String Algorithms and Data Structures
Suffix Arrays

CS 199-225

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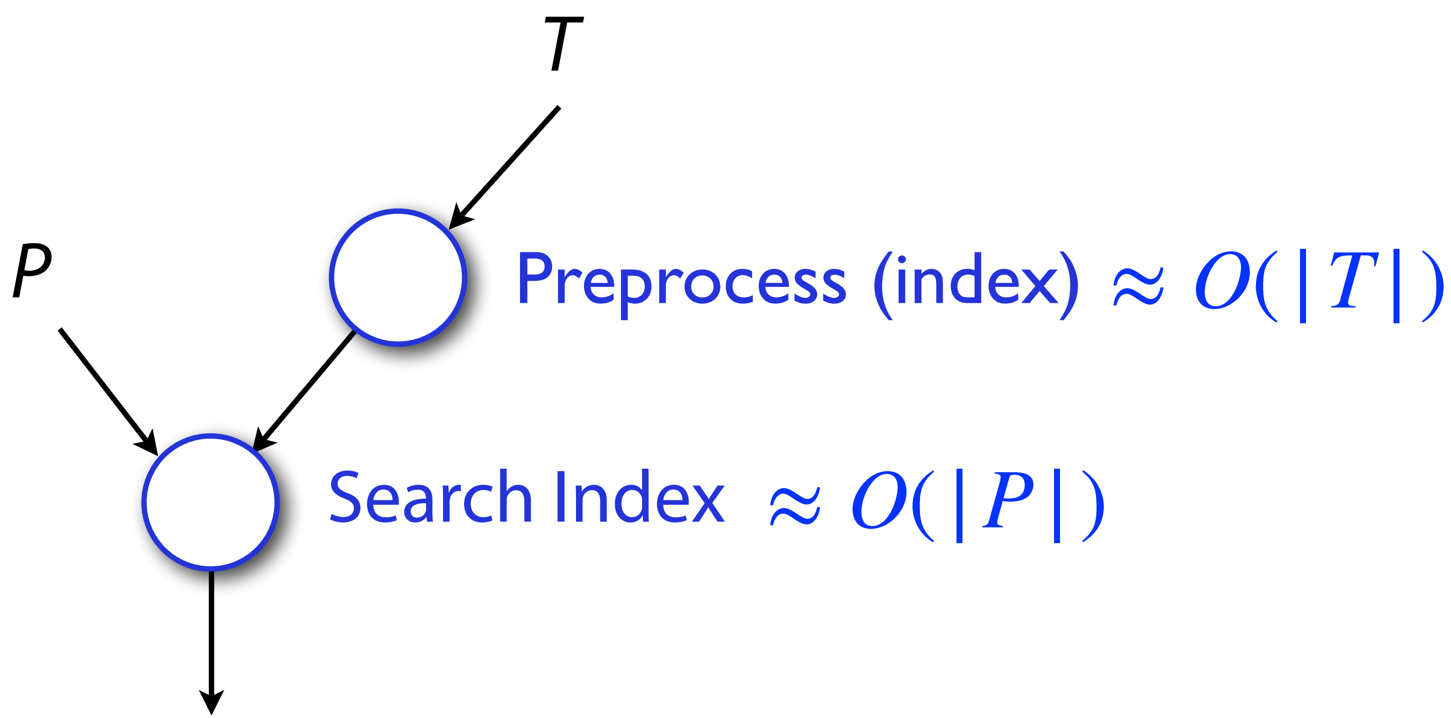
Informal Early Feedback Reminder

Will be closing the IEF form and opening a voting form soon!

