String Algorithms and Data Structures

Suffix Arrays

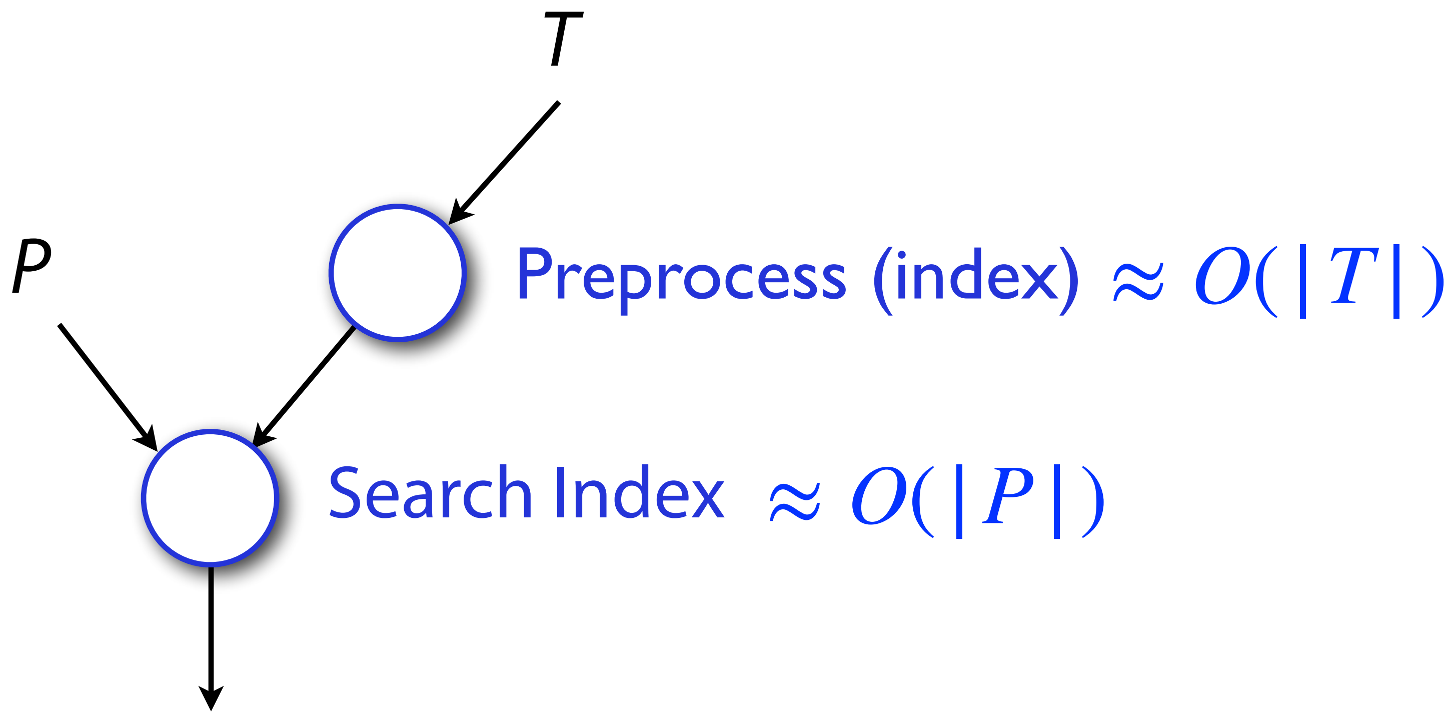
CS 199-225
Brad Solomon

October 17, 2022

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

Department of Computer Science

Exact pattern matching *w/ indexing*



T

P

Preprocess (index) $\approx O(|T|)$

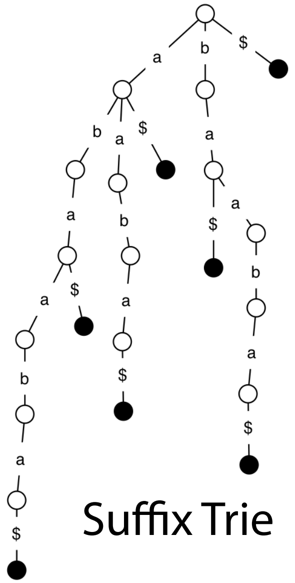
Search Index $\approx O(|P|)$

Find instances of *P* in *T*

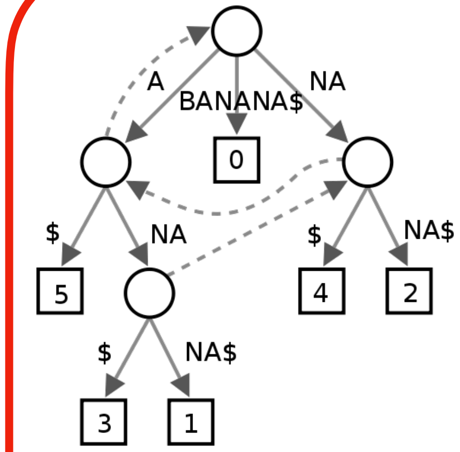
