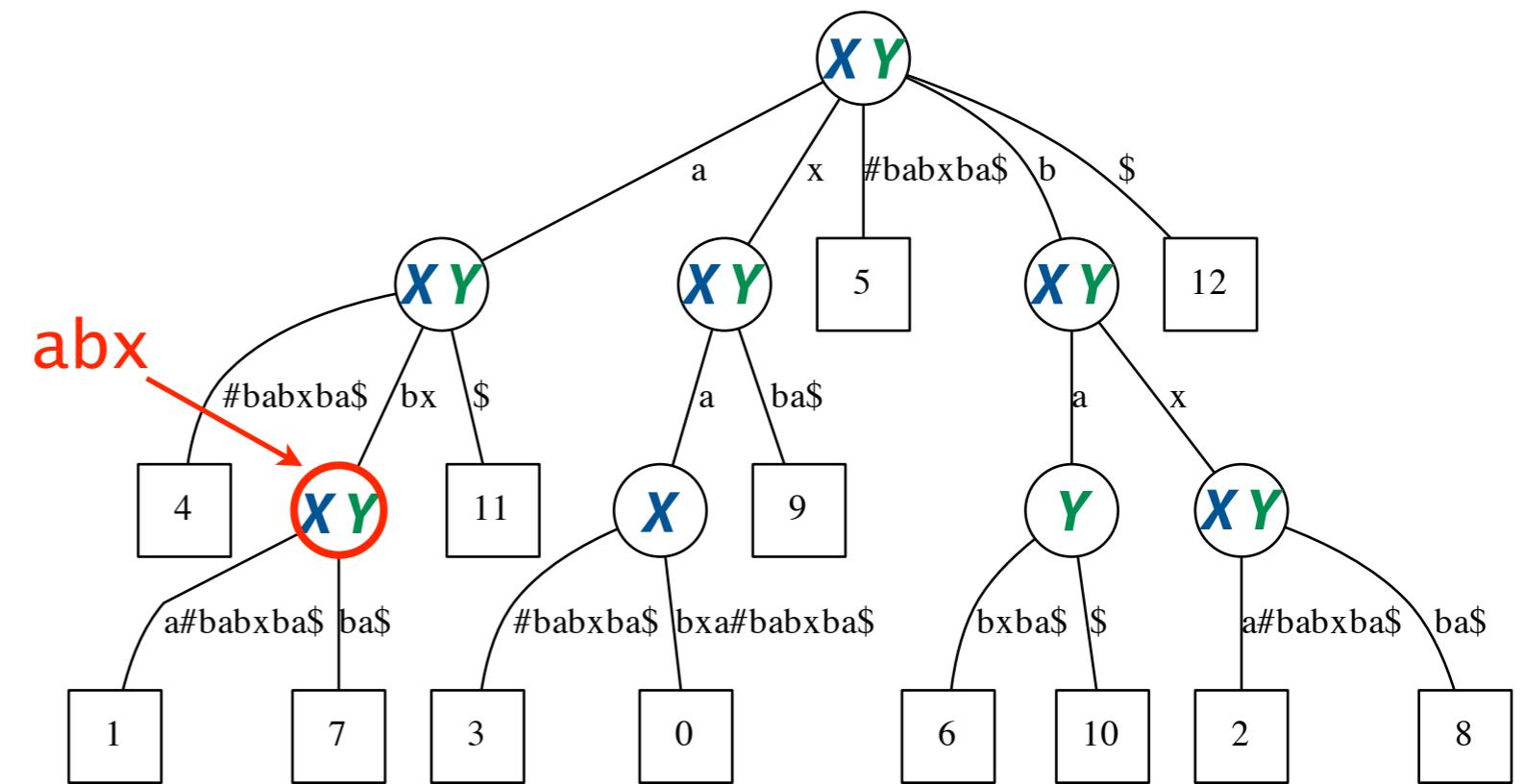
To find the longest common substring (LCS) of  $X$  and  $Y$ , make a new string  $X\#Y\$$  where  $\#$  and  $\$$  are both terminal symbols. Build a suffix tree for  $X\#Y\$$ .

$$\textcolor{blue}{X} = \text{xabxa}$$

$$\textcolor{green}{Y} = \text{babxba}$$

$$\textcolor{blue}{X}\#\textcolor{green}{Y}\$ = \text{xabxa}\#\text{babxba}\$$$

Consider leaves:  
offsets in  $[0, 4]$  are  
suffixes of  $\textcolor{blue}{X}$ , offsets in  
 $[6, 11]$  are suffixes of  $\textcolor{green}{Y}$