Exact pattern matching *w/ indexing*

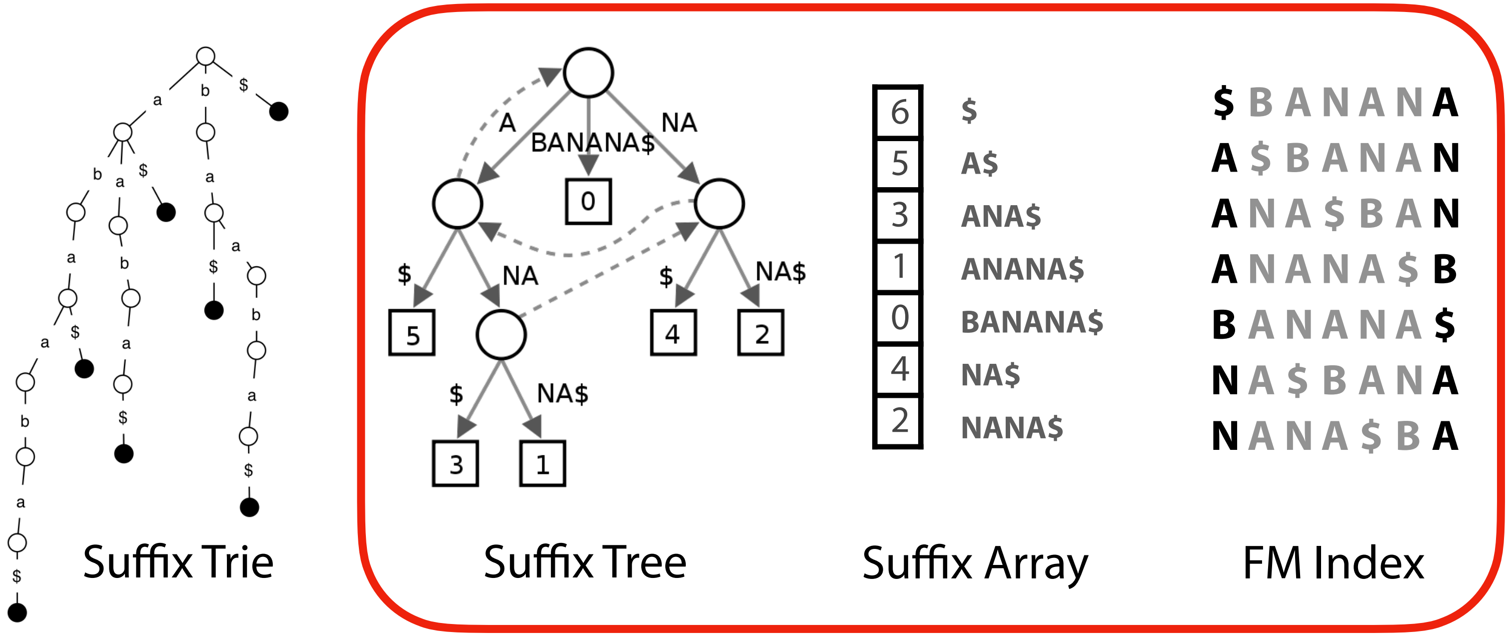


Find instances of *P* in *T*

Exact pattern matching *w/ indexing*

There are many data structures built on ***suffixes***

Modern methods still use these today



Suffix Trie

A rooted tree storing a collection of suffixes as (key, value) pairs

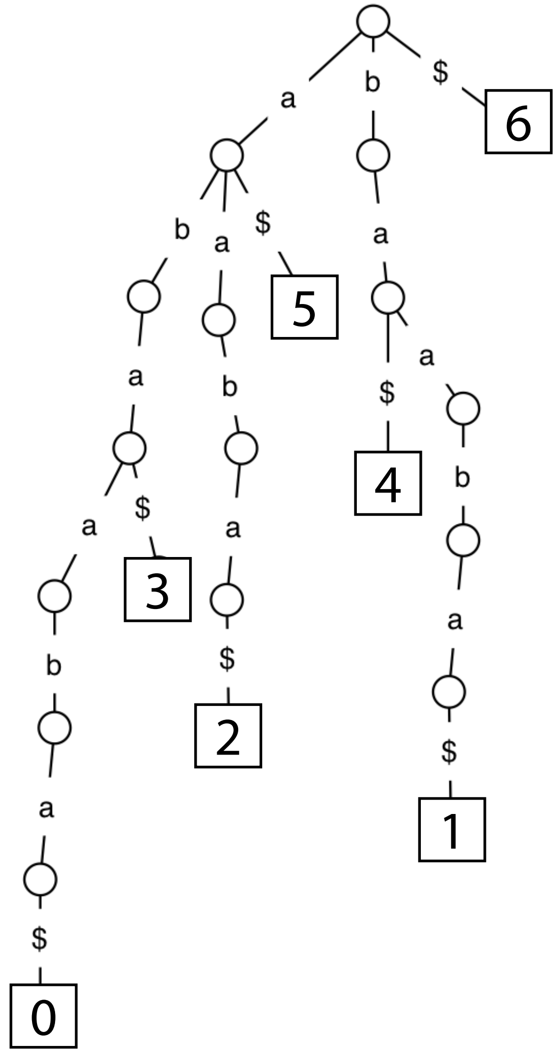
The tree is structured such that:

Each key is "spelled out" along some path starting at root

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

For given node, at most one child edge has label c, for any $c \in \Sigma$

Each key's value is stored at a leaf



Suffix Tree

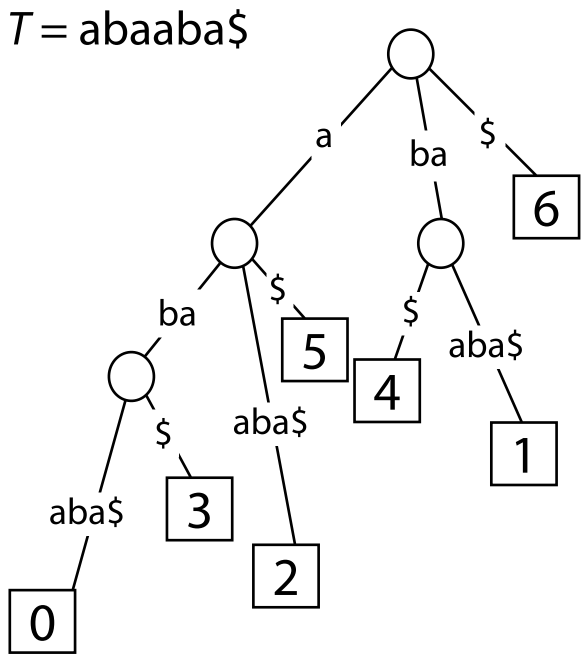
A rooted tree storing a collection of suffixes as (key, value) pairs

The tree has many similarities to the trie but:

Each edge is labeled with *a string s*

For given node, at most one child edge *starts with character c*, for any $c \in \Sigma$

Each internal node contains >1 children

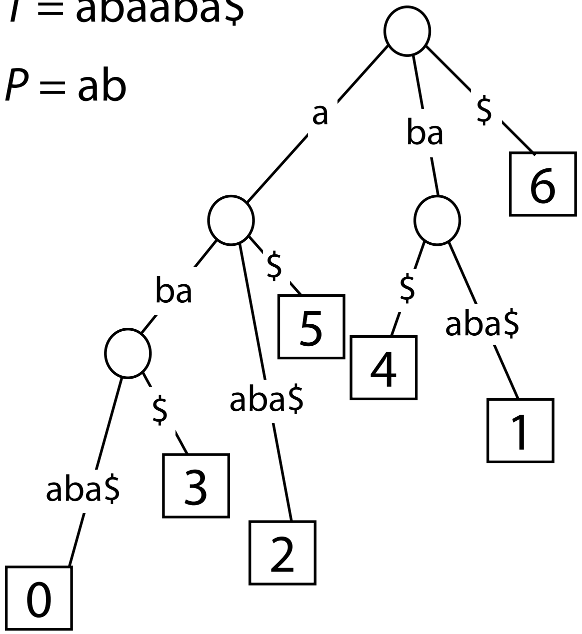


Searching a suffix tree

How efficient is search?