Exact pattern matching *w/ indexing*

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

Modern methods still use these today



Suffix Trie



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

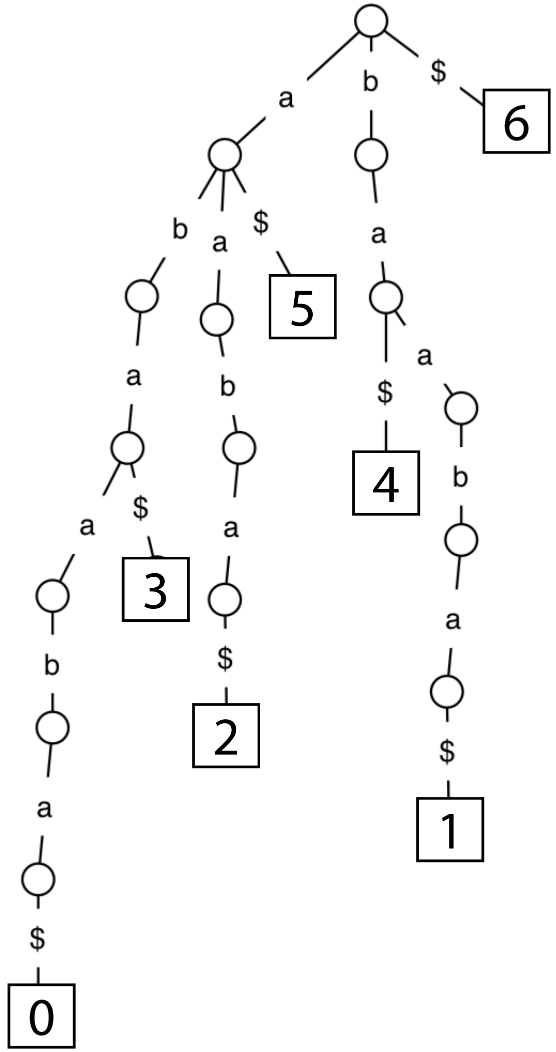
FM Index

Suffix Trie

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

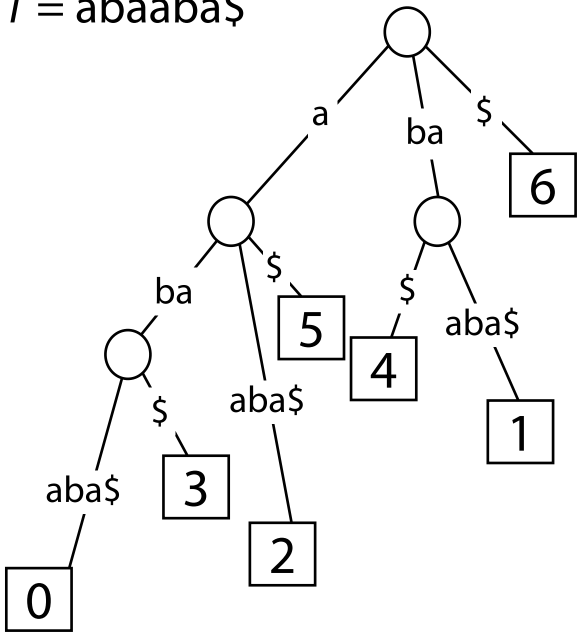
A rooted tree storing a collection of suffixes as (key, value) pairs

