

Suffix-based indexing

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Introduction to suffix indexing structures

- So far we've discussed substring indices
- Today we'll cover data structures that index the suffixes of a string: suffix tries, suffix tree, suffix array

Tries

A trie (pronounced “try”) is a 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 a *set* or a *map* where keys are strings

Tries: example

Make this map into a trie:

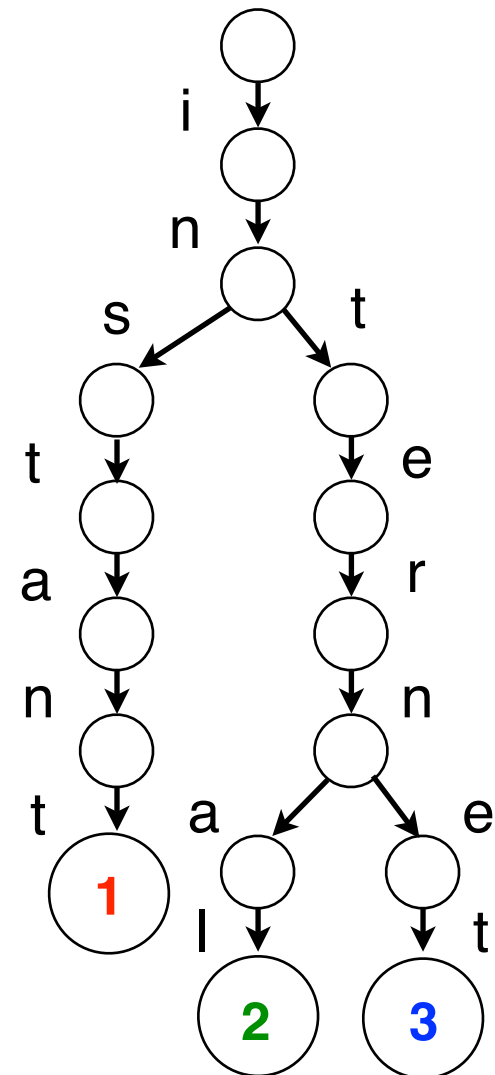
Key	Value
instant	1
internal	2
internet	3

The smallest tree such that:

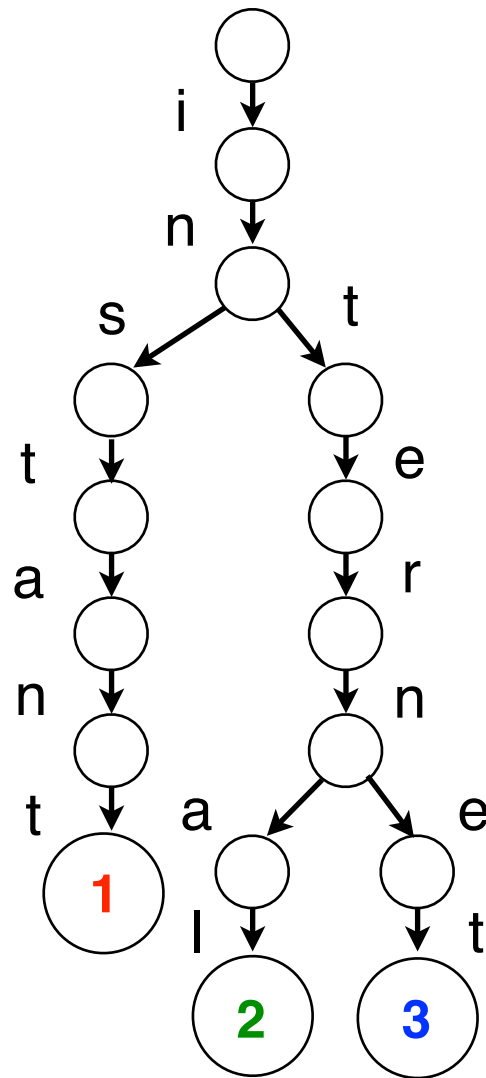
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Tries: example



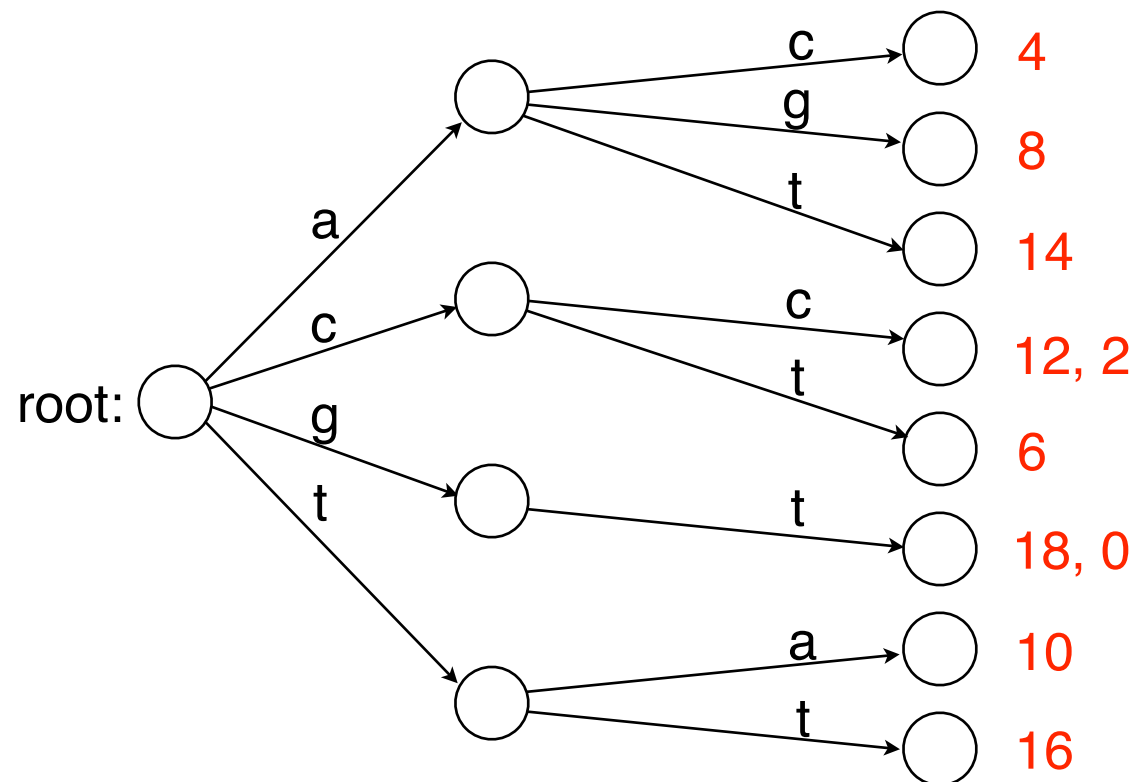
Checking for presence of a key P ,
where $n = |P|$, is **$O(n)$** time

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

Tries: another example

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

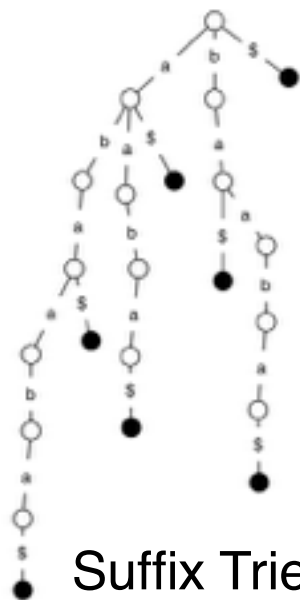
ac	4
ag	8
at	14
cc	12
cc	2
ct	6
gt	18
gt	0
ta	10
tt	16



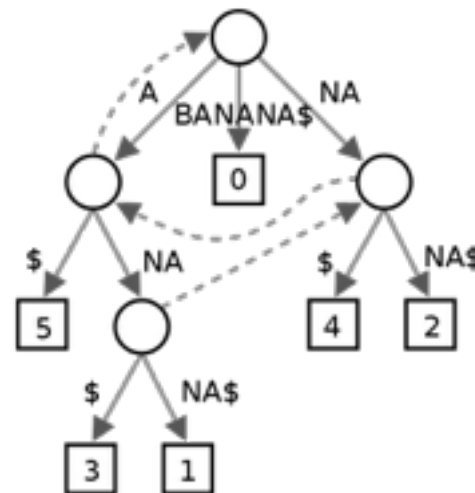
Indexing with suffixes

Until now, our indexes have been 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	ANA\$
1	ANANA\$
0	BANANA\$
4	NA\$
2	NANA\$