T = abaaba$

P = ab

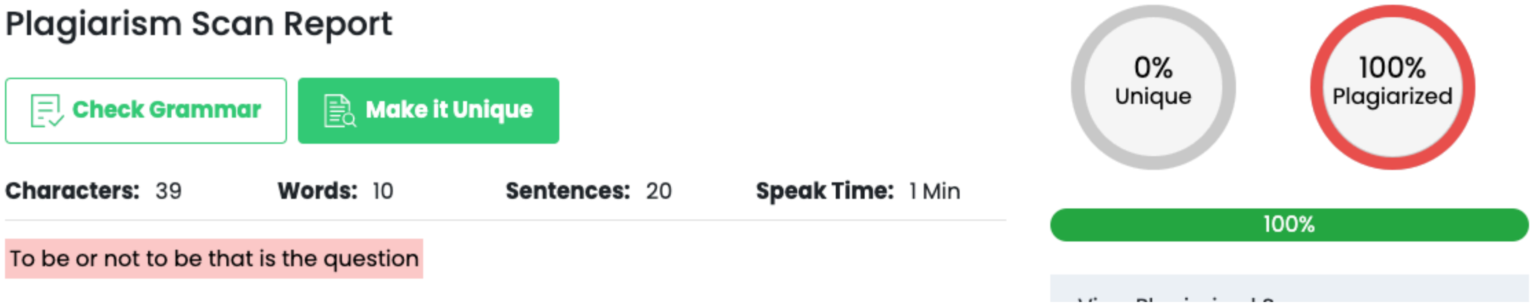


Suffix trie vs suffix tree: bounds

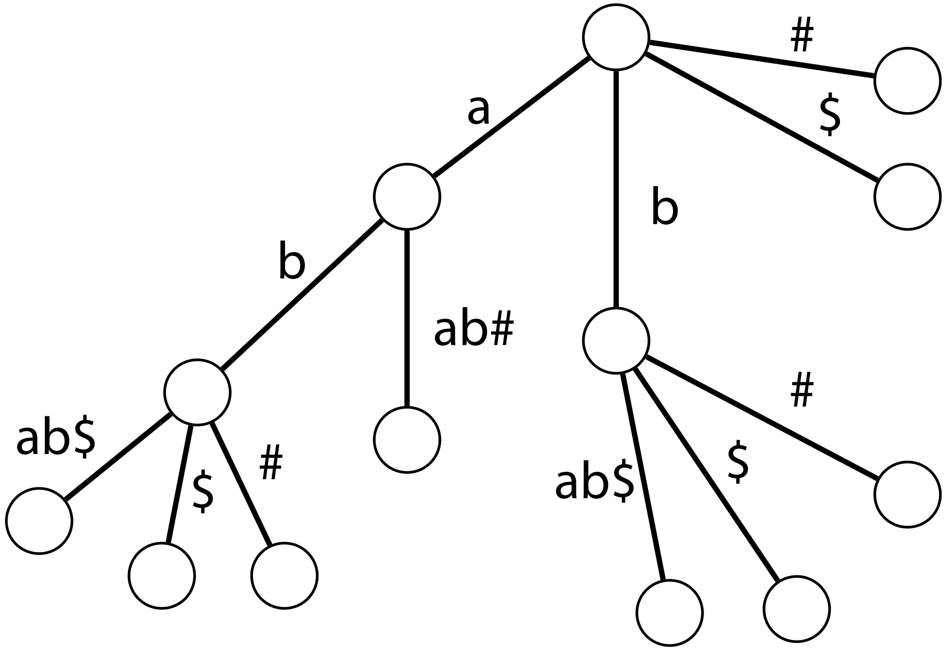
	Suffix trie	**Suffix tree**
Time: Does P occur?	$O(n)$	$O(n)$
Time: Report k locations of P	$O(n + m^2)$	$O(n + k)$
Space	$O(m^2)$	$O(m)$