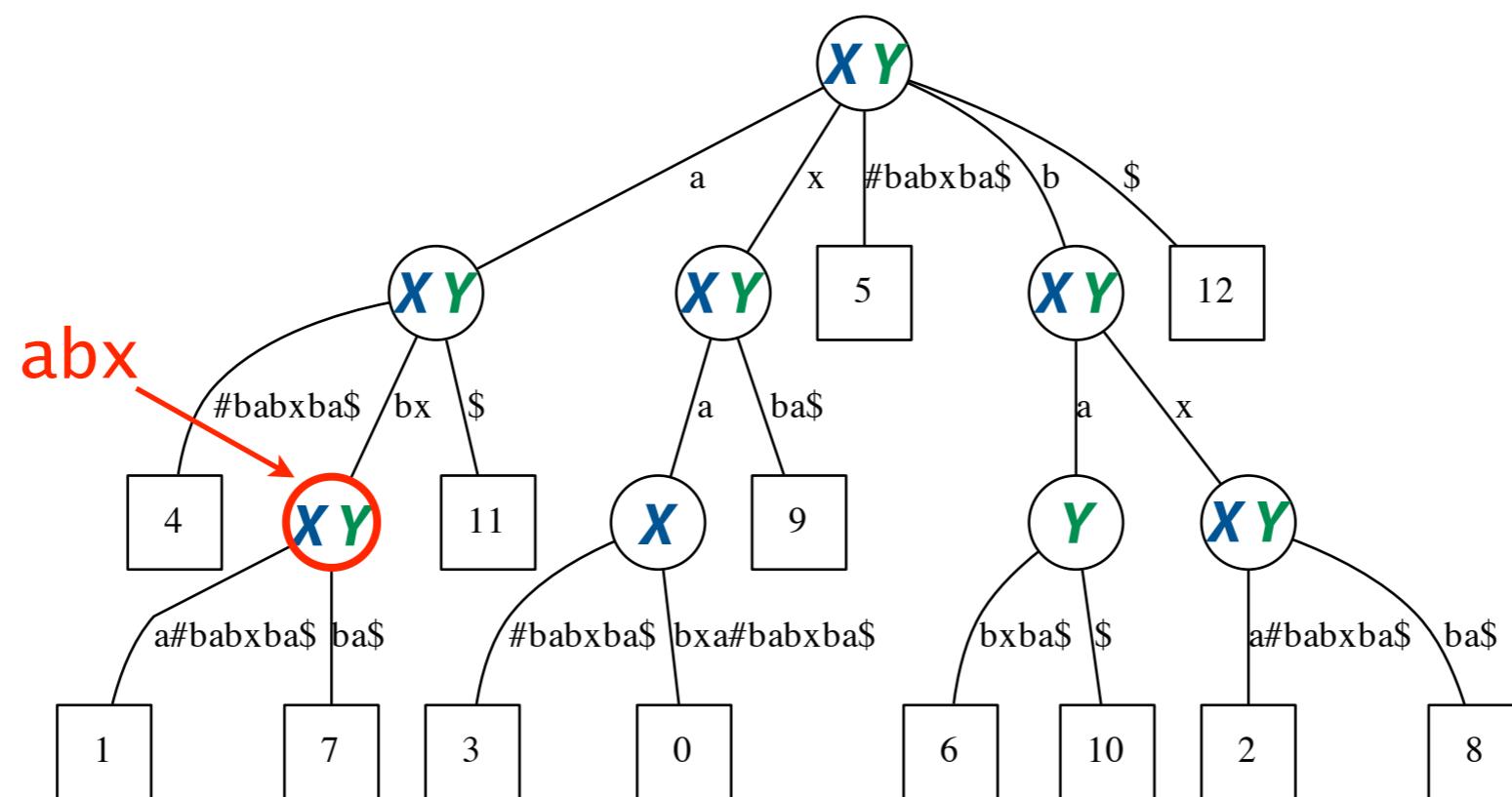
Traverse the tree and annotate each node according to whether leaves below it include suffixes of  $\textcolor{blue}{X}$ ,  $\textcolor{green}{Y}$  or both

The deepest node annotated with both  $\textcolor{blue}{X}$  and  $\textcolor{green}{Y}$  has LCS as its label.  
 $O(|\textcolor{blue}{X}| + |\textcolor{green}{Y}|)$  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

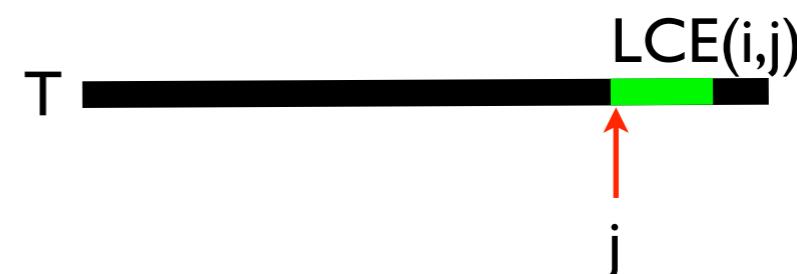
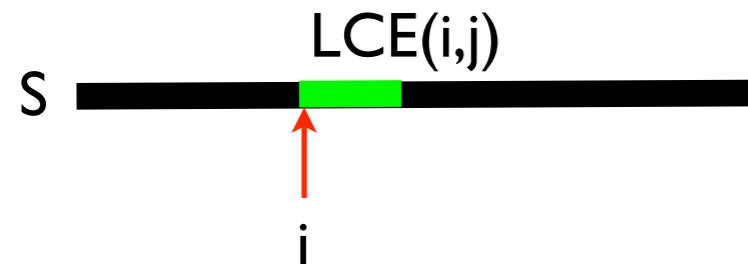
Such a tree is called a *generalized suffix tree*. These are introduced in *Gusfield 6.4*.



# Longest Common Extension

Longest common extension: We are given strings S and T. In the future, many pairs  $(i, j)$  will be provided as queries, and we want to quickly find:

the longest substring of S starting at i that matches a substring of T starting at j.



Build generalized suffix tree for S and T.

$O(|S| + |T|)$

Preprocess tree so that lowest common ancestors (LCA) can be found in constant time.  
This can be done using range-minimum queries (RMQ)

$O(|S| + |T|)$

Create an array mapping suffix numbers to leaf nodes.