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

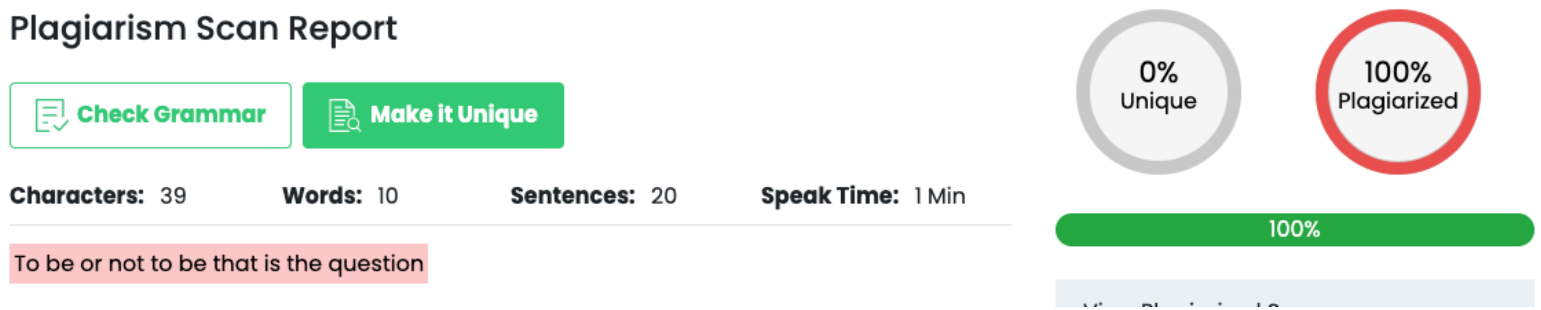


Suffix trie vs suffix tree: bounds

	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	$O(m^2)$	$O(m)$

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

Suffix trees in the real world



Plagiarism Scan Report

Characters: 39 **Words:** 10 **Sentences:** 20 **Speak Time:** 1 Min

To be or not to be that is the question

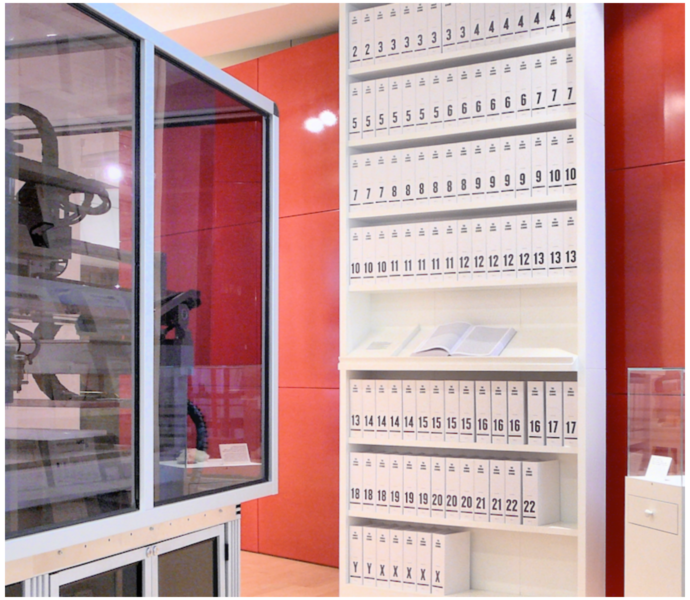
ancestry

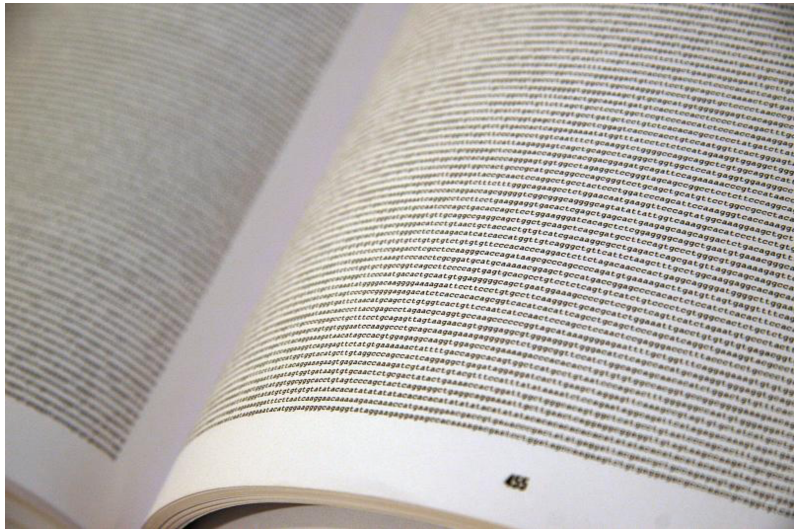
23andMe

Genome A: TCGAT**GCGAGGATCA**TTA

Genome B: AAGTC**GCGAGGATCA**CCG

Suffix trees in the real world: MUMmer





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

Delcher, Arthur L., et al. "Fast algorithms for large-scale genome alignment and comparison." *Nucleic Acids Research* 30.11 (2002): 2478-2483.