Suffix Array

\$	B	A	N	A	N	A
A	\$	B	A	N	A	N
A	N	A	\$	B	A	N
A	N	A	N	A	\$	B
B	A	N	A	N	A	\$
N	A	\$	B	A	N	A
N	A	N	A	\$	B	A

FM Index

Suffix trie

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

T :

```
GTTATAGCTGATCGCGGGCGTAGCGG$
GTTATAGCTGATCGCGGGCGTAGCGG$
TTATAGCTGATCGCGGGCGTAGCGG$
TATAGCTGATCGCGGGCGTAGCGG$
ATAGCTGATCGCGGGCGTAGCGG$
TAGCTGATCGCGGGCGTAGCGG$
AGCTGATCGCGGGCGTAGCGG$
GCTGATCGCGGGCGTAGCGG$
CTGATCGCGGGCGTAGCGG$
TGATCGCGGGCGTAGCGG$
GATCGCGGGCGTAGCGG$
ATCGCGGGCGTAGCGG$
TCGCGGGCGTAGCGG$
CGCGGGCGTAGCGG$
GCGGGCGTAGCGG$
CGGCGTAGCGG$
GGCGTAGCGG$
GCGTAGCGG$
CGTAGCGG$
GTAGCGG$
TAGCGG$
AGCGG$
GCGG$
CGG$
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 :

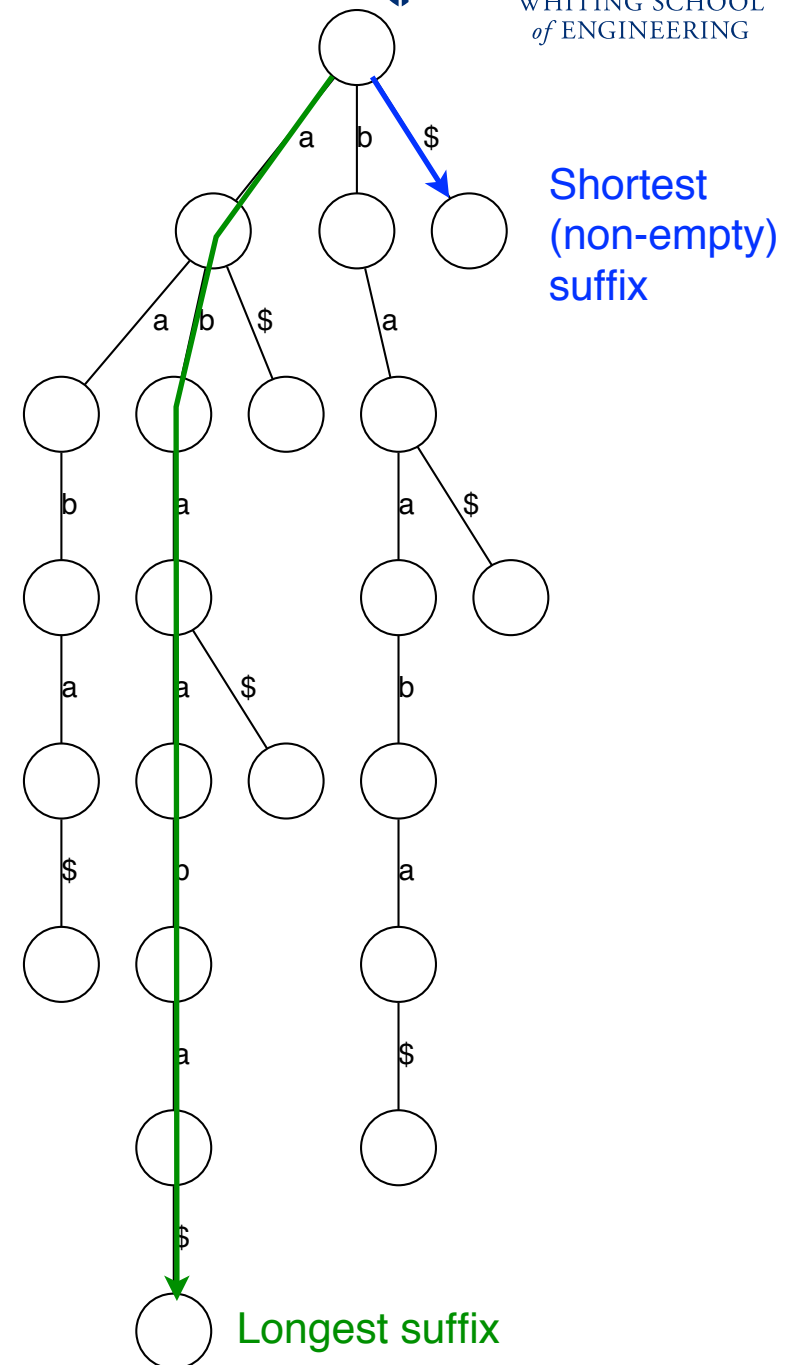
```
GTTATAGCTGATCGCGGCGTAGCGG$
GTTATAGCTGATCGCGGCGTAGCGG$
TTATAGCTGATCGCGGCGTAGCGG$
TATAGCTGATCGCGGCGTAGCGG$
ATAGCTGATCGCGGCGTAGCGG$
TAGCTGATCGCGGCGTAGCGG$
AGCTGATCGCGGCGTAGCGG$
GCTGATCGCGGCGTAGCGG$
CTGATCGCGGCGTAGCGG$
TGATCGCGGCGTAGCGG$
GATCGCGGCGTAGCGG$
ATCGCGGCGTAGCGG$
TCGCGGCGTAGCGG$
CGCGGCGTAGCGG$
GCGGCGTAGCGG$
CGGCGTAGCGG$
GGCGTAGCGG$
GCGTAGCGG$
```

Suffix trie

T : abaaba $T\$$: 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 \$?

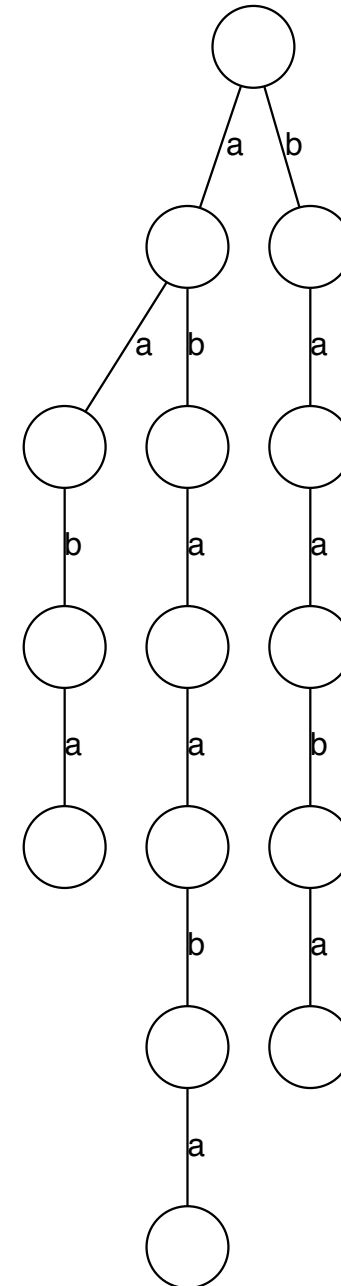


Suffix trie

T: abaaba

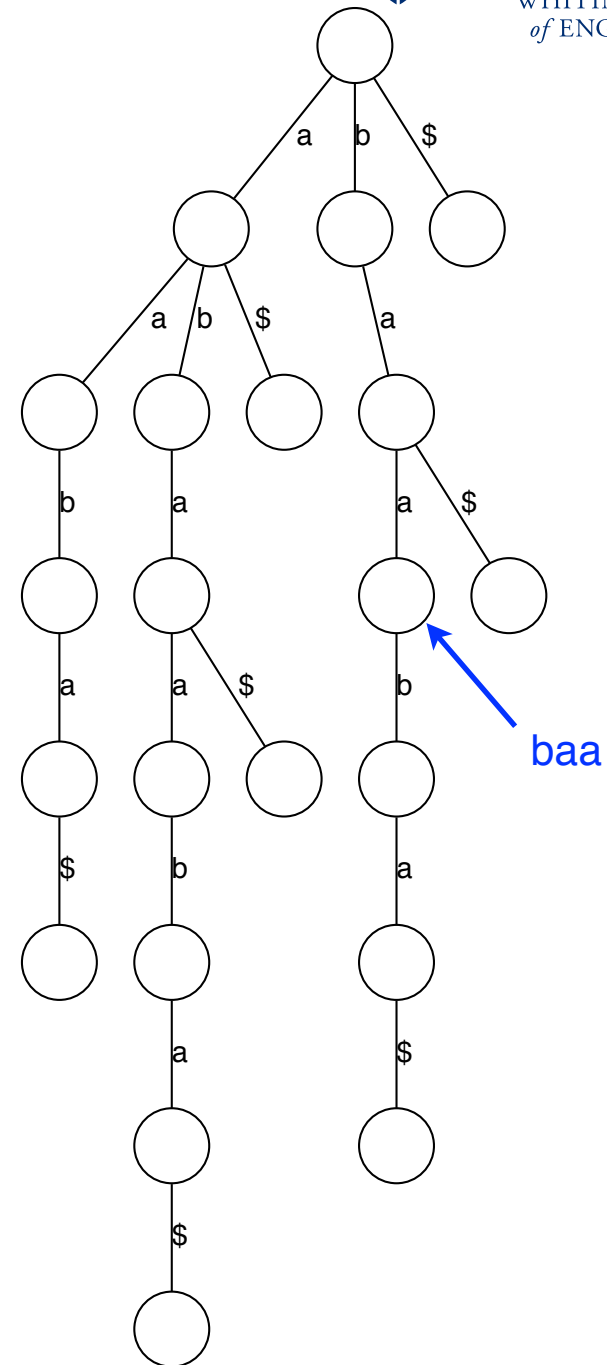
Each path from root to leaf represents a suffix; each suffix is represented by some path from root to leaf

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