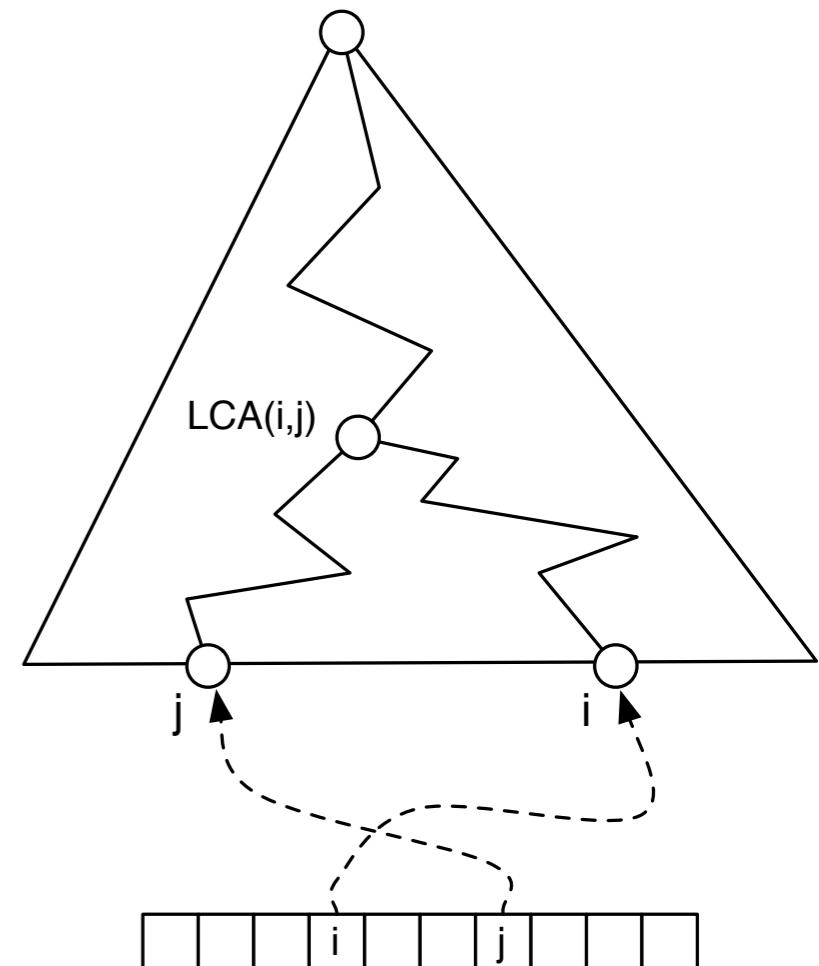
$O(|S| + |T|)$

Given query  $(i, j)$ :

$O(1)$   
 $O(LCE(i, j))$

Find the leaf nodes for i and j