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

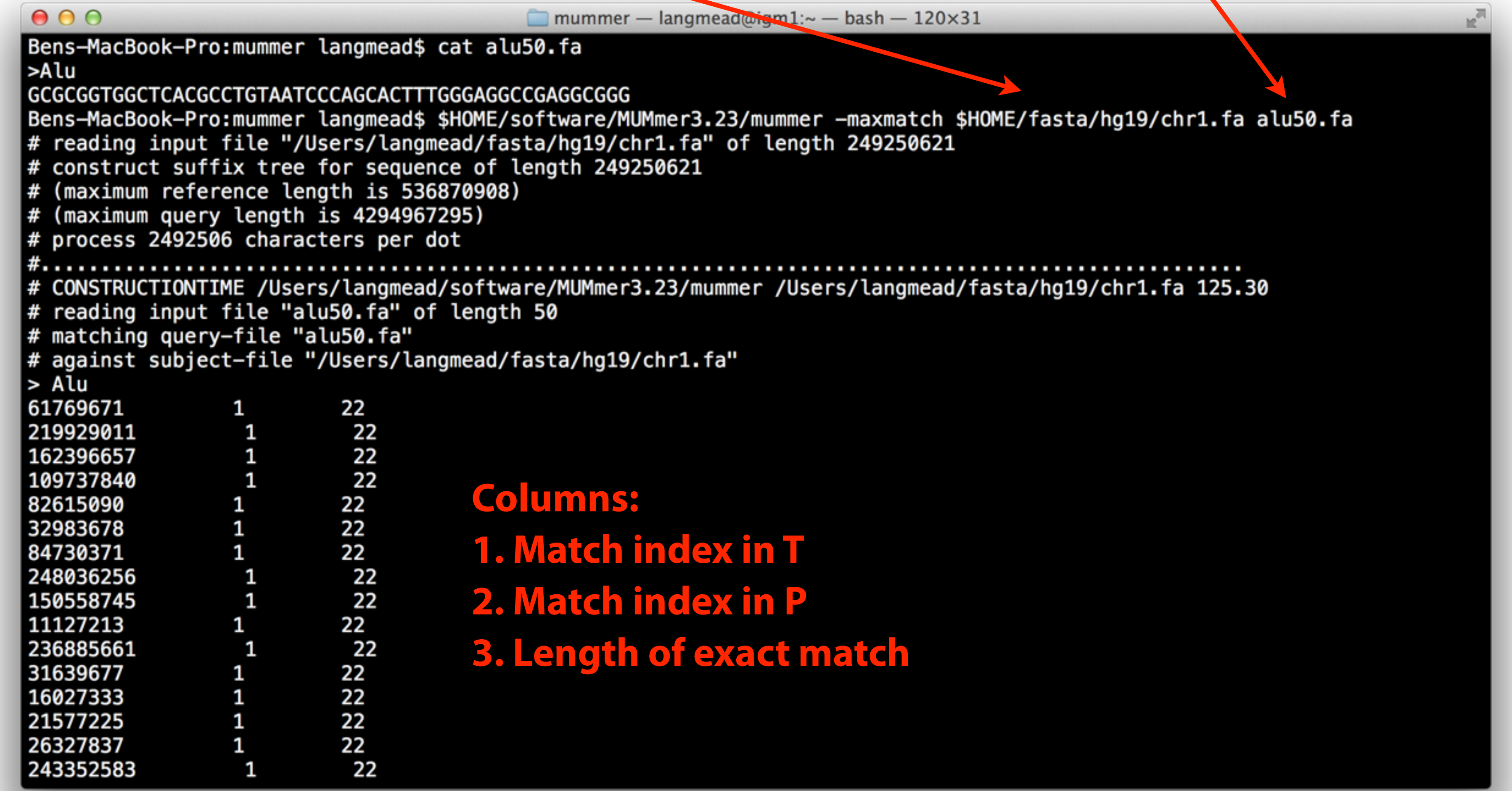
Suffix trees in the real world: MUMmer

File containing genome (T)

File containing query (P)