$m = \mid T \mid,\ n = \mid P \mid,\ k = \#$ occurrences of P in T

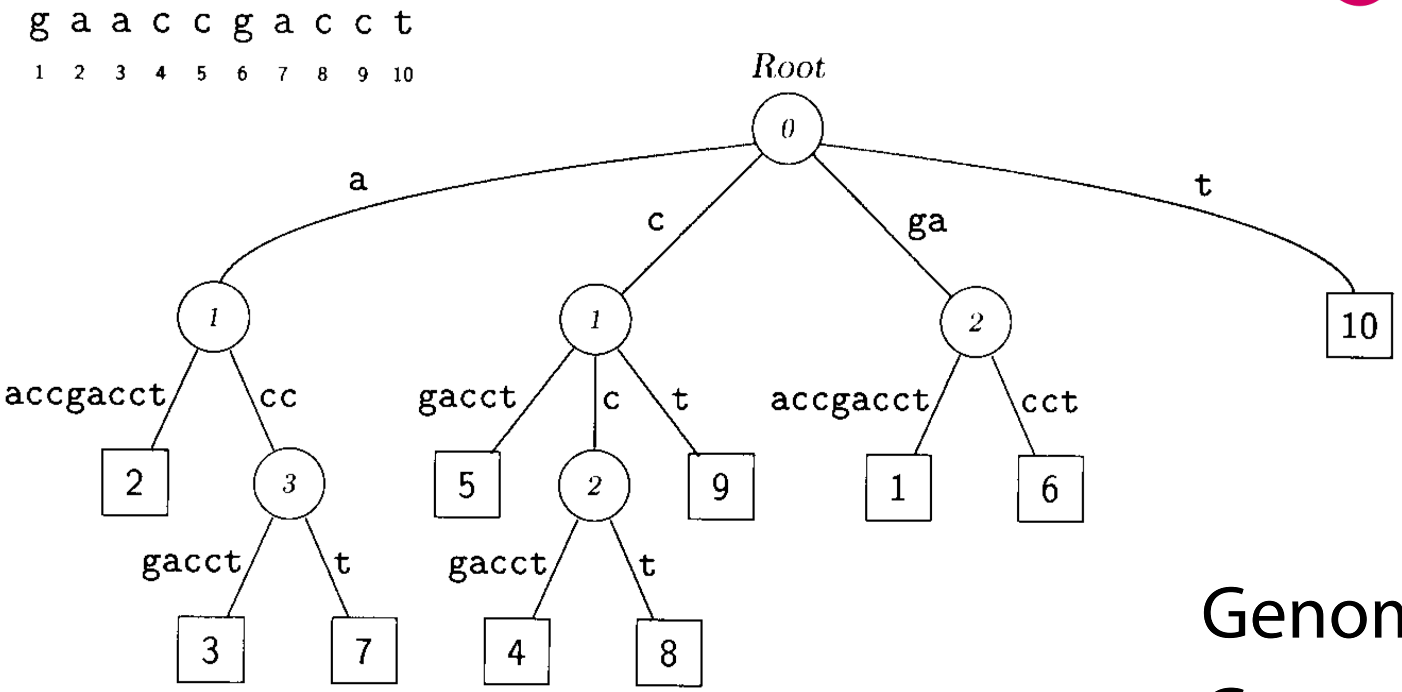
Suffix trees in the real world



X = ABAB   Y = AAB   Generalized Suffix Tree: ABAB$AAB#



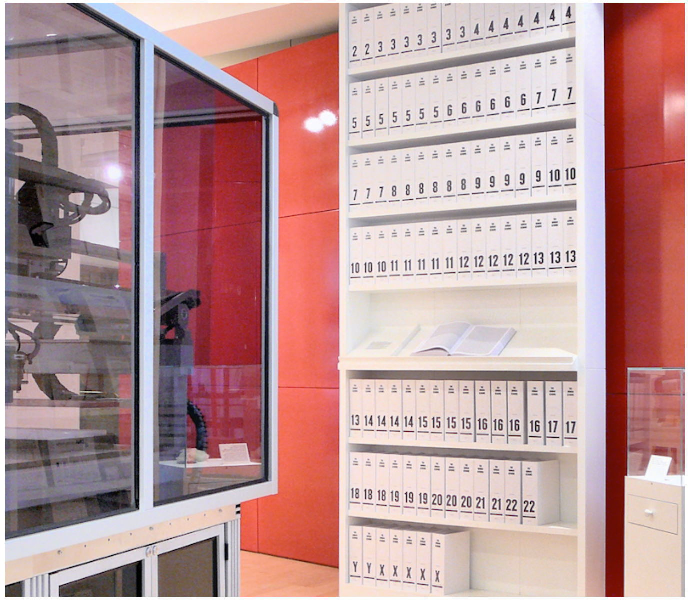
Suffix trees in the real world

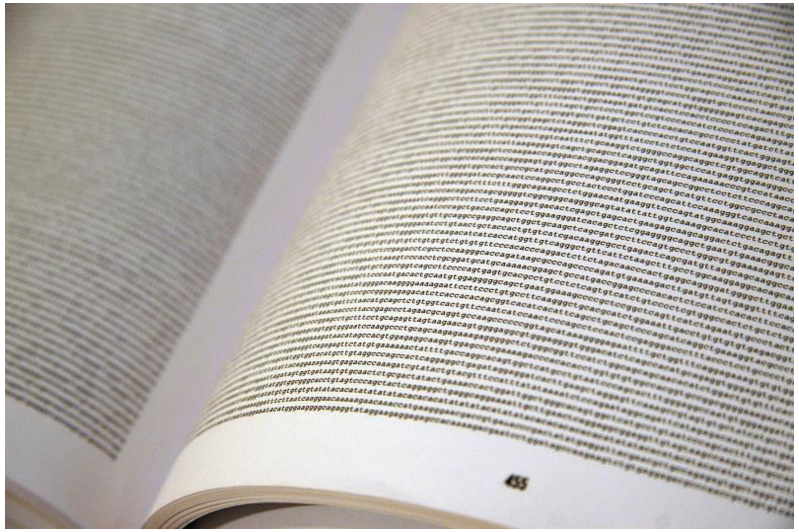


Genome A: TCGATGCGAGGATCATTA

Genome B: AAGTCGCGAGGATCACCG

Suffix trees in the real world: MUMmer





Delcher, Arthur L., et al. "Alignment of whole genomes." *Nucleic Acids Research* 27.11 (1999): 2369-2376.

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Kurtz, Stefan, et al. "Versatile and open software for comparing large genomes." *Genome Biol* 5.2 (2004): R12.

~ 4,000 citations

http://mummer.sourceforge.net

Suffix trees in the real world: MUMmer

File containing genome (T)

File containing query (P)

Indexing phase: ~2 minutes

Matching phase: very fast

```
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
```

Columns:

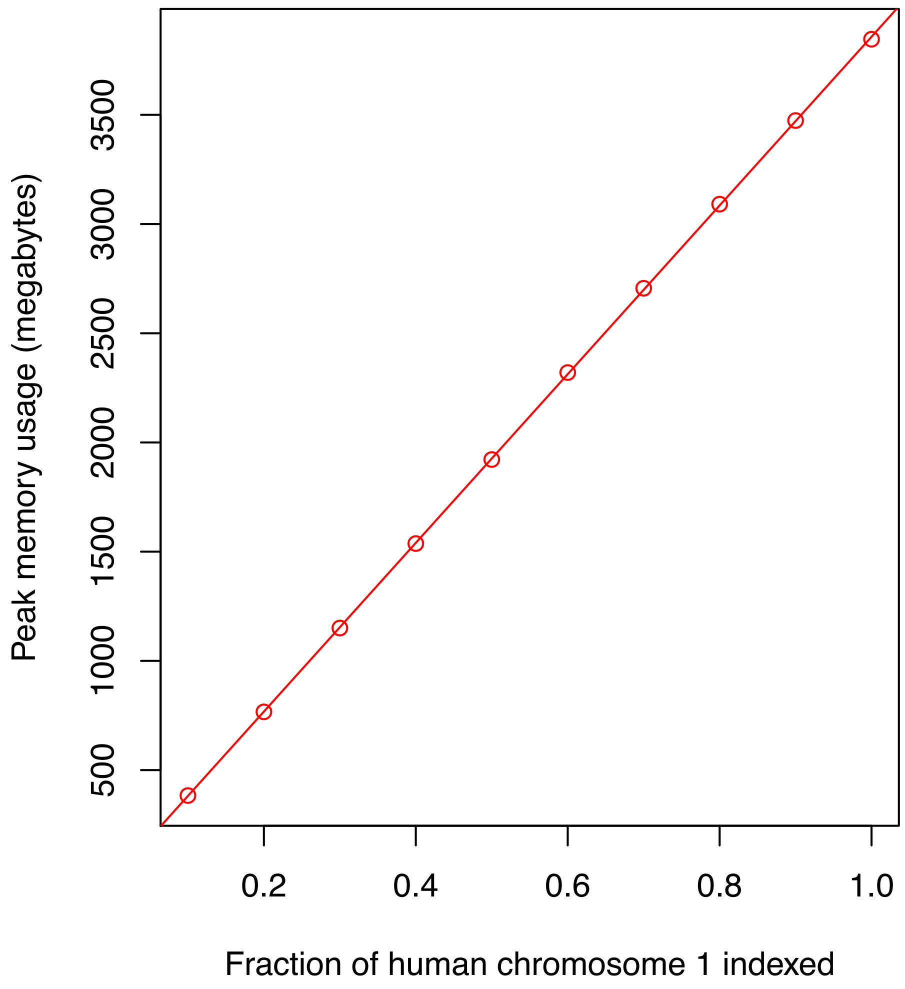
1. Match index in T

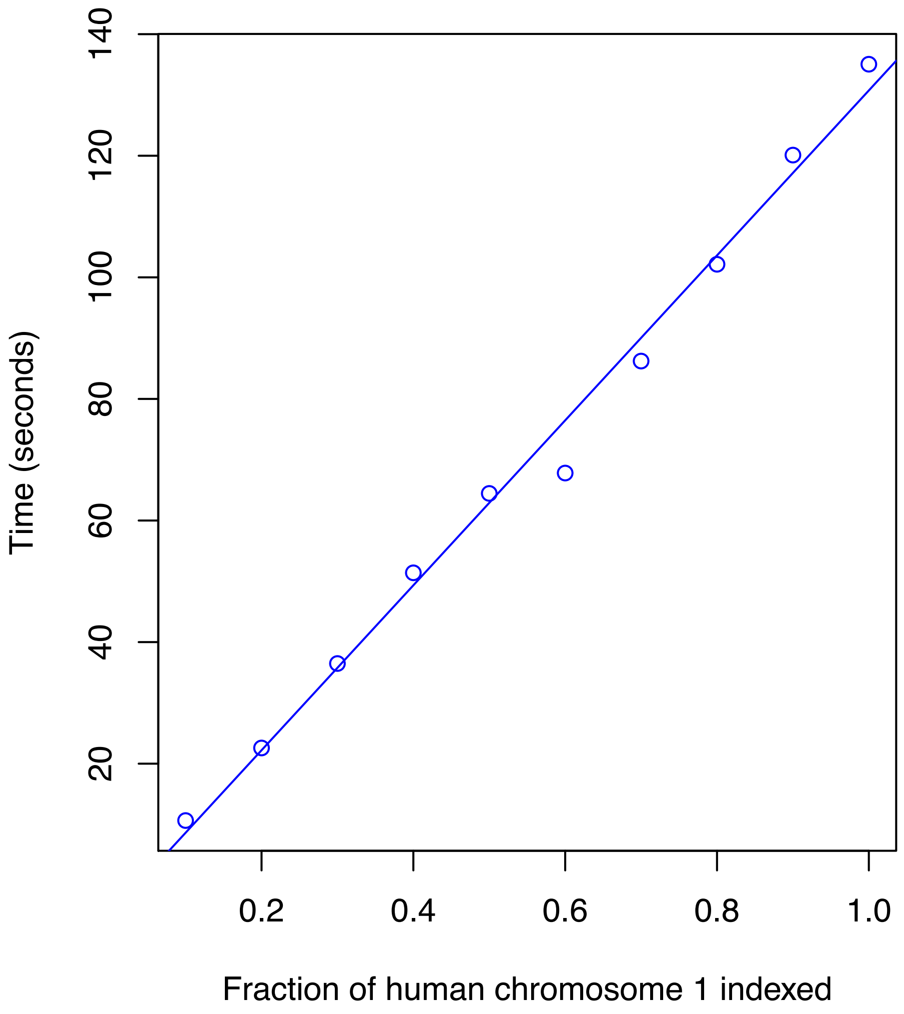
2. Match index in P

3. Length of exact match

Example by Ben Langmead

Suffix trees in the real world: MUMmer



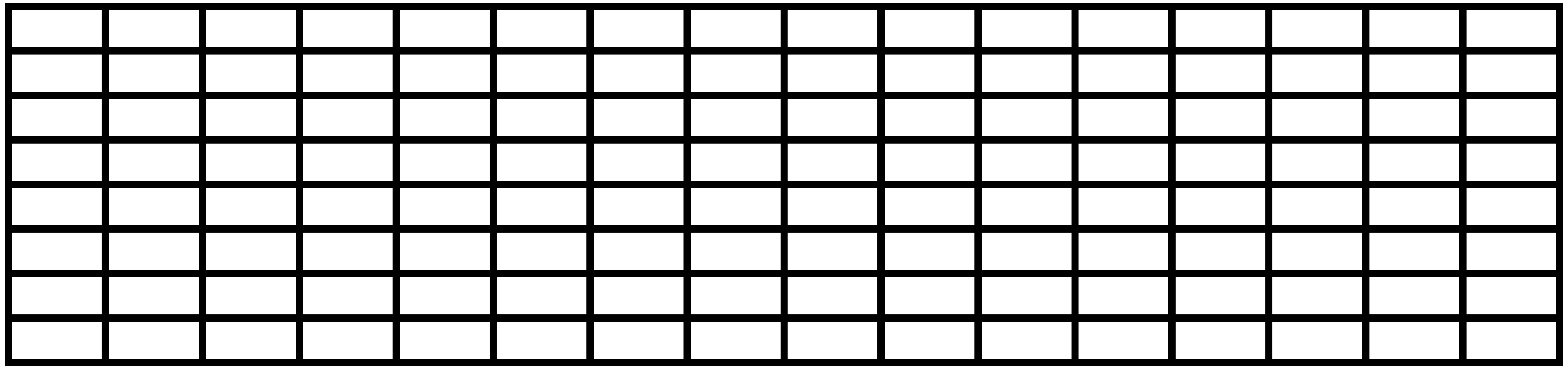


For whole chromosome 1, took 2m:14s and used 3.94 GB memory

Suffix trees in the real world: constant factor

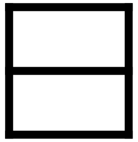
Suffix Trees are O(|T|) but there's a hidden constant factor at work:

MUMmer constant factor ≈ **15.76 bytes per nt**



Suffix tree of human genome: **>45 GB**

'Raw' two-bit encoding ≈ **2 bits per nt**

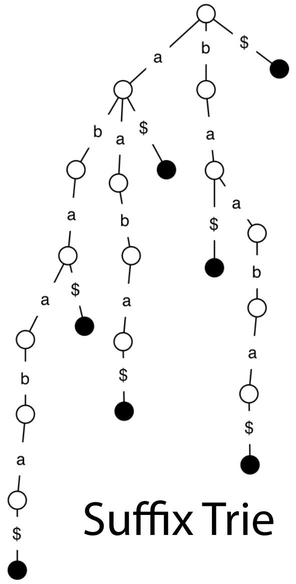


Raw encoding of human genome: **~0.75 GB**

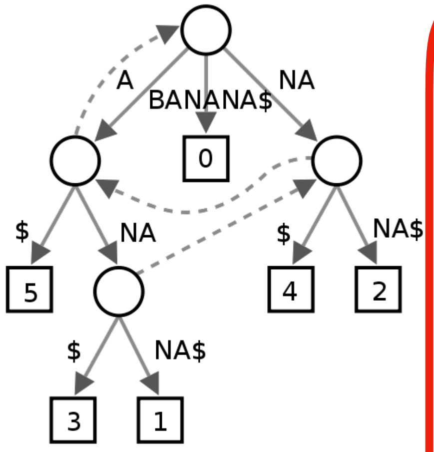
Exact pattern matching *w/ indexing*

There are many data structures built on ***suffixes***

More efficient to store, less efficient* to use



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

Lexicographic Order

A systematic way of organizing strings by the content and arrangement of its characters

Lexicographic Order

A systematic way of organizing strings by the **content** and arrangement of its characters

Strings are compared by their individual characters.

Alphabetical Order `A < B < … < Z`

ASCII Order `$ < 0 < A < a`

ASCII Value	Character
36	$
…	…
48	0
…	…
65	A
…	…
97	a

Lexicographic Order

A systematic way of organizing strings by the content and **arrangement** of its characters

Characters are compared in order from left to right

A B C D

B B

A B A B

B B B

Lexicographic Order

A systematic way of organizing strings by the **content** and **arrangement** of its characters

What is the *lexicographically* smallest string?

A) “`beep`”

B) “`zzz`”

C) “`aardvarks`”

D) “`apples`”

Lexicographic Order

A systematic way of organizing strings by the **content** and **arrangement** of its characters

What is the *lexicographically* smallest string?

A) “bah$”

B) “x”

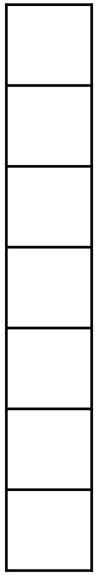
C) “bb$”

D) “b$b”

Suffix Array

Suffix array of *T* is an array of integers specifying lexicographic (alphabetical) order of *T*'s suffixes

***T* = a b a a b a $**
0 1 2 3 4 5 6



Suffix Array

Suffix array of T is an array of integers specifying lexicographic (alphabetical) order of T's suffixes

T = a b a a b a $
0 1 2 3 4 5 6

As with suffix tree, T is part of index

SA(T) =		
	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 $

m integers

Note: Red is not stored

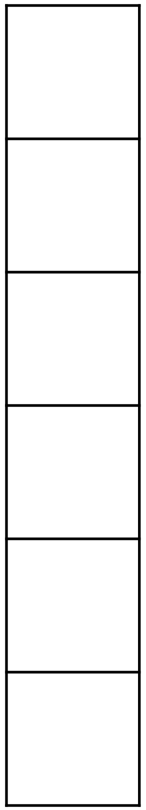
vector<int> build_sarray(string T)

Input:

```
    0 1 2 3 4 5
T:  C G T G C $
    C G T G C $
      G T G C $
        T G C $
          G C $
            C $
              $
```

m suffixes

Output:



`vector<int> build_sarray(string T)`

Input:

	0	1	2	3	4	5
T:	C	G	T	G	C	$
	C	G	T	G	C	$
		G	T	G	C	$
			T	G	C	$
				G	C	$
					C	$
						$

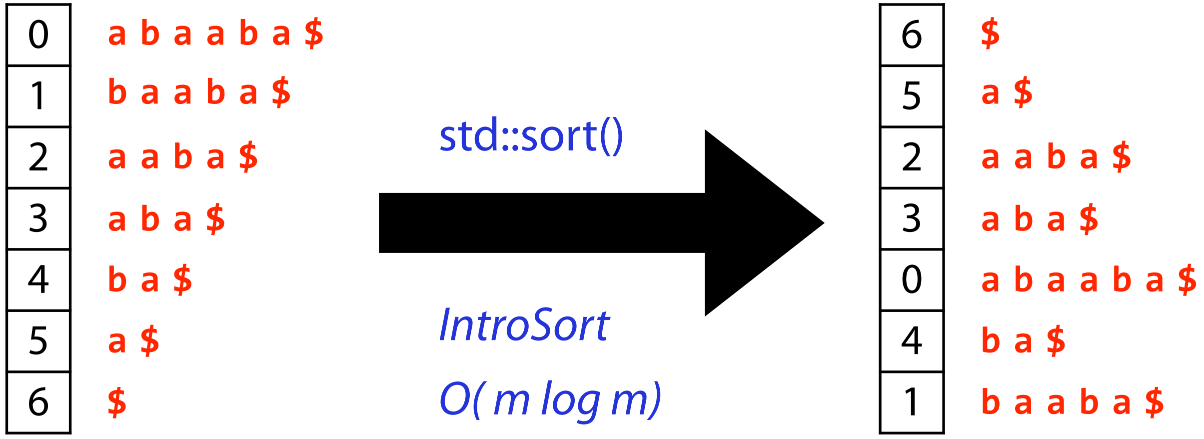
m suffixes

Output:

5
4
0
3
1
2

Suffix array: build by sorting (from array)

Use your favorite sort, e.g., quickSort, heapSort, insertSort, …



Expected time:

Suffix array: build by 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.

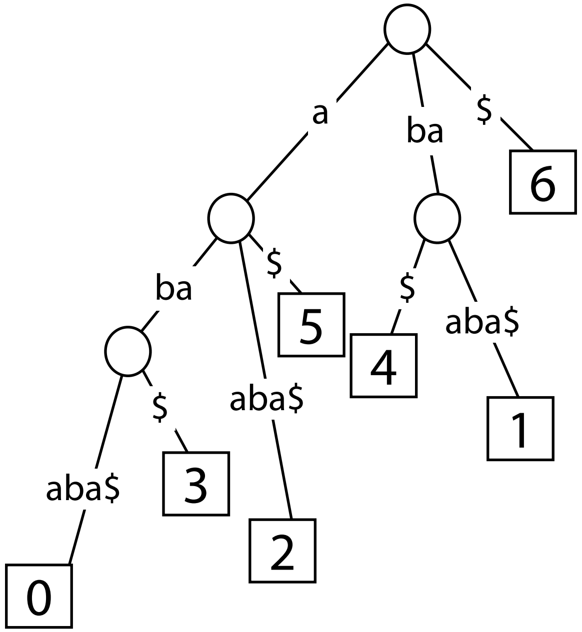
There exist several ***O*(*m*)** algorithms that *divide-and-conquer*

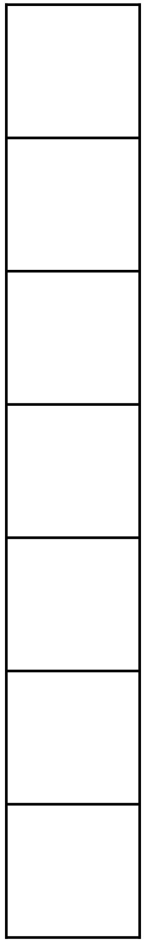
Kärkkäinen J, Sanders P. "Simple linear work suffix array construction." Automata, Languages and Programming (2003): 187-187.

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

Suffix array: build by suffix tree

(a) Build suffix tree, (b) traverse in lexicographic order, (c) upon reaching leaf, append suffix to array





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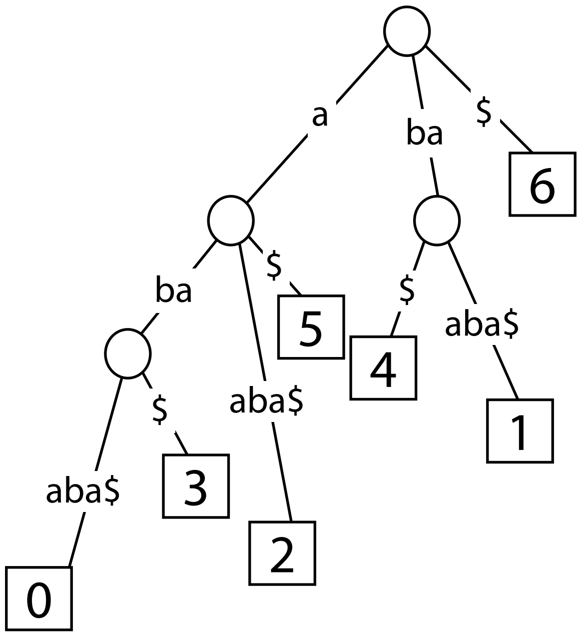
(a) Build suffix tree, (b) traverse in lexicographic order, (c) upon reaching leaf, append suffix to array



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 $

Assignment 7: a_sarray

Learning Objective:

Construct a suffix array by sorting suffixes

Implement exact pattern matching using a suffix array

Be as efficient or inefficient as you like!

Challenge yourself: Try to build in O($m^2 \log m$) or better.

Searching a suffix array

To find all exact matches using a suffix array:

T = abaaba$

P = baa

Starts with b? →	6	$
Starts with b? →	5	a $
Starts with b? →	2	a a b a $
Starts with b? →	3	a b a $
Starts with b? →	0	a b a a b a $
Starts with b? →	4	b a $
	1	b a a b a $

Searching a suffix array

To find all exact matches using a suffix array:

T = abaaba$

P = baa

6	$
5	a $
2	a a b a $
3	a b a $
0	a b a a b a $
Matches baa? → 4	b a $
Starts with b? Matches baa? → 1	b a a b a $

Searching a suffix array

To find all exact matches using a suffix array:

1. Recreate suffix from int value

2. Compare each character in order

3. On mismatch, move to next suffix

What is our time complexity?