Return string of LCA for i and j



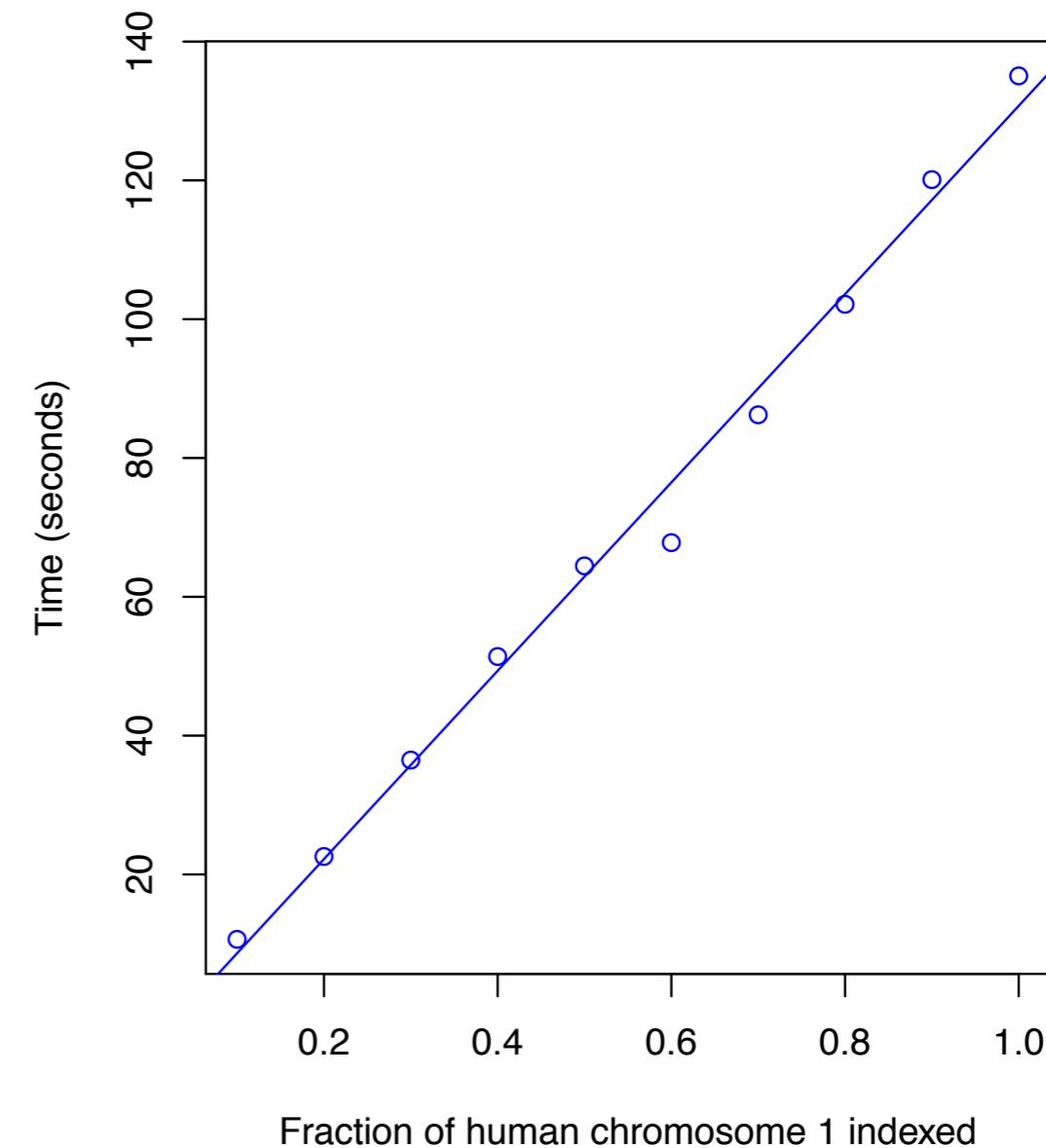
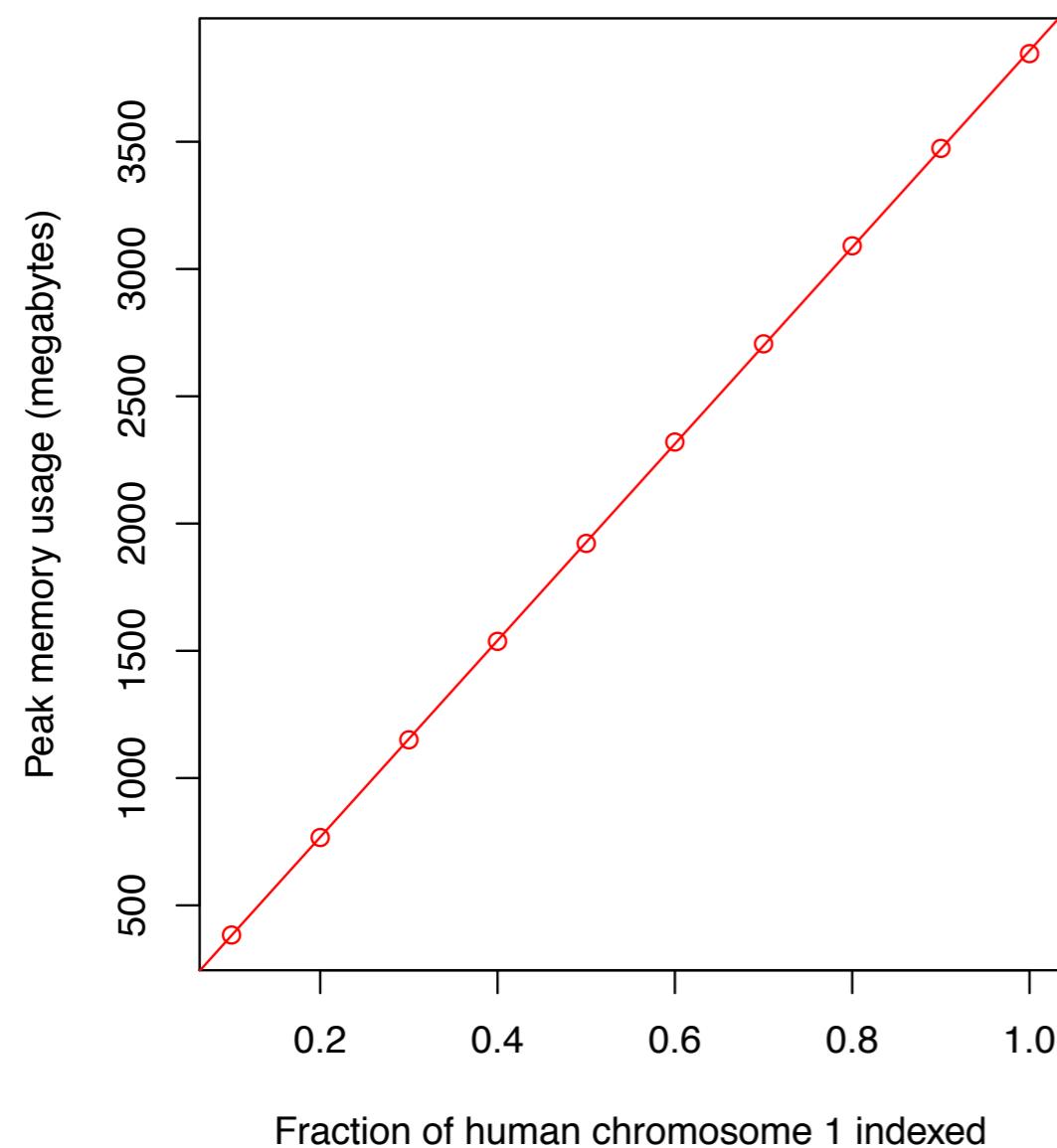
# Suffix trees in the real world: MUMmer