Indexing phase: ~2 minutes

Matching phase: very fast



```
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:

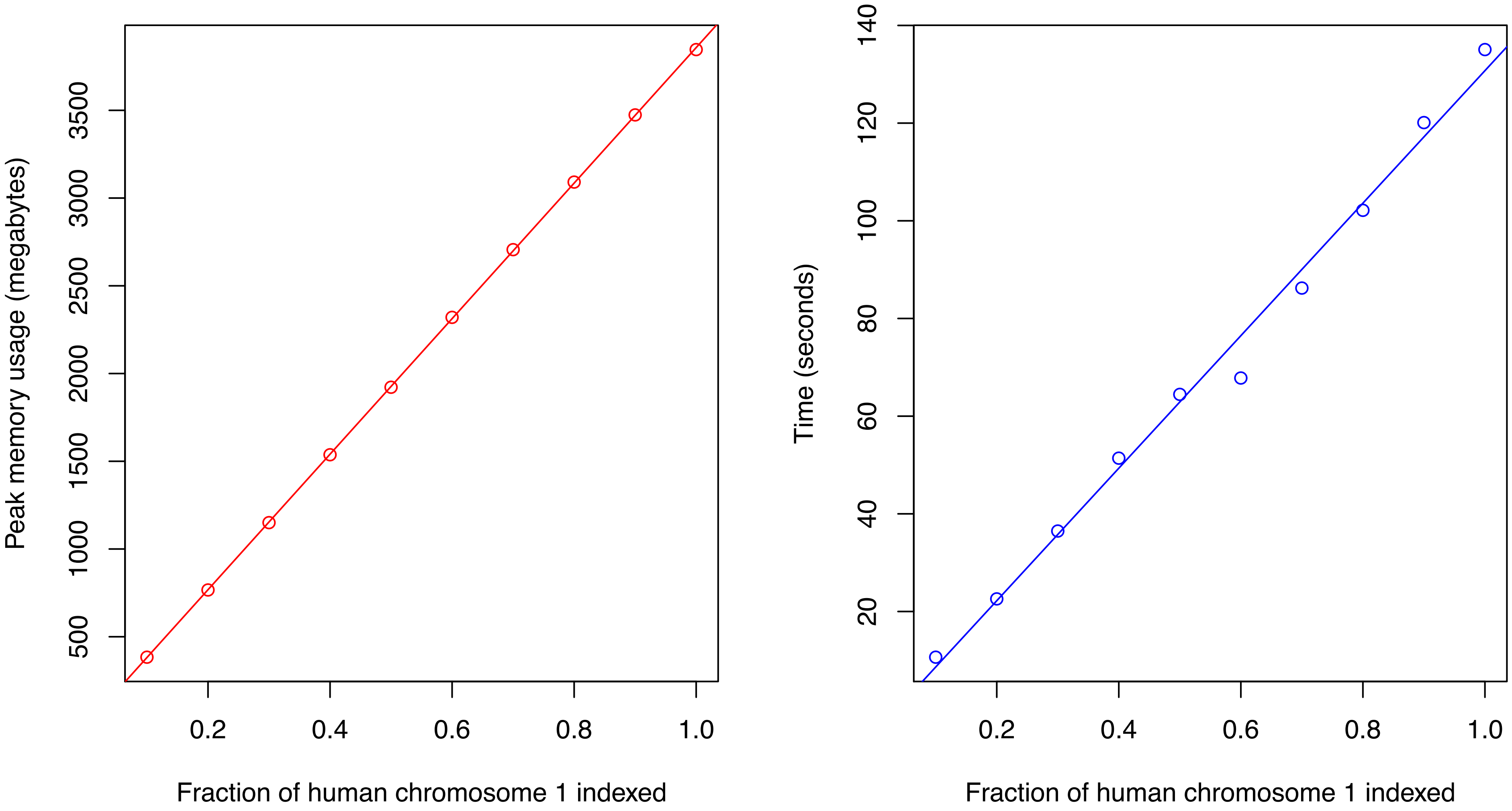
1. Match index in T

2. Match index in P

3. Length of exact match

Example by Ben Langmead

Suffix trees in the real world: MUMmer

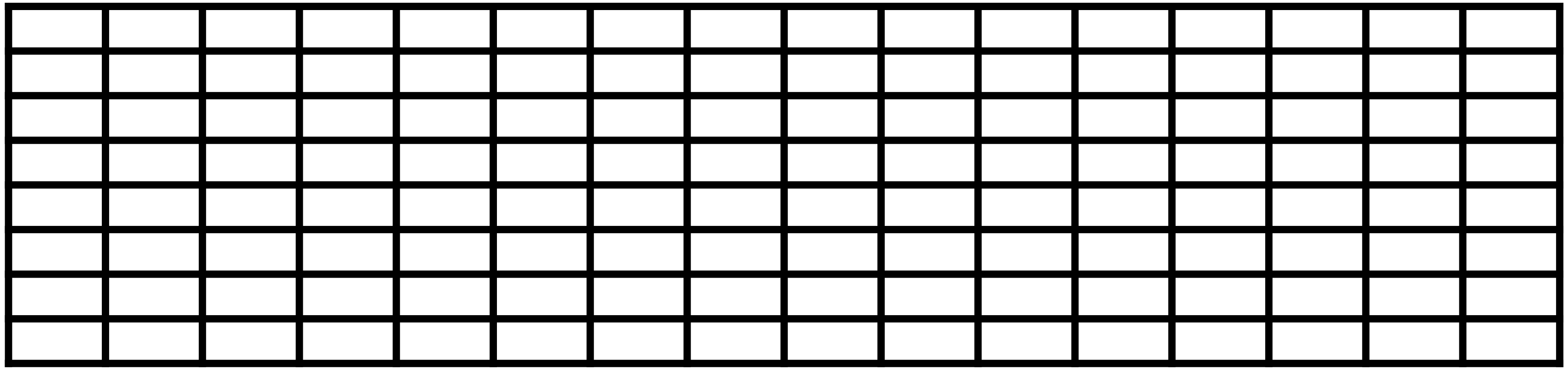


For whole chromosome 1, took 2m:14s and used 3.94 GB memory

Suffix trees in the real world: constant factor

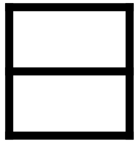