Suffix trie

We can think of nodes as having **labels**, where the label spells out characters on the path from the root to the node





Suffix trie

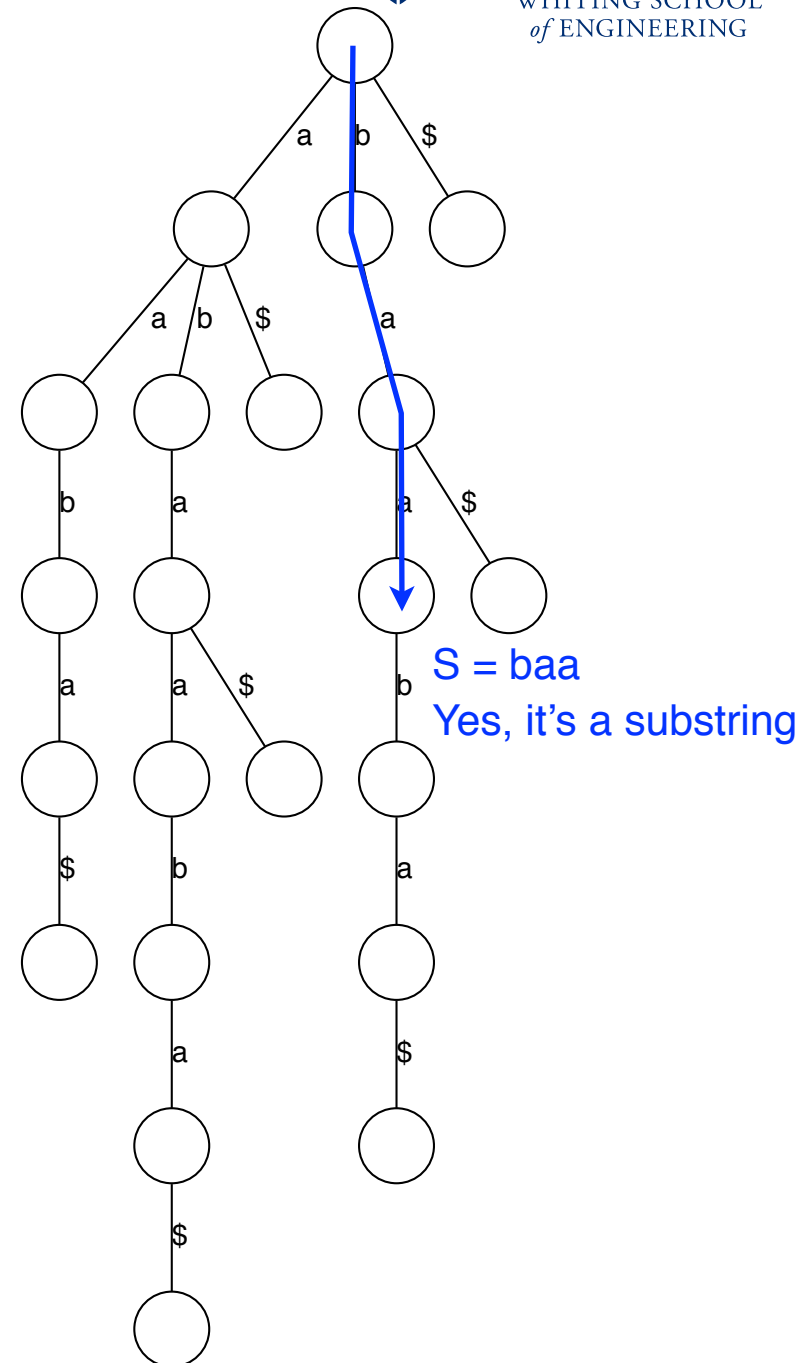
How do we check whether a string S is a substring of T ?

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

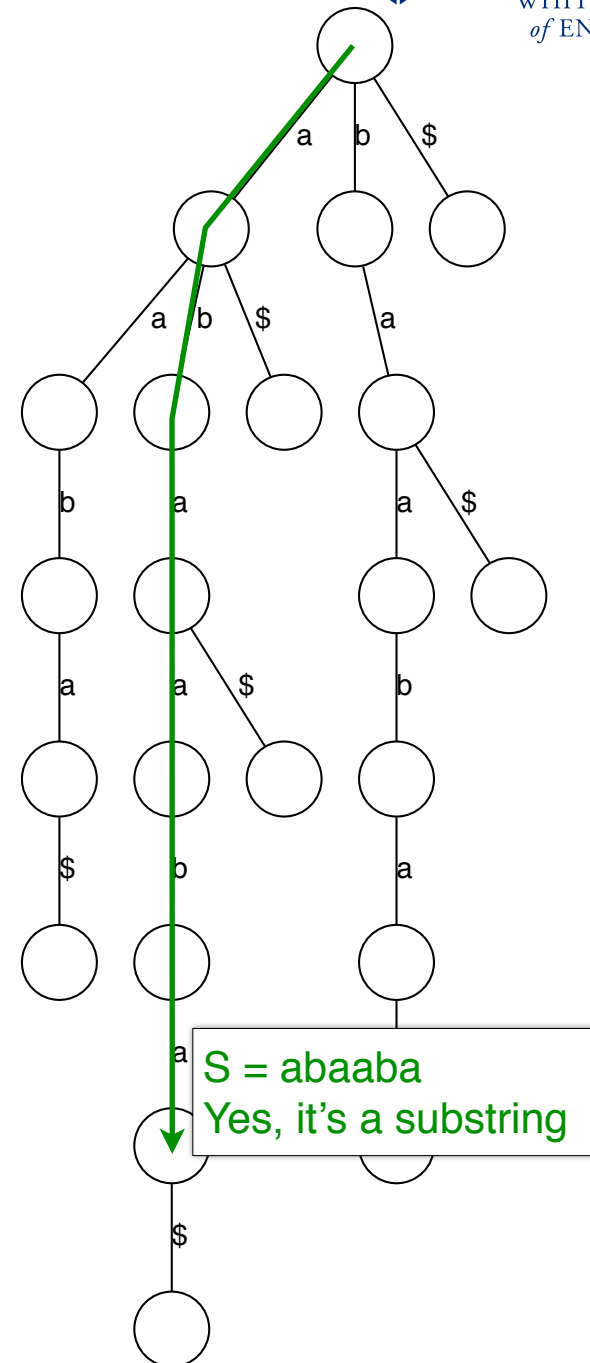
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Suffix trie

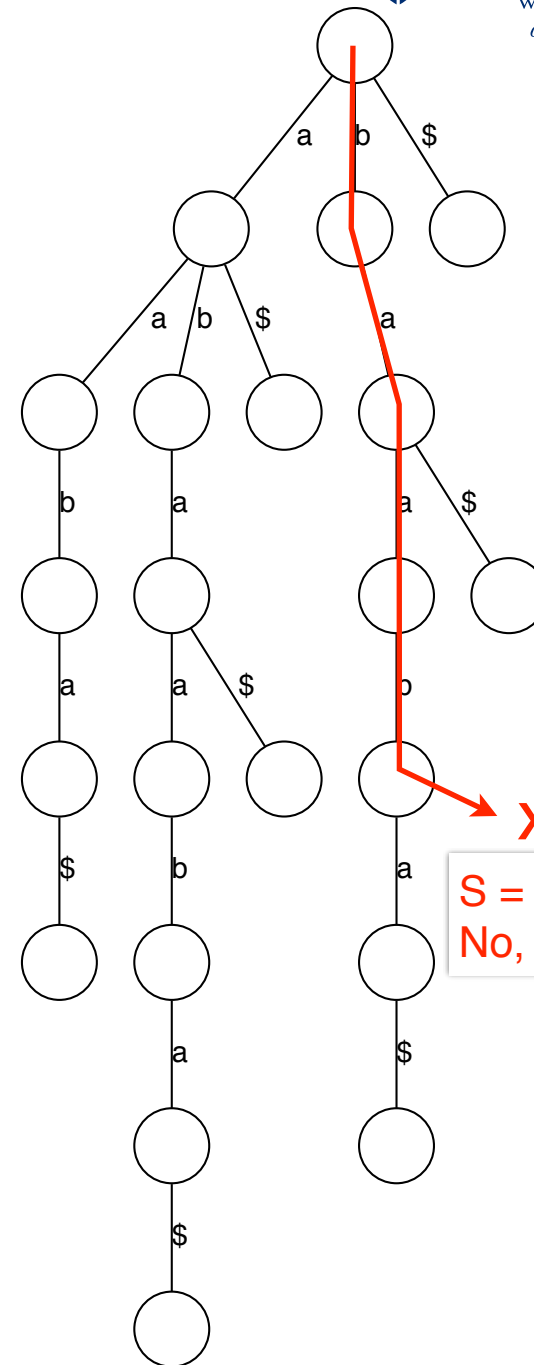
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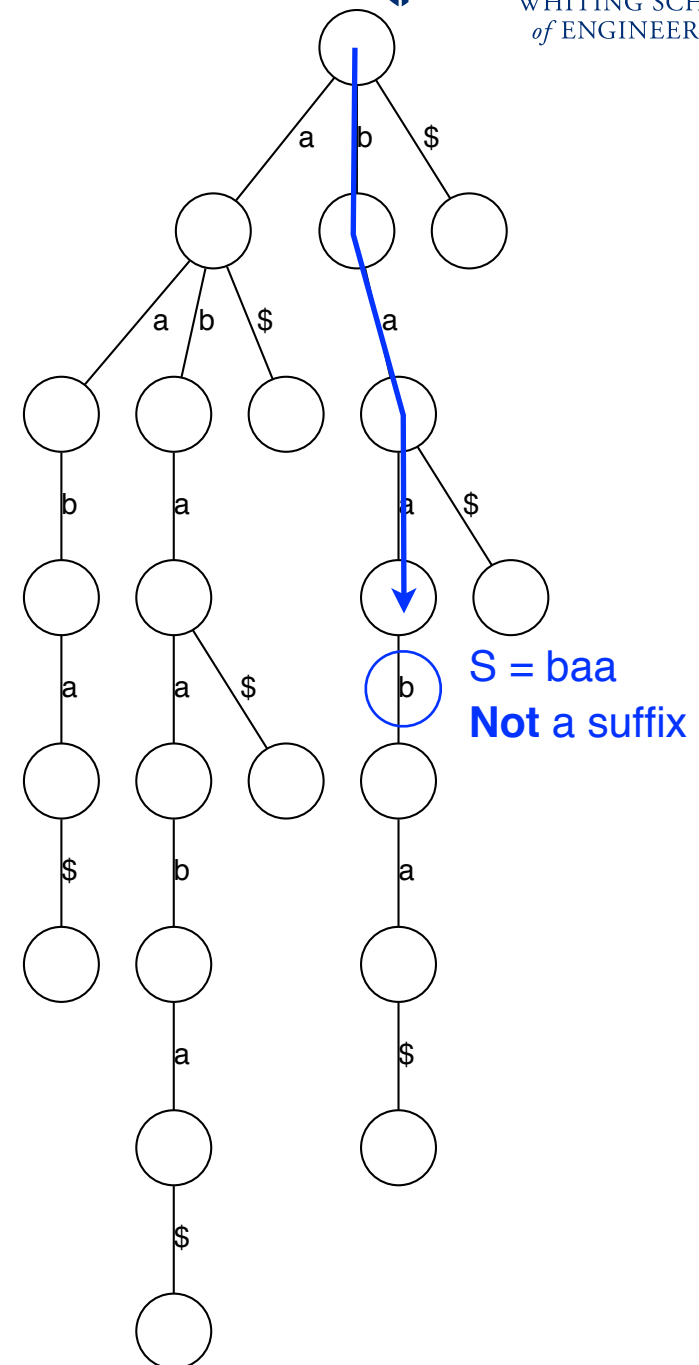
S = baabb
No, not a substring



Suffix trie

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

Same procedure as for substring, but additionally check whether the final node in the walk has an outgoing edge labeled \$

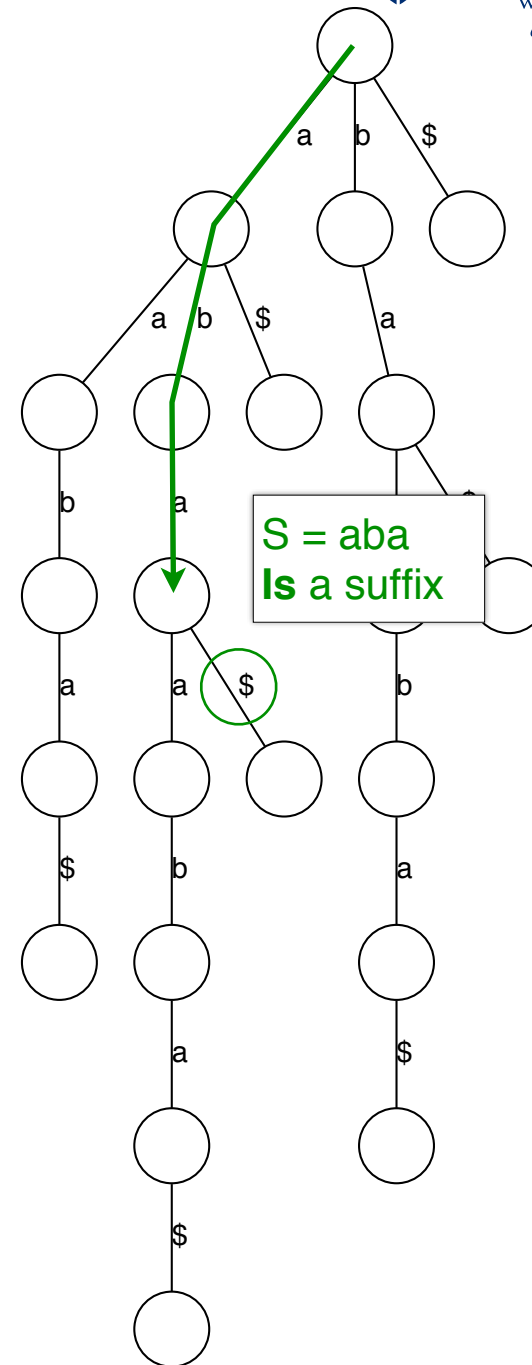




Suffix trie

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

Same procedure as for substring, but additionally check whether the final node in the walk has an outgoing edge labeled $\$$

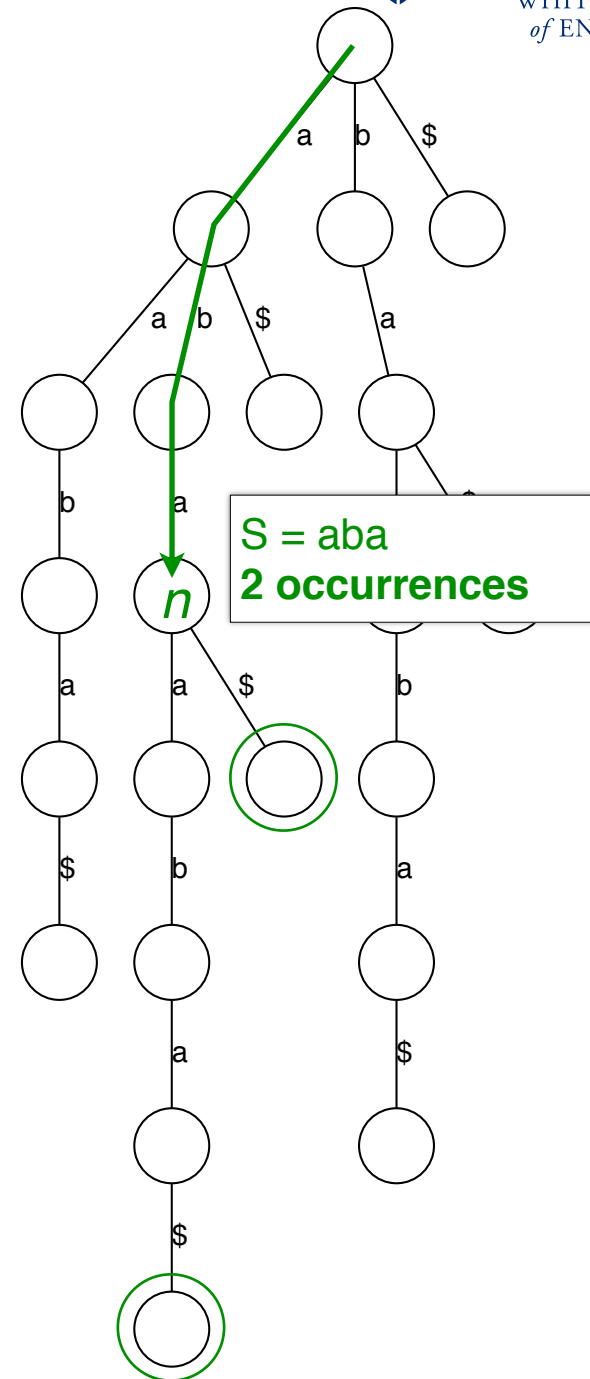


Suffix trie

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

Follow path corresponding to S .
 Either we fall off, in which case
 answer is 0, or we end up at node n
 and the answer = # of leaf nodes in
 the subtree rooted at n .

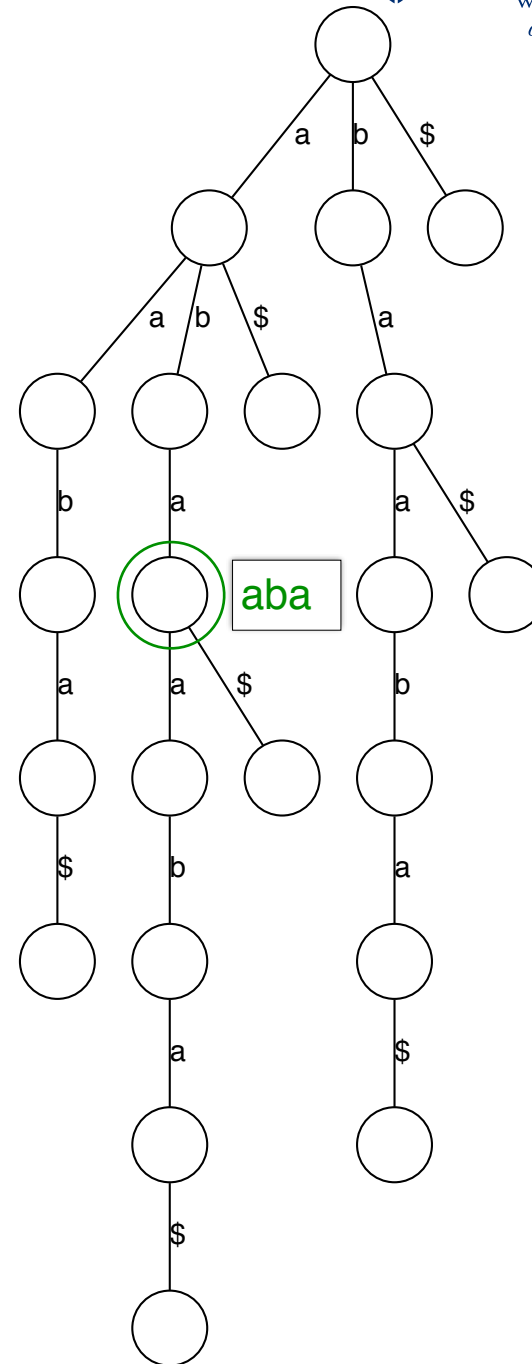
Leaves can be counted with depth-first traversal.



Suffix trie