# Indexing phase: ~2 minutes

Matching  
phase:  
very fast

# 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  
 **$\approx 15.75$  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  **$\approx 12.5$  bytes per node**

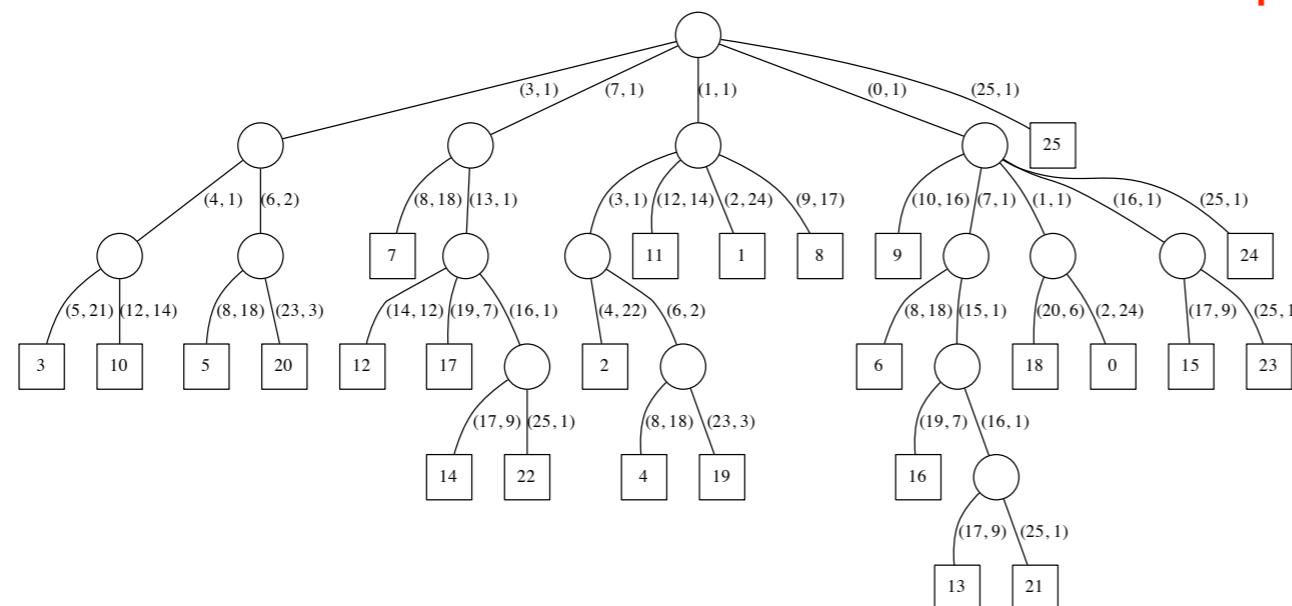
Kurtz, Stefan. "Reducing the space requirement of suffix trees." *Software Practice and Experience* 29.13 (1999): 1149-1171.