Suffix Trees are O(|T|) but there's a hidden constant factor at work:

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



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

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

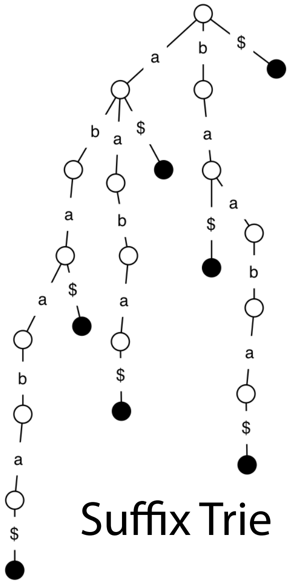


Raw encoding of human genome: **~0.75 GB**

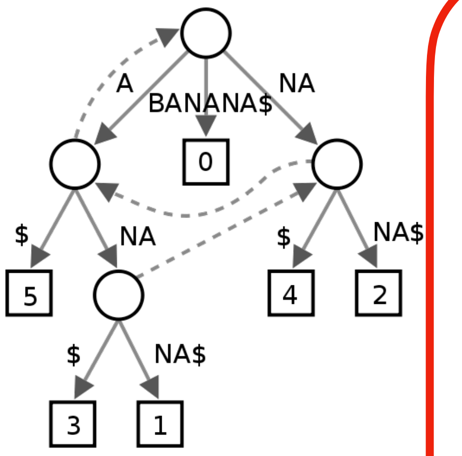
Exact pattern matching *w/ indexing*

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

$ BANAN**A**
A $BANA**N**