How do we find the **longest repeated substring** of T ?

Find the deepest node with more than one child

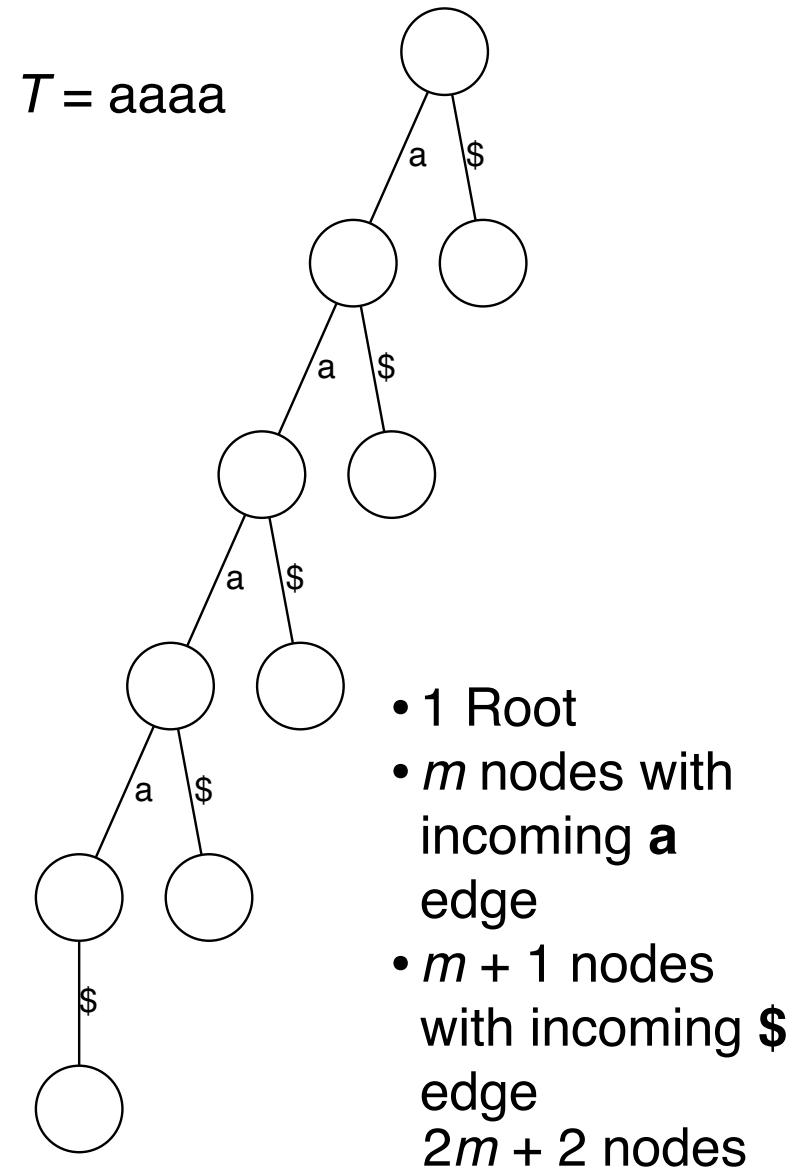


Suffix trie

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 ?

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



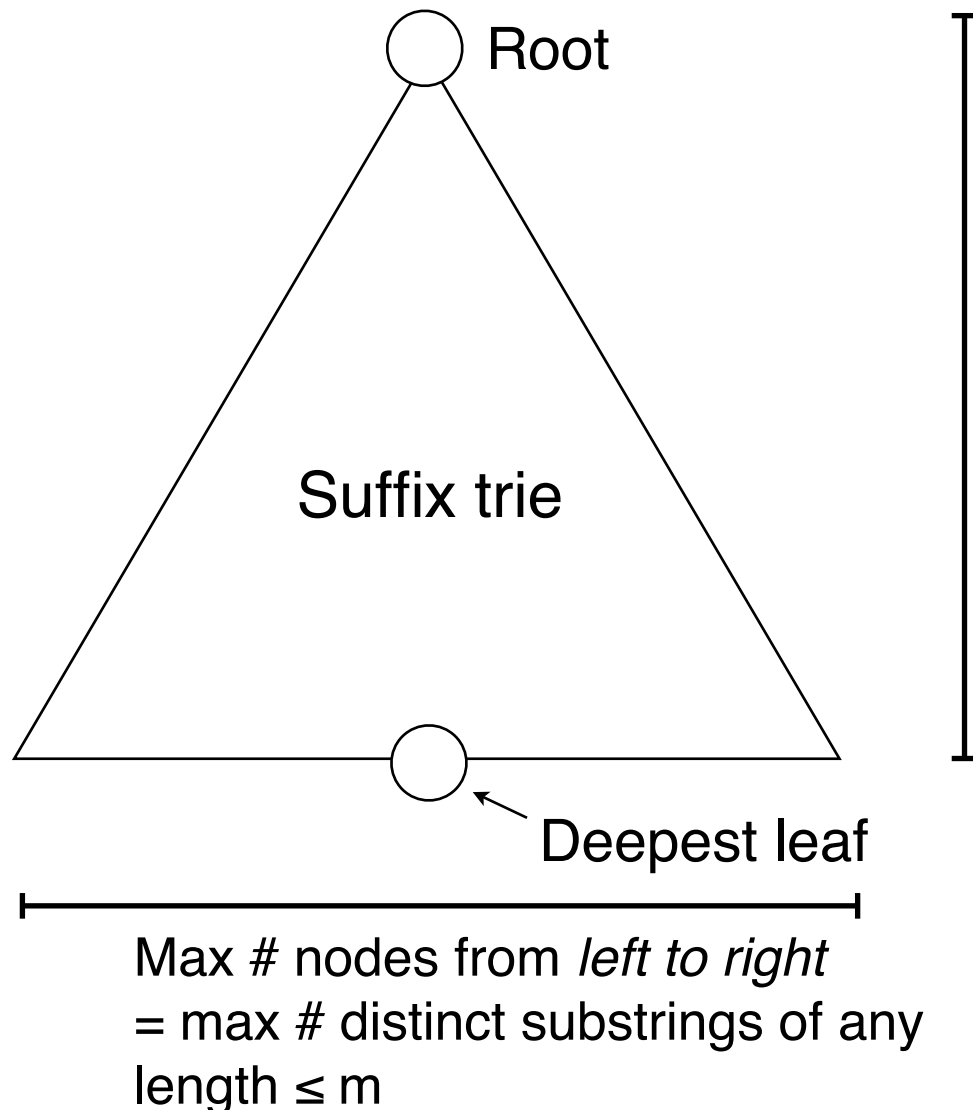
Yes: $a^n b^n$

- $$n^2 + 4n + 2 \text{ nodes, where } m = 2n$$



Suffix trie: upper bound on size

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



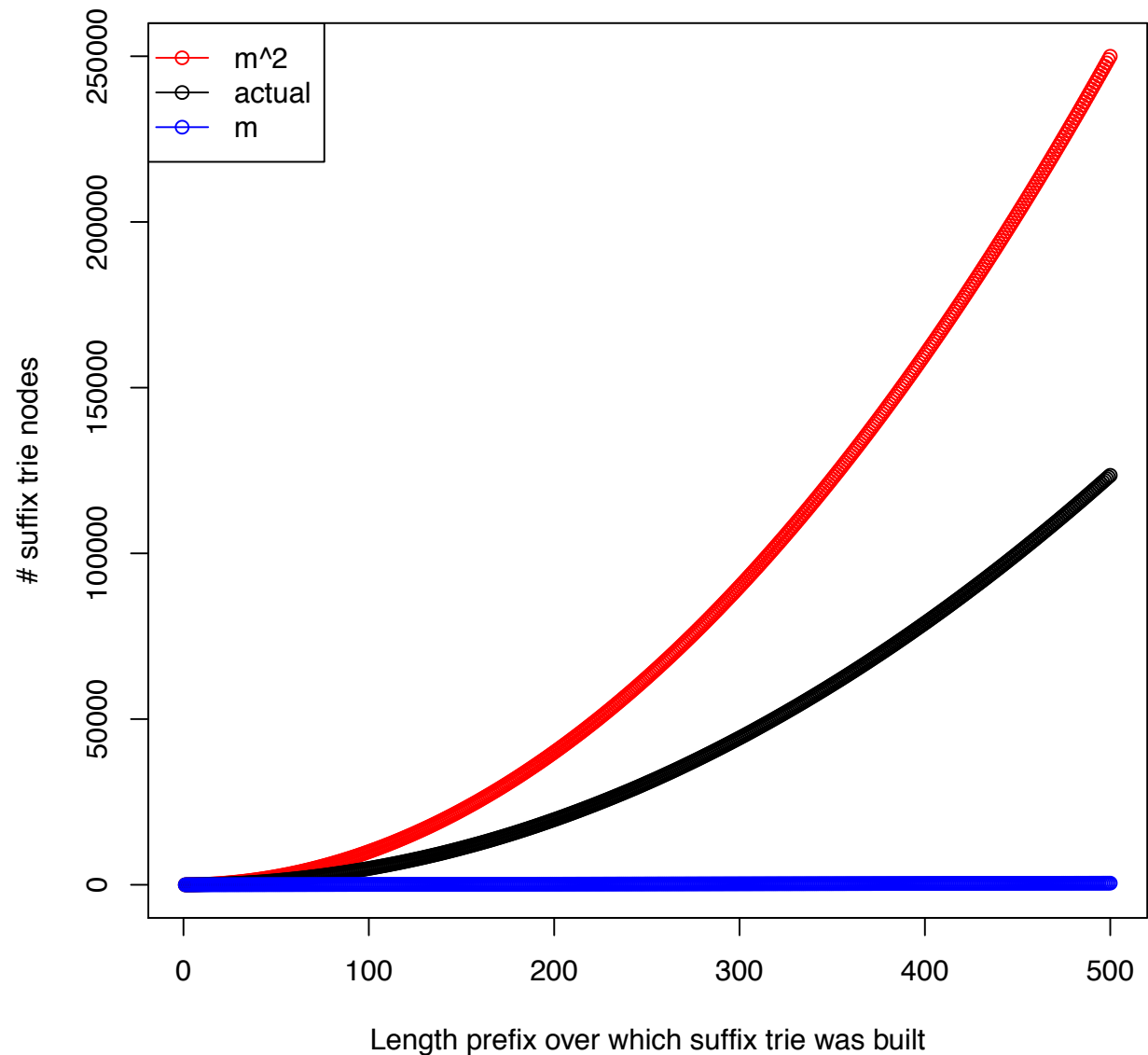
Max # nodes from *top to bottom*
= length of longest suffix + 1
= $m + 1$

$O(m^2)$ 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



[illegible]

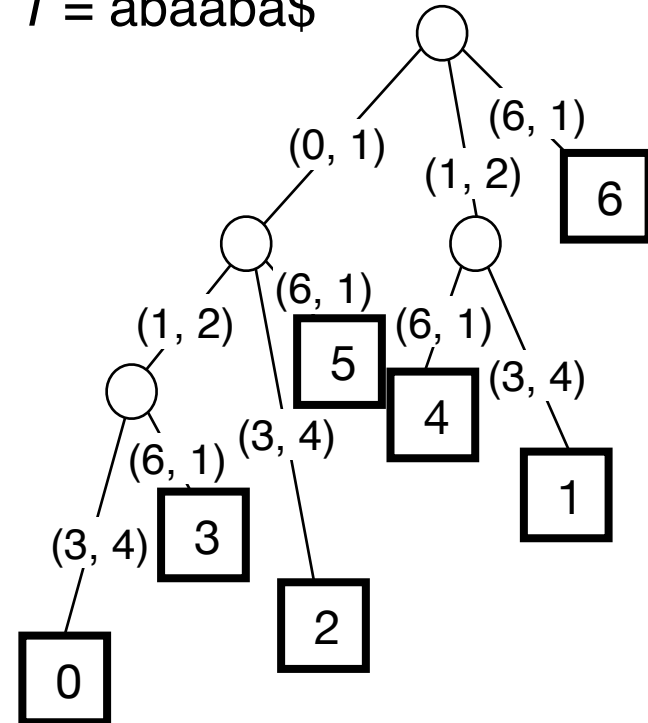
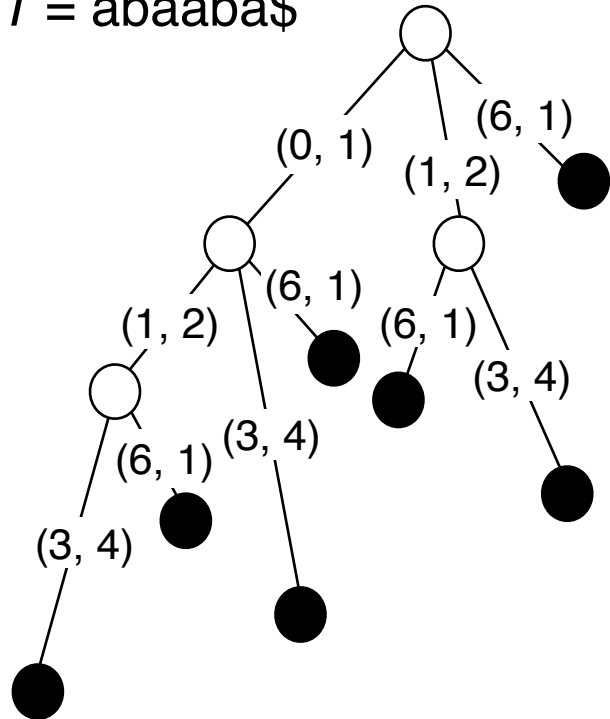
Reduces # nodes, edges,
guarantees internal nodes have >1
child

$\leq 2m - 1$ nodes total, or $O(m)$ nodes

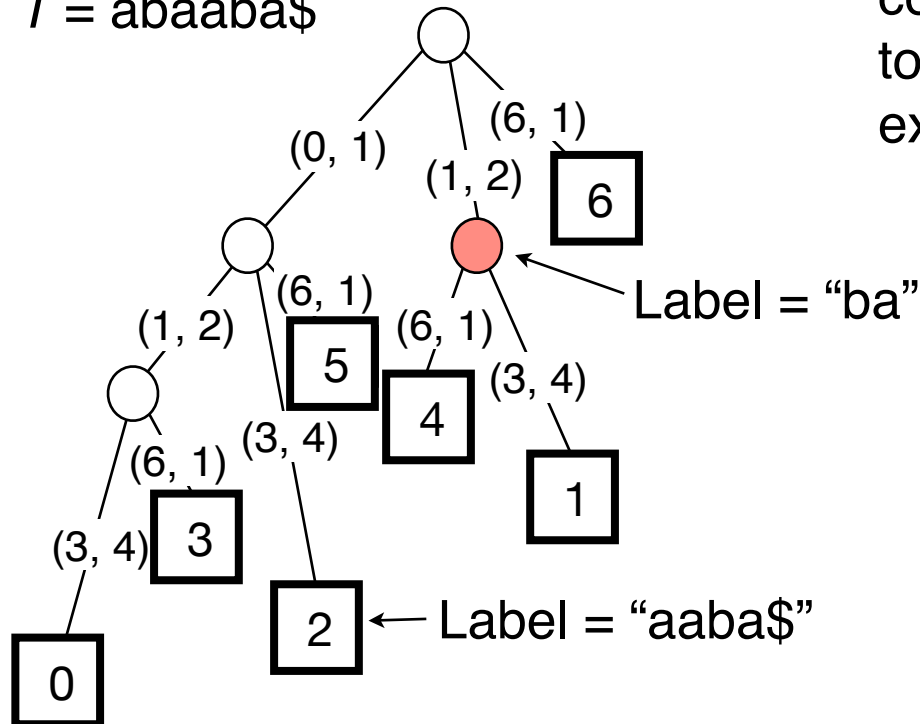
Is the total size $O(m)$ now? **No**: total length of edge labels is quadratic in m

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



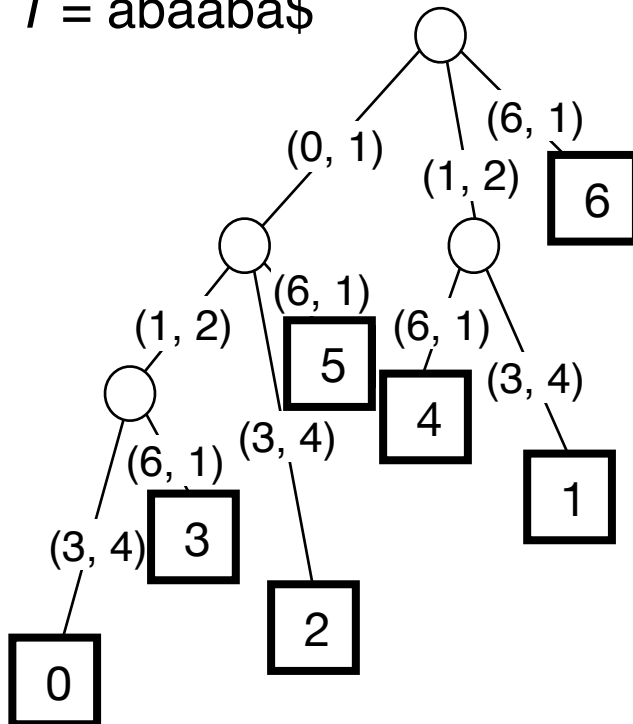


Again, each node's *label* equals the concatenated edge labels from the root to the node. These aren't stored explicitly.



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

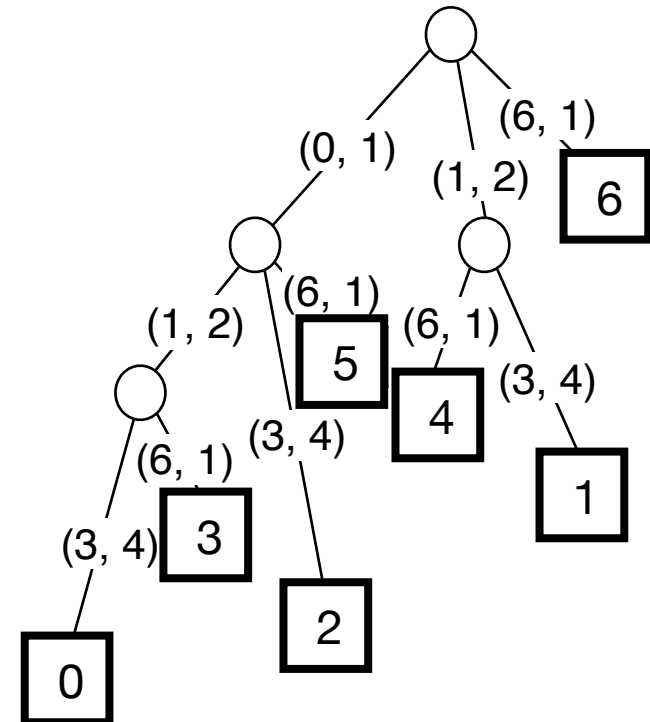
Suffix tree: building

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

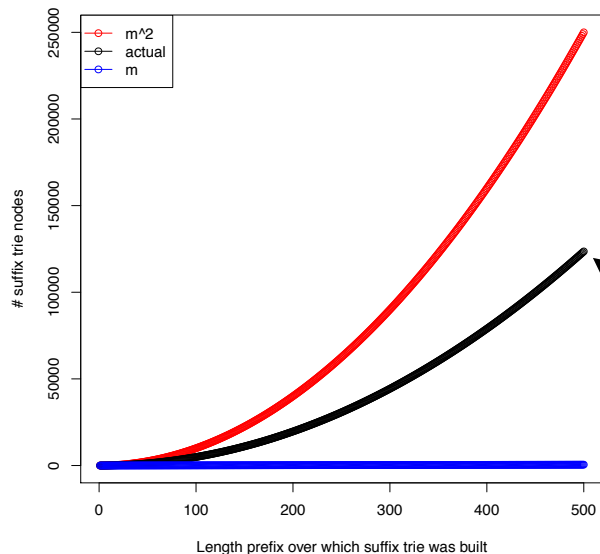