# 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

GTTATAGCTGATCGCGGCGTAGCGG\$  $m$  chars  
GTTATAGCTGATCGCGGCGTAGCGG\$  
TTATAGCTGATCGCGGCGTAGCGG\$  
TATAGCTGATCGCGGCGTAGCGG\$  
ATAGCTGATCGCGGCGTAGCGG\$  
TAGCTGATCGCGGCGTAGCGG\$  
AGCTGATCGCGGCGTAGCGG\$  
GCTGATCGCGGCGTAGCGG\$  
CTGATCGCGGCGTAGCGG\$  
TGATCGCGGCGTAGCGG\$  
GATCGCGGCGTAGCGG\$  
ATCGCGGCGTAGCGG\$  
TCGCGGCGTAGCGG\$  
CGCGGCGTAGCGG\$  
GCGGCGTAGCGG\$  
CGGCCTAGCGG\$  
GGCGTAGCGG\$  
CGTAGCGG\$  
GTAGCGG\$  
TAGCGG\$  
AGCGG\$  
GCGG\$  
C GG\$  
GG\$  
G\$

$m(m+1)/2$  chars

Bonus Content (not required) :  
Suffix tree construction

# WOTD (Write-Only Top-Down) Construction

Giegerich, Robert, and Stefan Kurtz. "A comparison of imperative and purely functional suffix tree constructions." *Science of Computer Programming* 25.2 (1995): 187-218.

Build a suffix tree for string  $s\$$

Recursive construction:

For every branching node **node**( $u$ ), subtree of **node**( $u$ ) is determined by all suffixes of  $s\$$  where  $u$  is a prefix.

Recursively construct subtree for all suffixes where  $u$  is a prefix.

**Definition:** *remaining suffixes of  $u$*

$$R(\text{node}(u)) = \{ v \mid uv \text{ is a suffix of } s\$ \}$$

# WOTD (Write-Only Top-Down) Construction

Build a suffix tree for string s\$

Recursive construction:

For every branching node **node**(u), subtree of **node**(u) is determined by all suffixes of s\$ where u is a prefix.

Recursively construct subtree for all suffixes where u is a prefix.

**Definition:** *remaining suffixes* of u

$$R(\text{node}(u)) = \{ v \mid uv \text{ is a suffix of } s\$ \}$$

**Definition:** *c-group* of node(u)

$$\text{group}(\text{node}(u), c) = \{ w \in \Sigma^* \mid cw \in R(\text{node}(u)) \}$$

# WOTD (Write-Only Top-Down) Construction

```
def WOTD(T : tree, node(u): node):
    for each c ∈ Σ ∪ {$}:
        G = group(node(u), c)
        ucv = lcp(G)
        if |G| == 1:      ← non-branching suffix
            add leaf node(ucv) as a child of node(u)
        else:
            add inner node(ucv) as a child of node(u)
            WOTD(T, node(ucv))

branching suffix
```

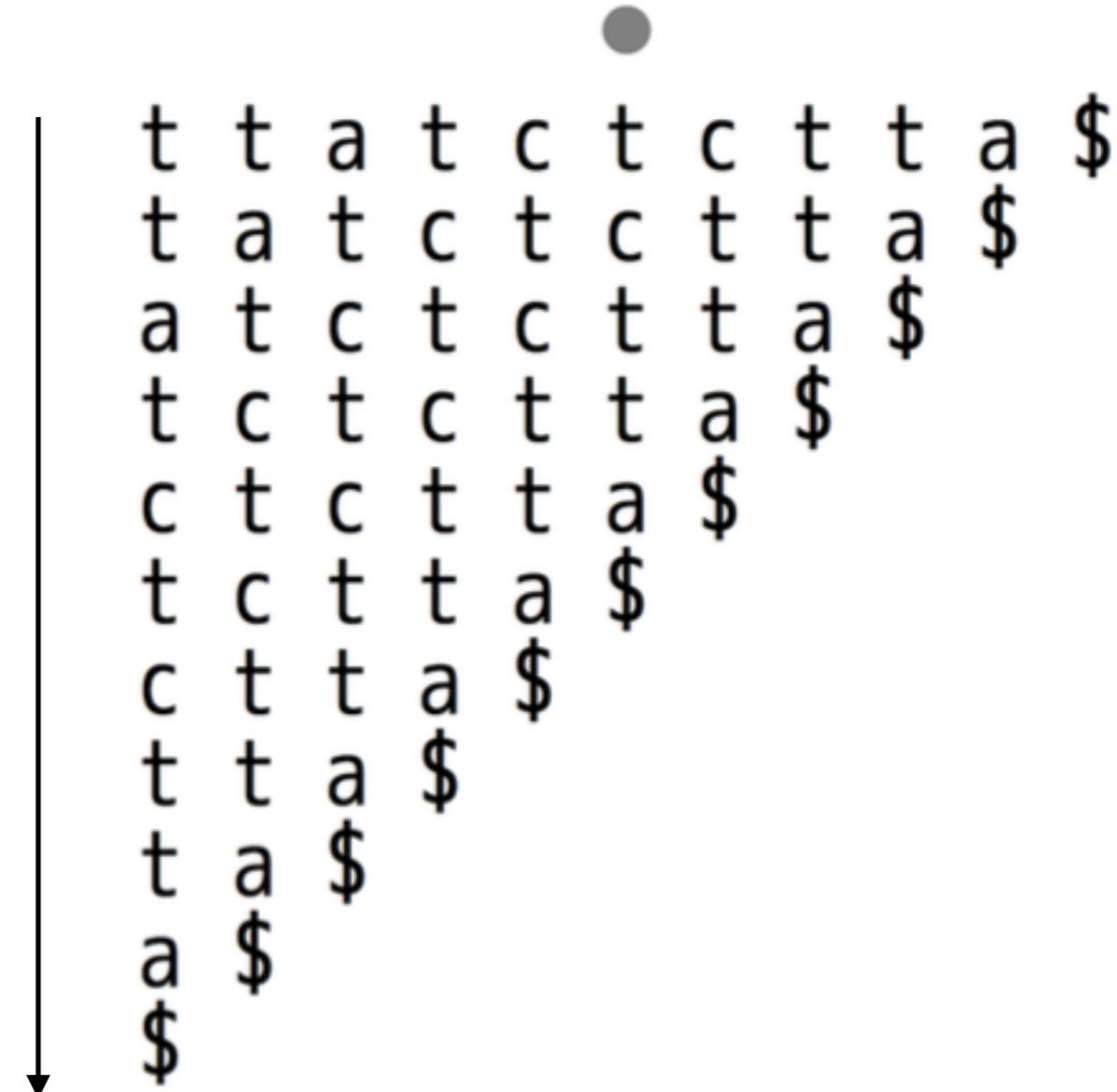
Start the algorithm by calling  $\text{WOTD}(T, \text{node}(\epsilon))$