$T = \text{abaaba\$}$ $m = |T|$

$P = \text{baa}$ $n = |P|$

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 $

Return {1}

Searching a suffix array

To find all exact matches using a suffix array w/ binary search:

T = abaaba\$ $m = |T|$

P = baa $n = |P|$

	6	\$
	5	a \$
	2	a a b a \$
Match here? →	3	a b a \$
	0	a b a a b a \$
Match here? →	4	b a \$
Match here? →	1	b a a b a \$

Return {1}

Searching a suffix array

To find all exact matches using a suffix array w/ binary search:

T = abaaba\$ $m = |T|$

P = aba $n = |P|$

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 $

Binary search match! → 3

Return {3}!

But what about our other match?

Searching a suffix array

To find all exact matches using a suffix array w/ binary search:

T = abaaba$ $m = |T|$

P = aba $n = |P|$

1. Pick suffixes using binary search

2. Compare suffixes as normal

3. After match, check neighbors

6	$	
5	a $	
2	a a b a $	No match
3	a b a $	
0	a b a a b a $	Match
4	b a $	No match
1	b a a b a $	

Return {0,3}

Assume we have k=m matches

What is our time complexity?

Searching a suffix array

How can we do better?

$T = \text{abaaba\$}$ $\quad m = |T|$

$P = \text{a}$ $\quad n = |P|$

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 $

Range Search

Given a collection of objects, C, with comparable values and an object of interest, q, find ~~the first~~ ALL instance(s) of $q \in C$.

Input:

0	1	2	2	2	2	2	3	4	5

Output: Range of indices matching q if it exists, $(-1, -1)$ otherwise

Binary Search: Get first match

Find(3)

```
        if mid == q:

            # Match case:
            # Treat like query is larger
            # Remember last match!

        elif mid > q:

            # query is smaller case
        else:

            # query is larger case


    # Final Return Snippet
    if saw_match:
        return last_match
    else:
        return -1
```

2	3	3	3	3	4	4

Binary Search: Get last match

Find(2)

```
        if mid == q:

            # Match case:
            # Treat like query is smaller
            # Remember last match!

        elif mid > q:

            # query is smaller case
        else:

            # query is larger case


    # Final Return Snippet
    if saw_match:
        return last_match
    else:
        return -1
```

2	2	2	2	2	2	4

Searching a suffix array

How can we do better?

1. Identify the *first* and *last* matches to P w/ binary search

2. Return all values in that range!

Assume we have k=m matches

What is our time complexity?

T = abaaba$ $m = |T|$

P = a $n = |P|$

	6	$	
→	5	a $	First
	2	a a b a $	
	3	a b a $	
→	0	a b a a b a $	Last
	4	b a $	
	1	b a a b a $	

Assignment 7: a_sarray

Learning Objective:

Construct a suffix array by sorting suffixes

Implement exact pattern matching using a suffix array

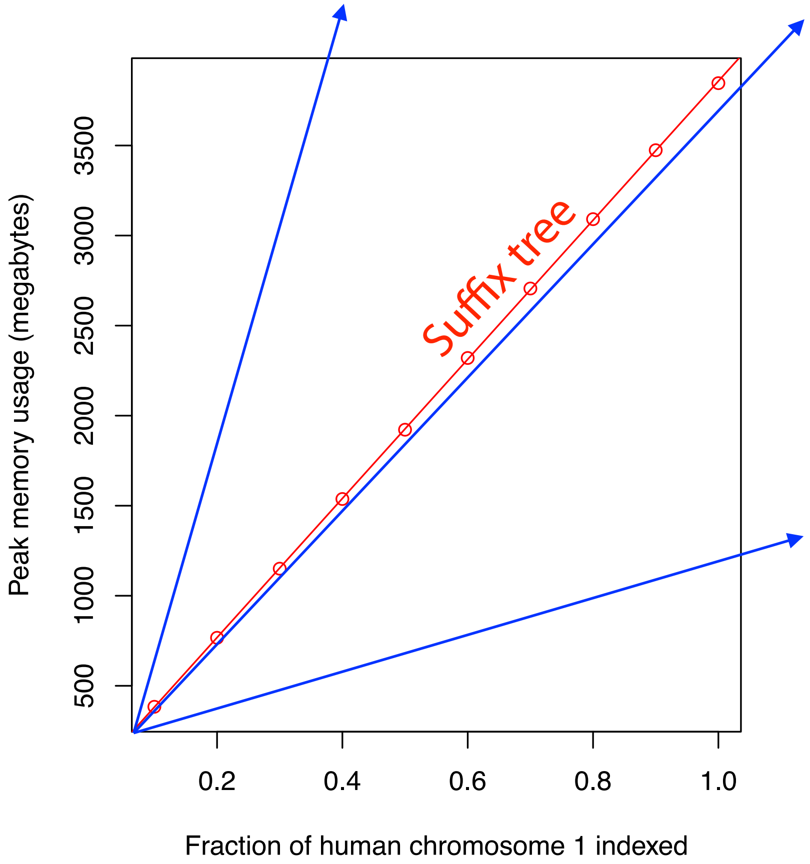
Be as efficient or inefficient as you like!

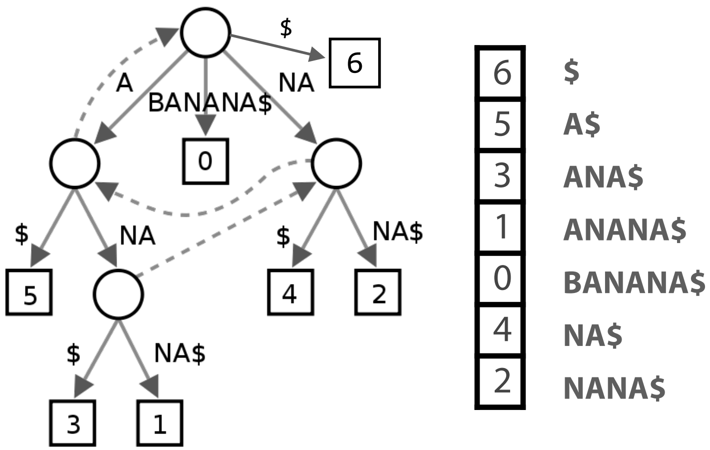
Challenge yourself: Try to search in $O(n \log m + k)$