Suffix tree: actual growth

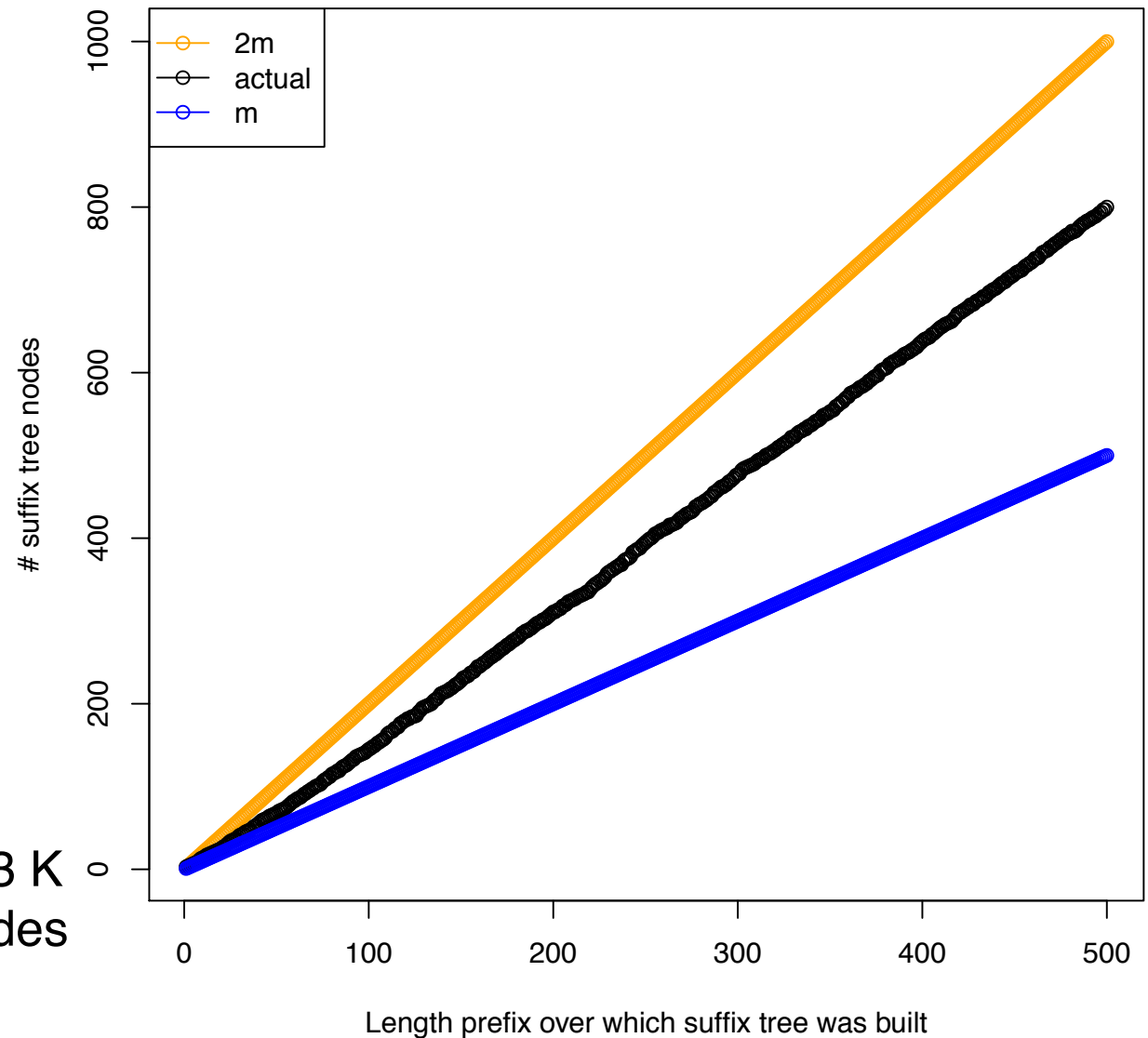
Built suffix trees for the first 500 prefixes of the lambda phage virus genome

Black curve shows # nodes increasing with prefix length

Compare with suffix trie:



123 K
nodes



Suffix tree: building

Method of choice: Ukkonen's algorithm

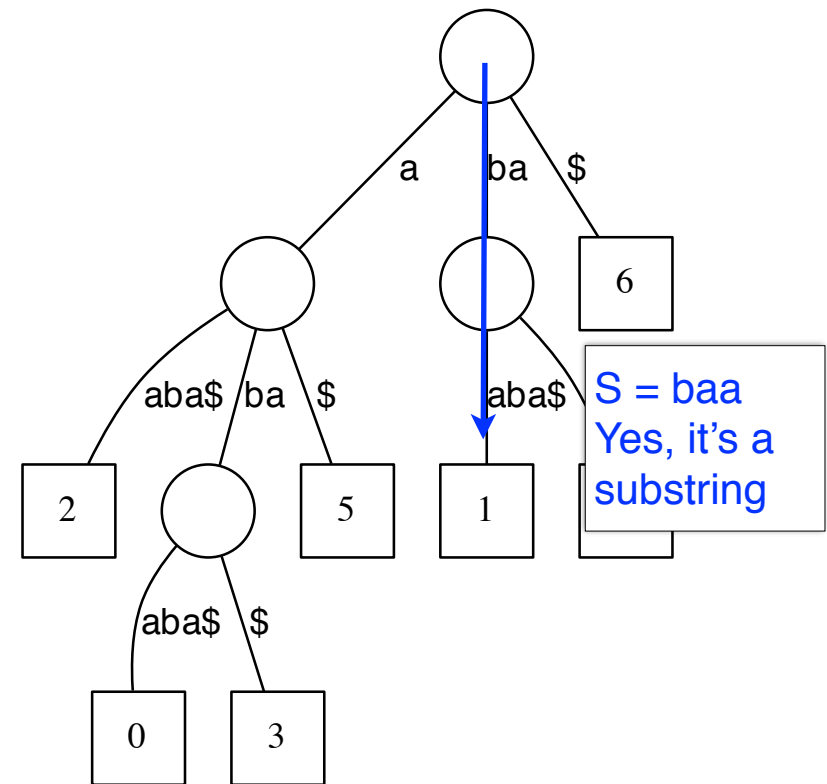
Ukkonen, Esko. "On-line construction of suffix trees."
Algorithmica 14.3 (1995): 249-260.

$O(m)$ 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

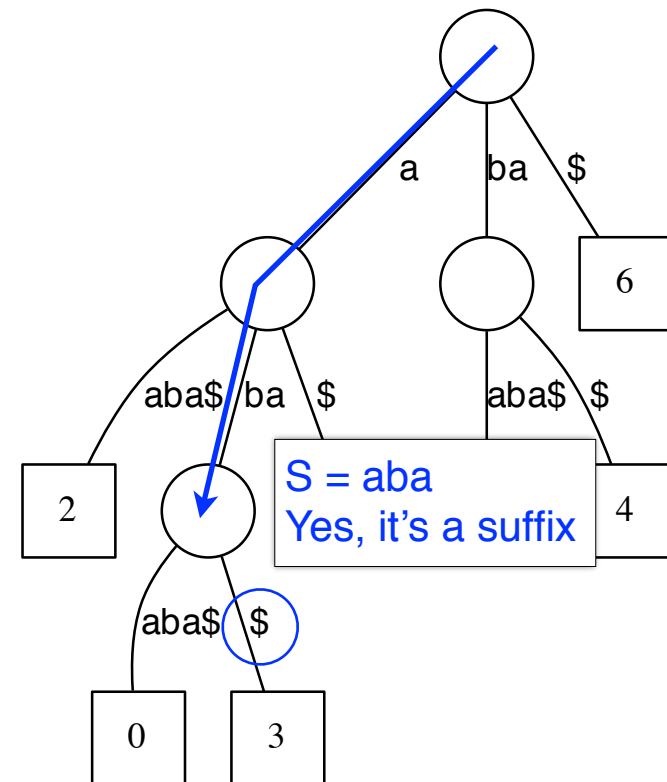
Essentially same procedure as for suffix trie, except we have to deal with coalesced edges



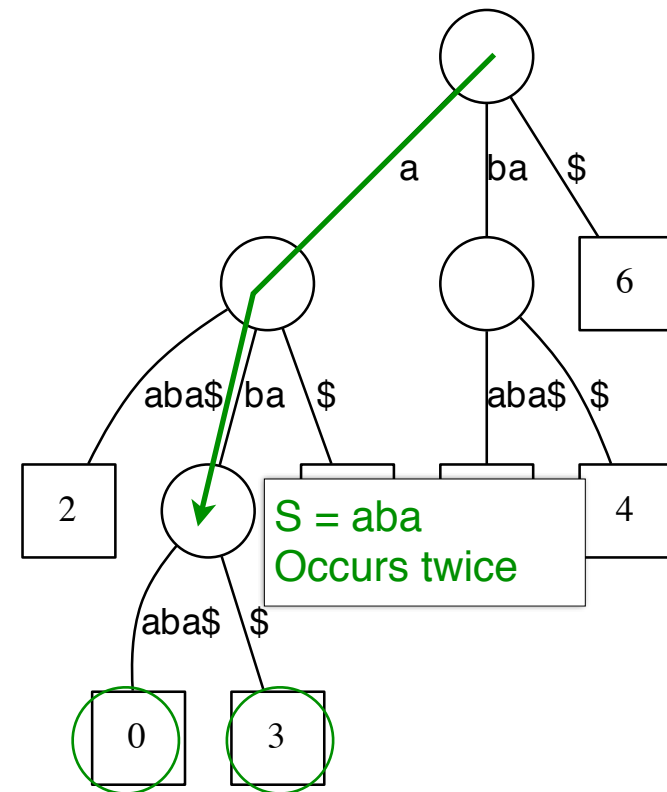
Suffix tree

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



Same procedure as for suffix trie



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

 $O(n)$ $O(k)$

abaaba
ab ab

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**

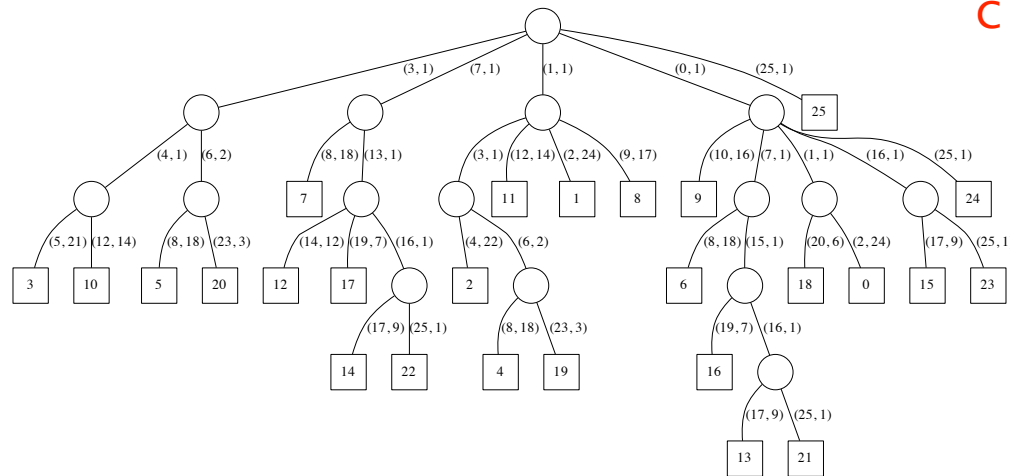
Kurtz, Stefan. "Reducing the space requirement of suffix trees." *Software Practice and Experience* 29.13 (1999): 1149-1171.

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

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



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

GTTATAGCTGATCGCGGCGTAGCGG\$
 GTTATAGCTGATCGCGGCGTAGCGG\$
 TTATAGCTGATCGCGGCGTAGCGG\$
 TATAGCTGATCGCGGCGTAGCGG\$
 ATAGCTGATCGCGGCGTAGCGG\$
 TAGCTGATCGCGGCGTAGCGG\$