root node

# WOTD Example

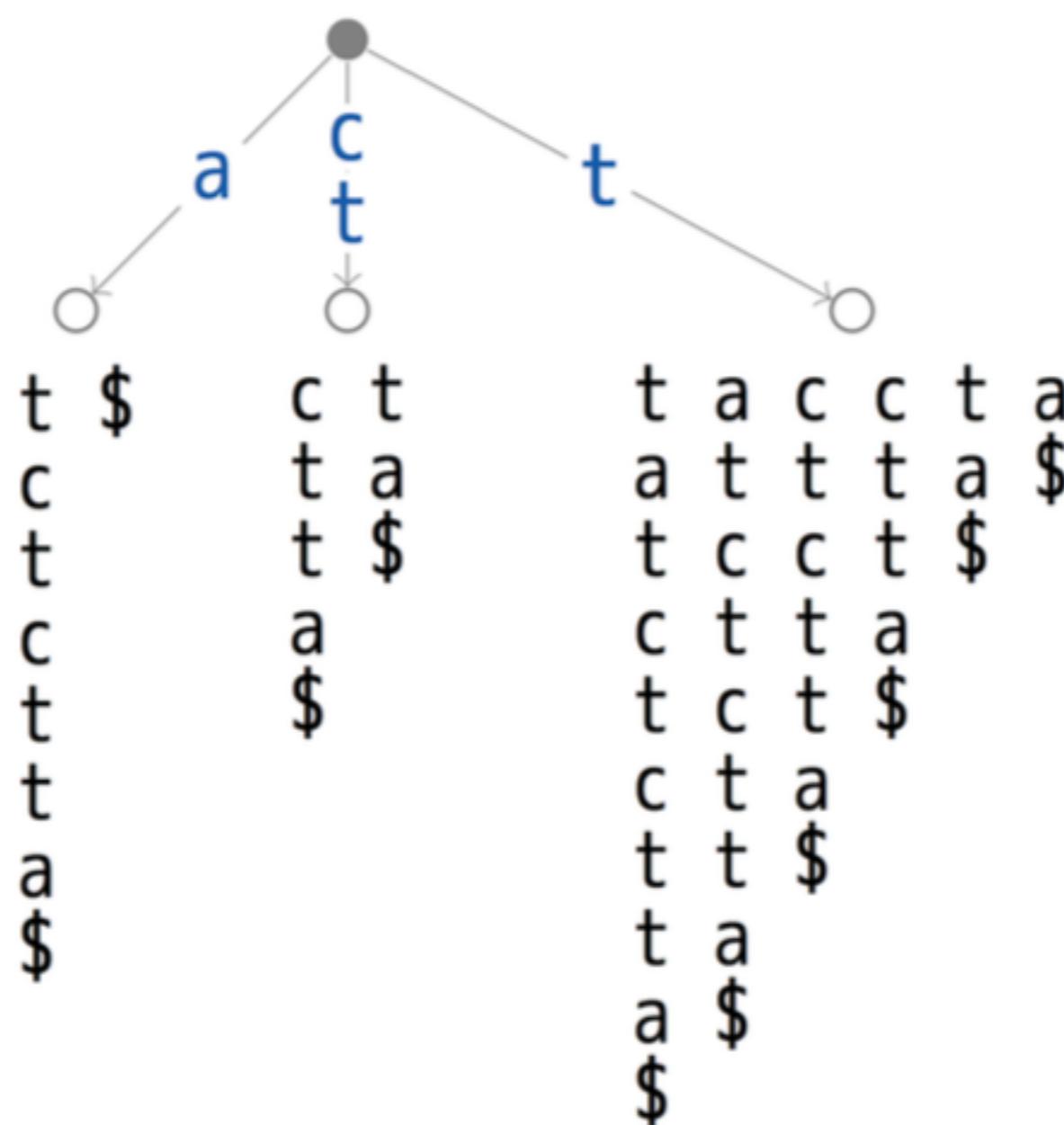
$s = ttatctcta\$$

suffixes are  
read top-to-bottom



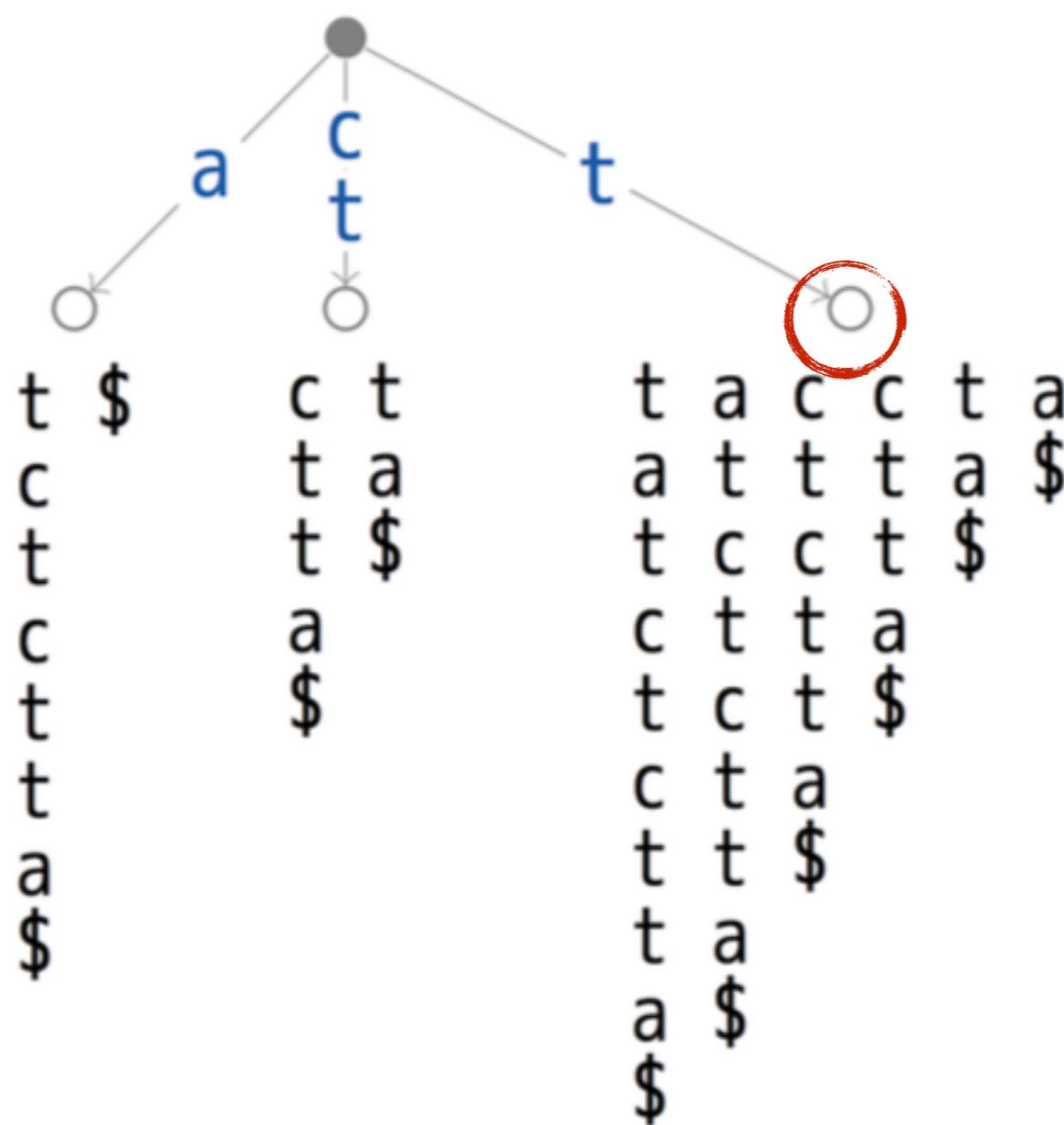
# WOTD Example

$s = ttatctctta$



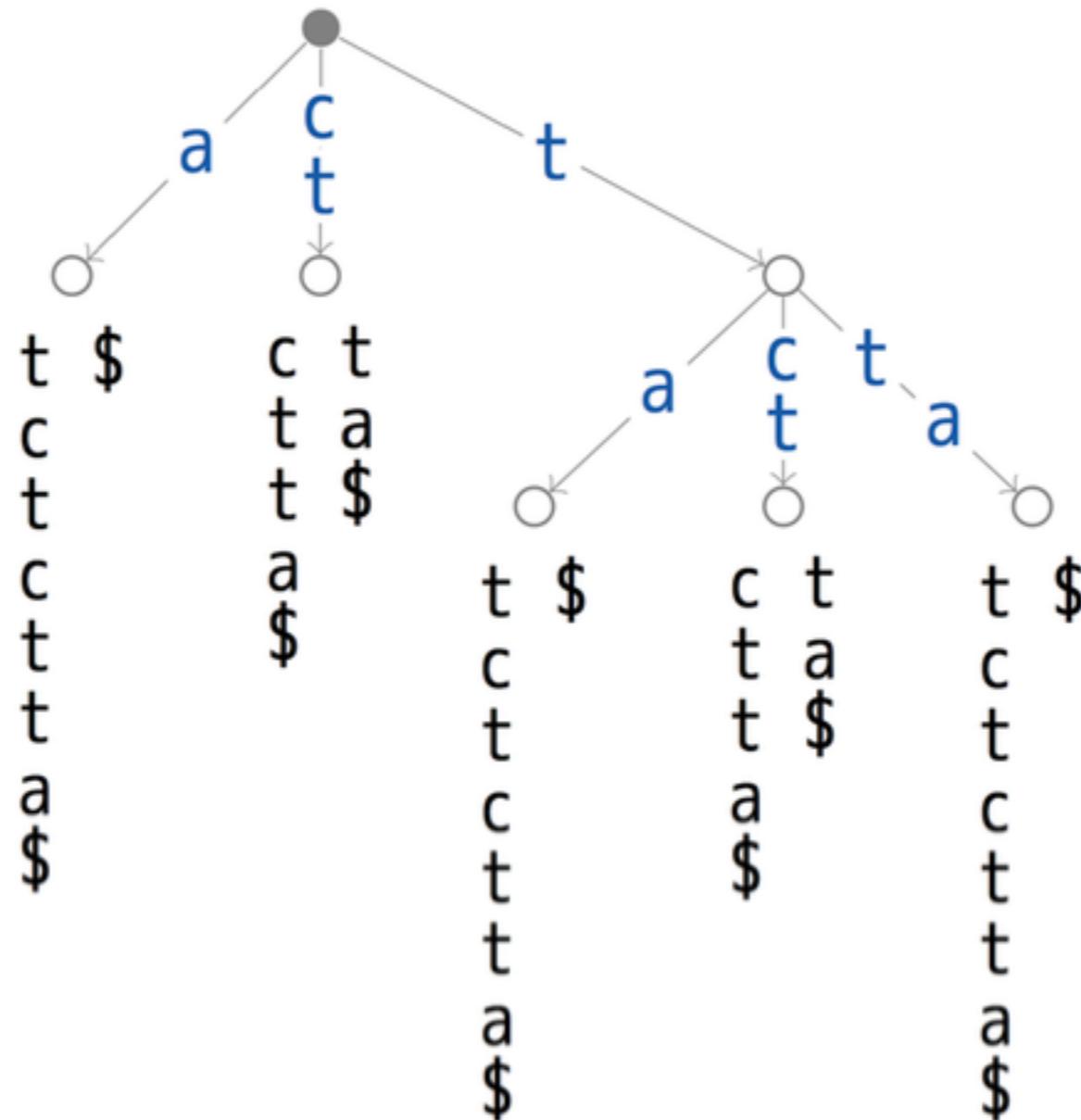
# WOTD Example

$s = ttatctctta$



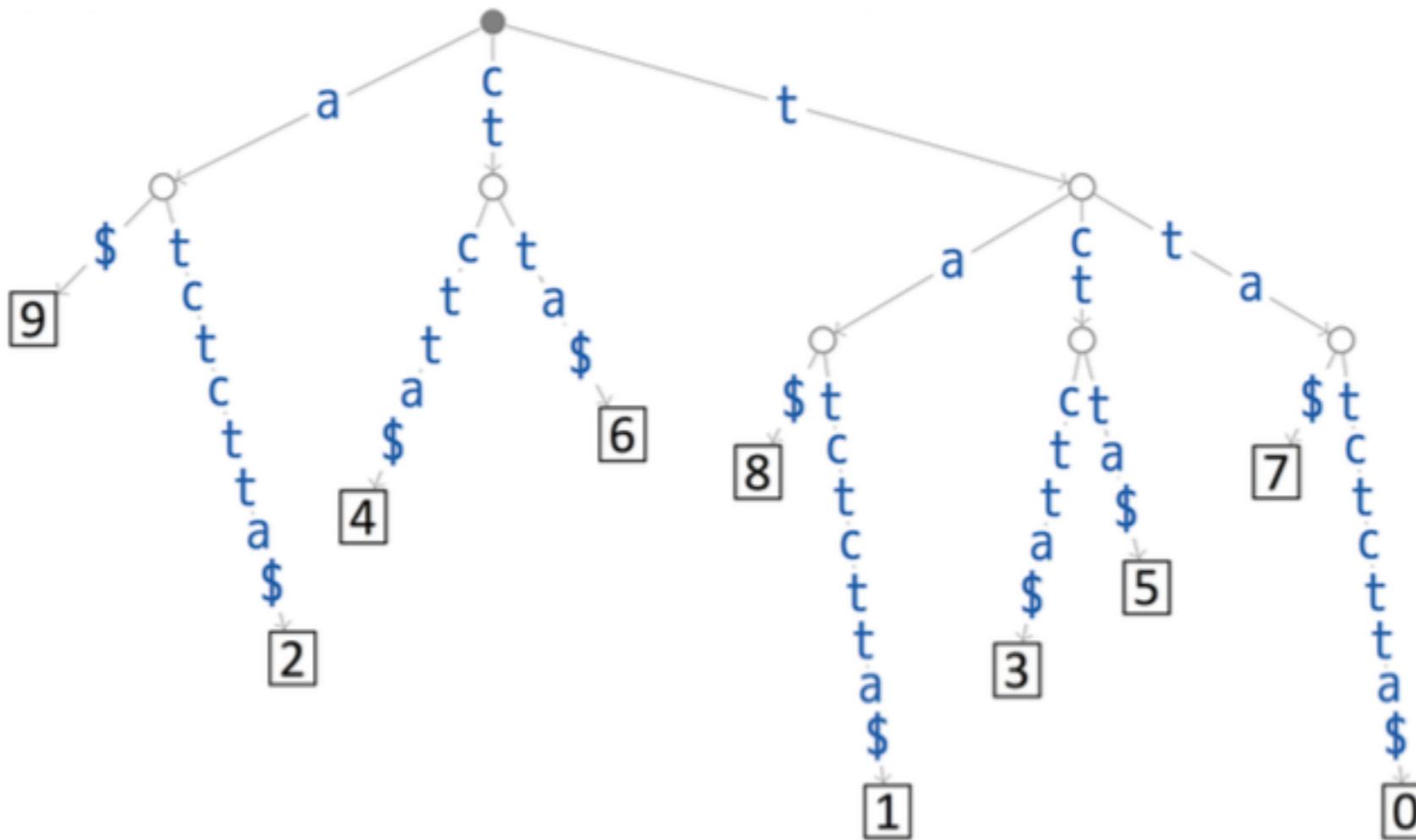
# WOTD Example

$s = ttatctctta$



# WOTD Example

$s = ttatctctta$



# WOTD Properties

- Worst case time still  $\in O(|T|^2)$
- Expected case time  $\in O(|T| \log |T|)$
- Write-only property & recursive construction lends itself well to parallelism
- Good caching properties (locality of reference for substrings belonging to a subtree)
- Top-down construction order allows lazy construction as discussed in:

Giegerich, Robert, Stefan Kurtz, and Jens Stoye. "Efficient implementation of lazy suffix trees." *Software: Practice and Experience* 33.11 (2003): 1035-1049.