Suffix tree vs suffix array: size

$O(m)$ space, like suffix tree

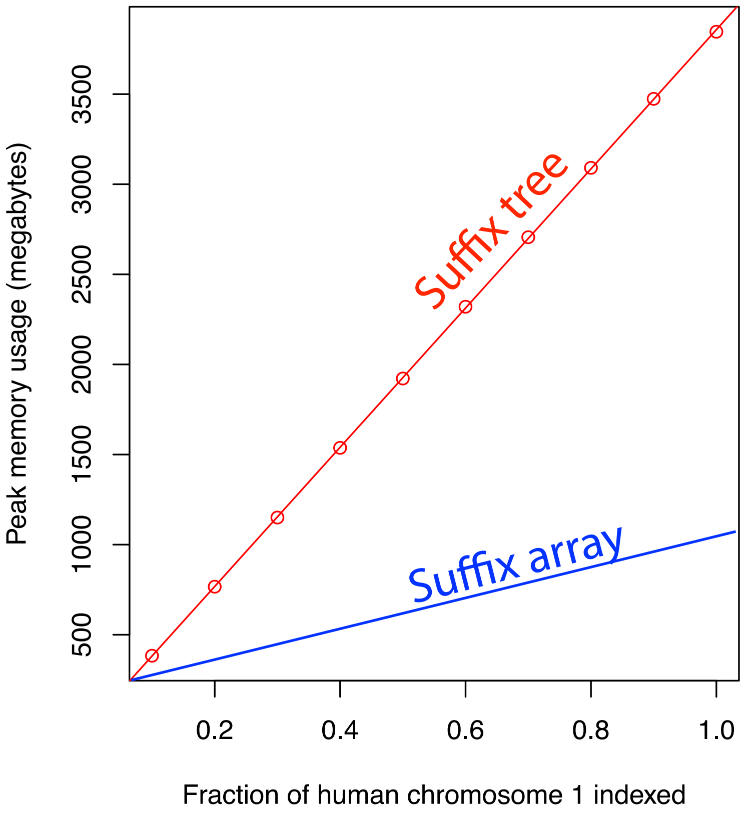
Is "constant factor" worse, better, same?

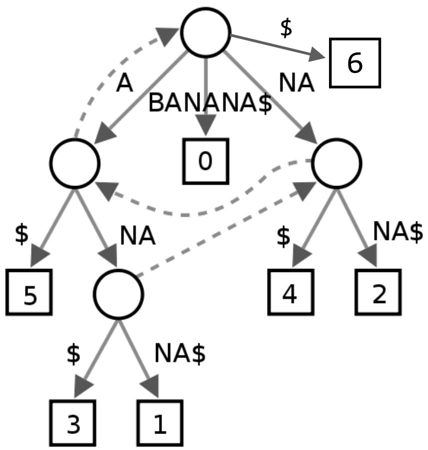




Suffix tree vs suffix array: size

32-bit integers sufficient for human genome, so fits in ~4 bytes/base × 3 billion bases ≈ **12 GB**. Suffix tree is **>45 GB**.





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

Suffix tree vs suffix array: search

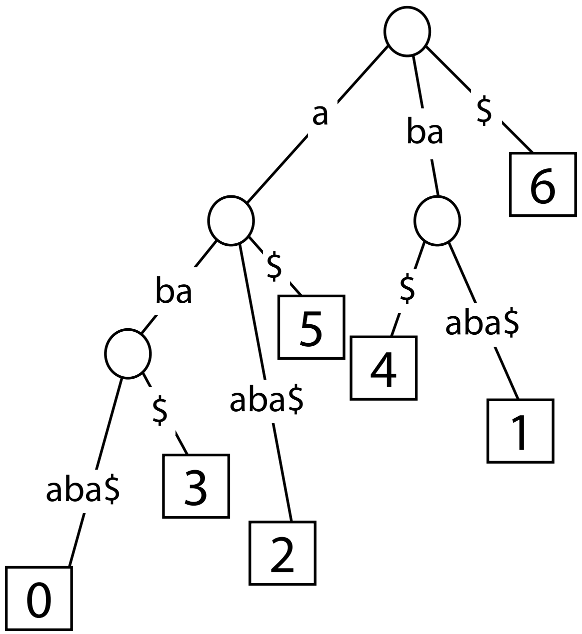
Suffix Array

O(n log m + k)*

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 $

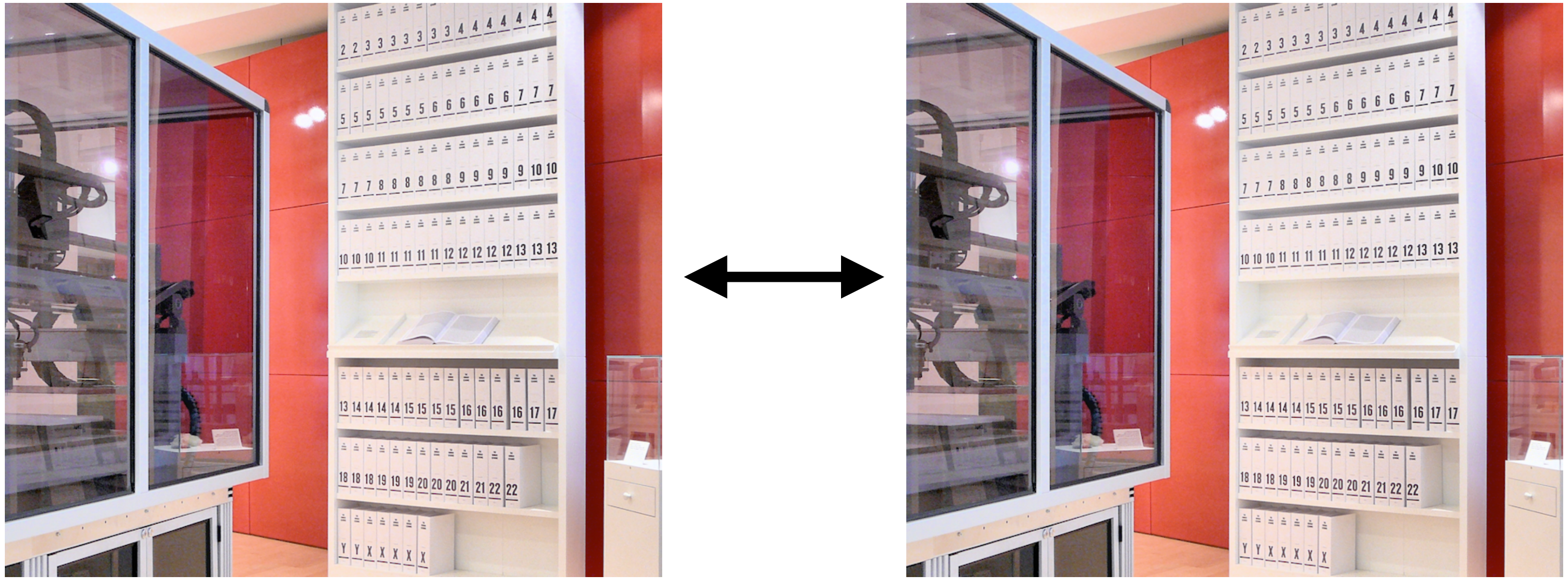
Suffix Tree

O(n + k)



* Can be improved to O(n + log m), (See Gusfield 7.17.4)

Suffix ***arrays*** in the real world: MUMmer



Delcher, Arthur L., et al. "Alignment of whole genomes." *Nucleic Acids Research* 27.11 (1999): 2369-2376.

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G. Marçais et al. "MUMmer4: A fast and versatile genome alignment system." *PLoS Comp Biol* (2018)

~ 4,000 citations

http://mummer.sourceforge.net

Exact pattern matching *w/ indexing*

There are many data structures built on ***suffixes***

The FM index is a compressed self-index (smaller* than original text)!