 AGCTGATCGCGGCGTAGCGG\$
 GCTGATCGCGGCGTAGCGG\$
 CTGATCGCGGCGTAGCGG\$
 TGATCGCGGCGTAGCGG\$
 GATCGCGGCGTAGCGG\$
 ATCGCGGCGTAGCGG\$
 TCGCGGCGTAGCGG\$
 CGCGGCGTAGCGG\$
 GCGGCGTAGCGG\$
 CGGCGTAGCGG\$
 GCGTAGCGG\$
 CGTAGCGG\$
 GTAGCGG\$
 TAGCGG\$
 AGCGG\$
 GCGG\$
 CGG\$
 GG\$
 G\$

m chars

$m(m+1)/2$
chars

Suffix array

$T\$ = \text{abaaba\$}$ ← As with suffix tree,
 T is part of index

SA(T) =
(SA = "Suffix Array")

6	\$] $m + 1$ integers
5	a \$	
2	a a b a \$	
3	a b a \$	
0	a b a a b a \$	
4	b a \$	
1	b a a b a \$	

Suffix array of T is an array of integers in $[0, m]$ specifying the lexicographic order of $T\$$'s suffixes

Suffix array

$O(m)$ space, same as suffix tree. Is constant factor smaller?

32-bit integer can distinguish characters in the human genome, so suffix array is ~12 GB, smaller than MUMmer's 47 GB suffix tree.

Suffix array: querying

Is P a substring of T ?

1. For P to be a substring, it must be a prefix of ≥ 1 of T 's suffixes
2. Suffixes sharing a prefix are consecutive in the suffix array

Use binary search

6	\$
5	a \$
2	a a b a \$
3	a b a \$
0	a b a a b a \$
4	b a \$
1	b a a b a \$

Suffix array: binary search

Python has `bisect` module for binary search

`bisect.bisect_left(a, x)`: Leftmost offset where we can insert `x` into `a` to maintain sorted order. `a` is already sorted!

`bisect.bisect_right(a, x)`: Like `bisect_left`, but returning *rightmost* instead of leftmost offset

```
from bisect import bisect_left, bisect_right

a = [1, 2, 3, 3, 3, 4, 5]
print(bisect_left(a, 3), bisect_right(a, 3)) # output: (2, 5)

a = [2, 4, 6, 8, 10]
print(bisect_left(a, 5), bisect_right(a, 5)) # output: (2, 2)
```

Python example: <http://nbviewer.ipython.org/6753277>

Suffix array: binary search

We can straightforwardly use binary search to find a range of elements in a sorted list that *equal* some query:

```
from bisect import bisect_left, bisect_right

strls = ['a', 'awkward', 'awl', 'awls', 'axe', 'axes', 'bee']

# Get range of elements that equal query string 'awl'
st, en = bisect_left(strls, 'awl'), bisect_right(strls, 'awl')

print(st, en) # output: (2, 3)
```

Python example: <http://nbviewer.ipython.org/6753277>

Suffix array: binary search

Can also use binary search to find a range of elements in a sorted list with some query as a *prefix*:

```
from bisect import bisect_left, bisect_right

strls = ['a', 'awkward', 'awl', 'awls', 'axe', 'axes', 'bee']

# Get range of elements with 'aw' as a prefix
st, en = bisect_left(strls, 'aw'), bisect_left(strls, 'ax')

print(st, en) # output: (1, 4)
```

Python example: <http://nbviewer.ipython.org/6753277>

Suffix array: binary search

We can do the same thing for a sorted list of suffixes:

```
from bisect import bisect_left, bisect_right

t = 'abaaba$'
suffixes = sorted([t[i:] for i in xrange(len(t))])

st, en = bisect_left(suffixes, 'aba'),
        bisect_left(suffixes, 'abb')

print(st, en) # output: (3, 5)
```

6	\$
5	a \$
2	a a b a \$
3	a b a \$
0	a b a a b a \$
4	b a \$
1	b a a b a \$

Python example: <http://nbviewer.ipython.org/6753277>

Suffix array: querying

Is P a substring of T ?

Do binary search, check whether P is a prefix of the suffix there

How many times does P occur in T ?

Two binary searches yield the range of suffixes with P as prefix; size of range equals # times P occurs in T

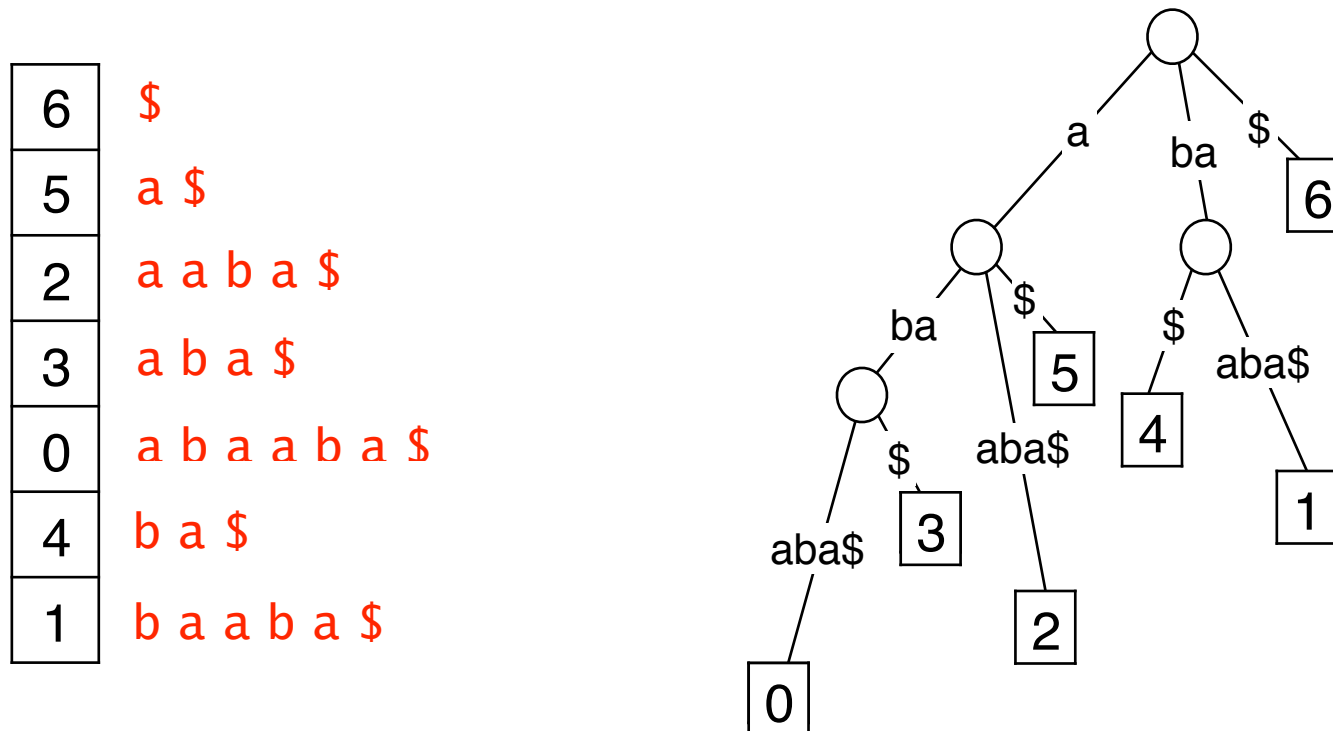
Worst-case time bound?

$O(\log_2 m)$ bisections, $O(n)$ comparisons per bisection, so $O(n \log m)$

6	\$
5	a \$
2	a a b a \$
3	a b a \$
0	a b a a b a \$
4	b a \$
1	b a a b a \$

Suffix array: querying

Contrast suffix array: $O(n \log m)$ with suffix tree: $O(n)$



But we can improve bound for suffix array...

Suffix array: querying

Consider further: binary search for suffixes with P as a prefix

Assume there's no \$ in P . So P can't be equal to a suffix.

Initialize $l = 0$, $c = \text{floor}(m/2)$ and $r = m$ (just past last elt of SA)

\uparrow \uparrow \uparrow
“left” “center” “right”

Notation: We'll use $SA[l]$ to refer to the suffix corresponding to suffix-array element l . We could write $\tau[SA[l]:]$, but that's too verbose.

Throughout the search, invariant is maintained:

$$SA[l] < P < SA[r]$$

Suffix array: querying

Throughout search, invariant is maintained:

$$SA[l] < P < SA[r]$$

What do we do at each iteration?

Let $c = \text{floor}((r + l) / 2)$

If $P < SA[c]$, either stop or let $r = c$ and iterate

If $P > SA[c]$, either stop or let $l = c$ and iterate

When to stop?

$P < SA[c]$ and $c = l + 1$ - answer is c

$P > SA[c]$ and $c = r - 1$ - answer is c

Suffix array: querying

```
def binarySearchSA(t, sa, p):  
    assert t[-1] == '$' # t already has terminator  
    assert len(t) == len(sa) # sa is the suffix array for t  
    if len(t) == 1: return 1  
    l, r = 0, len(sa) # invariant: sa[l] < p < sa[r]  
    while True:  
        c = (l + r) // 2  
        # determine whether p < T[sa[c]:] by doing comparisons  
        # starting from left-hand sides of p and T[sa[c]:]  
        plt = True # assume p < T[sa[c]:] until proven otherwise  
        i = 0  
        while i < len(p) and sa[c]+i < len(t):  
            if p[i] < t[sa[c]+i]:  
                break # p < T[sa[c]:]  
            elif p[i] > t[sa[c]+i]:  
                plt = False  
                break # p > T[sa[c]:]  
            i += 1 # tied so far  
        if plt:  
            if c == l + 1: return c  
            r = c  
        else:  
            if c == r - 1: return r  
            l = c
```

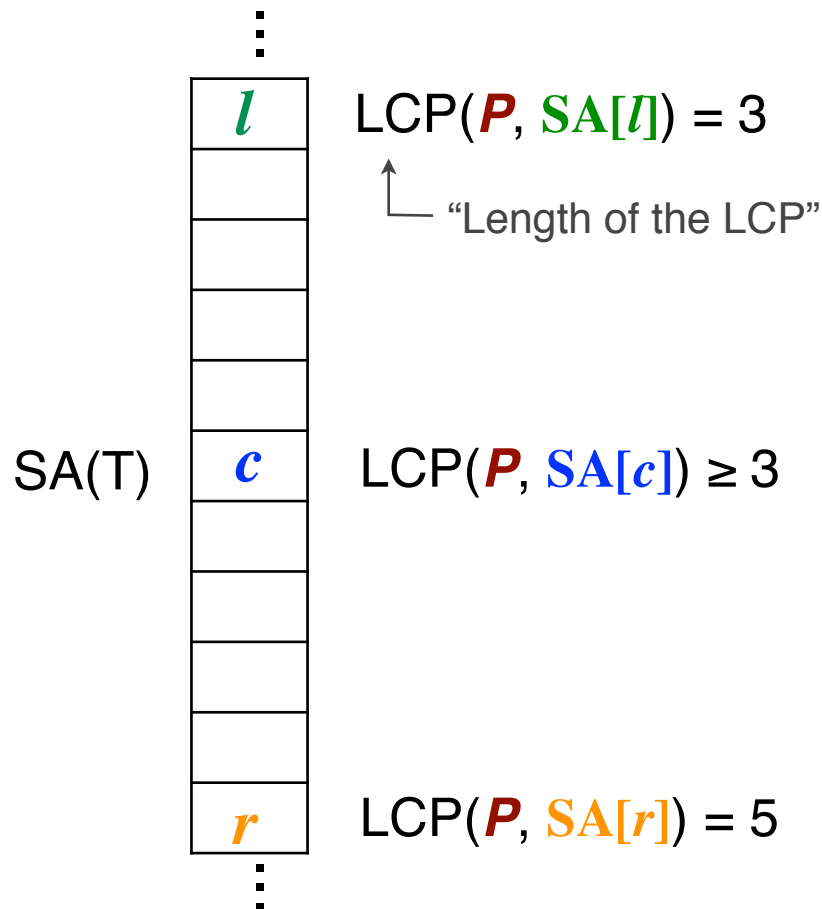
loop iterations \approx length
of Longest Common
Prefix (LCP) of P and
 $SA[c]$

If we already know something about
LCP of P and $SA[c]$, we can save
work

Python example: <http://nbviewer.ipython.org/6765182>

Suffix array: querying

Say we're comparing P to $SA[c]$ and we've already compared P to $SA[l]$ and $SA[r]$ in previous iterations.



More generally:

$$LCP(P, SA[c]) \geq \min(LCP(P, SA[l]), LCP(P, SA[r]))$$

We can skip character comparisons

Suffix array: querying

```
def binarySearchSA_lcp1(t, sa, p):  
    if len(t) == 1: return 1  
    l, r = 0, len(sa) # invariant: sa[l] < p < sa[r]  
    lcp_lp, lcp_rp = 0, 0  
    while True:  
        c = (l + r) // 2  
        plt = True  
        i = min(lcp_lp, lcp_rp)  
        while i < len(p) and sa[c]+i < len(t):  
            if p[i] < t[sa[c]+i]:  
                break # p < T[sa[c]:]  
            elif p[i] > t[sa[c]+i]:  
                plt = False  
                break # p > T[sa[c]:]  
            i += 1 # tied so far  
        if plt:  
            if c == l + 1: return c  
            r = c  
            lcp_rp = i  
        else:  
            if c == r - 1: return r  
            l = c  
            lcp_lp = i
```

Worst-case time bound is still $O(n \log m)$, but we're closer

Python example: <http://nbviewer.ipython.org/6765182>

Suffix array: querying review

We saw 2 ways to query (binary search) the suffix array:

1. Typical binary search. Ignores LCPs. $O(n \log m)$.
2. Binary search with some skipping using LCPs between P and T 's suffixes. Still $O(n \log m)$ worst case, but near $O(n + \log m)$ in practice.

Gusfield:
“Simple Accelerant”

If we precompute external LCP arrays we can accelerate the search to worst case $O(n + \log m)$ at the additional space cost of $2m$ integers. “Super Accelerant” algorithm

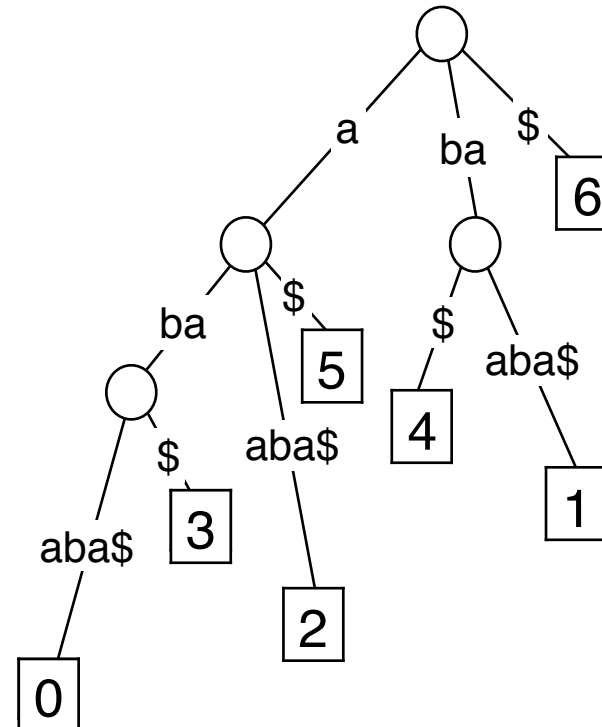
Suffix array: performance comparison

	Super accelerant	Simple accelerant	No accelerant
python -O	68.78 s	69.80 s	102.71 s
pypy -O	5.37 s	5.21 s	8.74 s
# character comparisons	99.5 M	117 M	235 M

Matching 500K 100-nt substrings to the ~ 5 million nt-long *E. coli* genome. Substrings drawn randomly from the genome.

Index building time not included

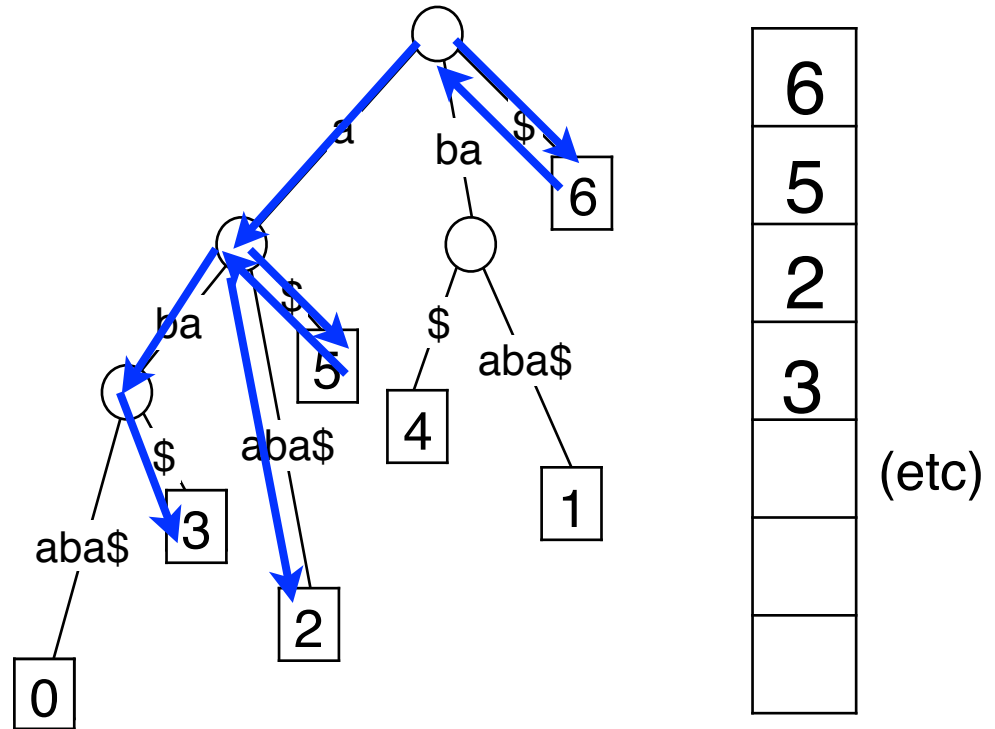
6	\$
5	a \$
2	a a b a \$
3	a b a \$
0	a b a a b a \$
4	b a \$
1	b a a b a \$



Suffix array: building

Idea: Build suffix tree, do a lexicographic depth-first traversal reporting leaf offsets as we go

Traverse $O(m)$ nodes and emit m integers, so $O(m)$ time assuming edges are already ordered



Suffix array: building

Suffix trees are big. Given T , how do we efficiently build T 's suffix array *without* first building a suffix tree?

6	\$
5	a \$
2	a a b a \$
3	a b a \$
0	a b a a b a \$
4	b a \$
1	b a a b a \$

Suffix array: sorting suffixes

One idea: Use your favorite sort, e.g., quicksort

0	a b a a b a \$
1	b a a b a \$
2	a a b a \$
3	a b a \$
4	b a \$
5	a \$
6	\$

```
def quicksort(q):  
    lt, gt = [], []  
    if len(q) <= 1:  
        return q  
    for x in q[1:]:  
        if x < q[0]:  
            lt.append(x)  
        else:  
            gt.append(x)  
    return quicksort(lt) + q[0:1] + quicksort(gt)
```

Expected time: $O(m^2 \log m)$

Not $O(m \log m)$ because a suffix comparison is $O(m)$ time

Suffix array: sorting suffixes

One idea: Use a sort algorithm that's aware that the items being sorted are strings, e.g. "multikey quicksort"

0	a b a a b a \$
1	b a a b a \$
2	a a b a \$
3	a b a \$
4	b a \$
5	a \$
6	\$

Essentially $O(m^2)$ time

Bentley, Jon L., and Robert Sedgewick. "Fast algorithms for sorting and searching strings." *Proceedings of the eighth annual ACM-SIAM symposium on Discrete algorithms*. Society for Industrial and Applied Mathematics, 1997

Suffix array: sorting suffixes

Another idea: Use a sort algorithm that's aware that the items being sorted are all suffixes of the same string

Original suffix array paper suggested an $O(m \log m)$ algorithm

Manber U, Myers G. "Suffix arrays: a new method for on-line string searches." *SIAM Journal on Computing* 22.5 (1993): 935-948.

Other popular $O(m \log m)$ algorithms have been suggested

Larsson NJ, Sadakane K. Faster suffix sorting. Technical Report LU-CS-TR: 99-214, LUNDFD6/(NFCS-3140)/1-43/(1999), Department of Computer Science, Lund University, Sweden, 1999.

More recently $O(m)$ algorithms have been demonstrated!

Kärkkäinen J, Sanders P. "Simple linear work suffix array construction." *Automata, Languages and Programming* (2003): 187-187.

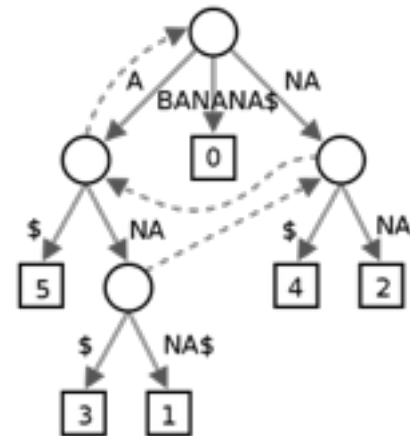
Ko P, Aluru S. "Space efficient linear time construction of suffix arrays." *Combinatorial Pattern Matching*. Springer Berlin Heidelberg, 2003.

Suffix array: summary

Suffix array gives us index that is:

(a) Just m integers, with $O(n \log m)$ worst-case query time, but close to $O(n + \log m)$ in practice

or **(b)** $3m$ integers, with $O(n + \log m)$ worst case



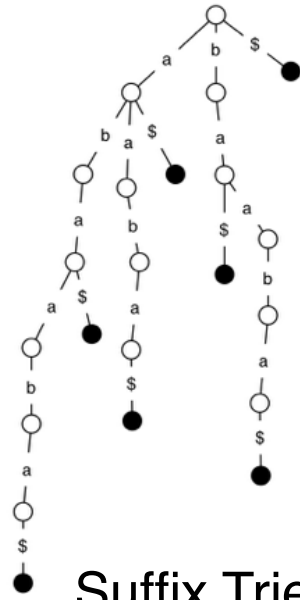
Suffix Tree

6	\$
5	A\$
3	ANA\$
1	ANANA\$
0	BANANA\$
4	NA\$
2	NANA\$

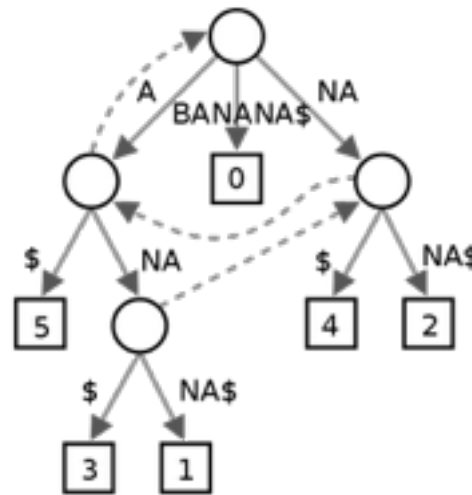
Suffix Array

(a) will often be preferable: index for entire human genome fits in ~12 GB instead of > 45 GB

Summary



$O(n)$ queries
 $O(m^2)$ space



$O(n)$ queries
 $O(m)$ space

6	\$
5	A\$
3	ANA\$
1	ANANA\$
0	BANANA\$
4	NA\$
2	NANA\$

Suffix Array

$O(n \log m)$ queries
 $O(m)$ space

Paper discussion: MUMmer

- Short break then I'll present the main ideas from the MUMmer paper