A NA$BA**N**
A NANA$**B**
B ANANA**$**
N A$BAN**A**
N ANA$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

A B A B

B 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”

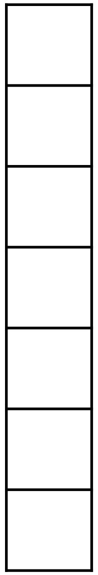
C) “bb$”

D) “b$b”

Suffix Array

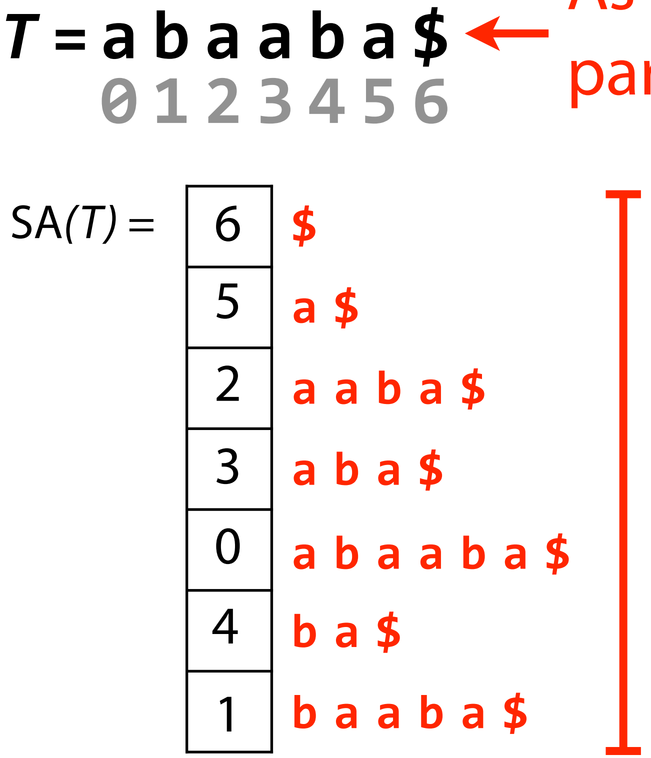
Suffix array of *T* is an array of integers specifying lexicographic (alphabetical) order of *T*'s suffixes

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 $
              $
```

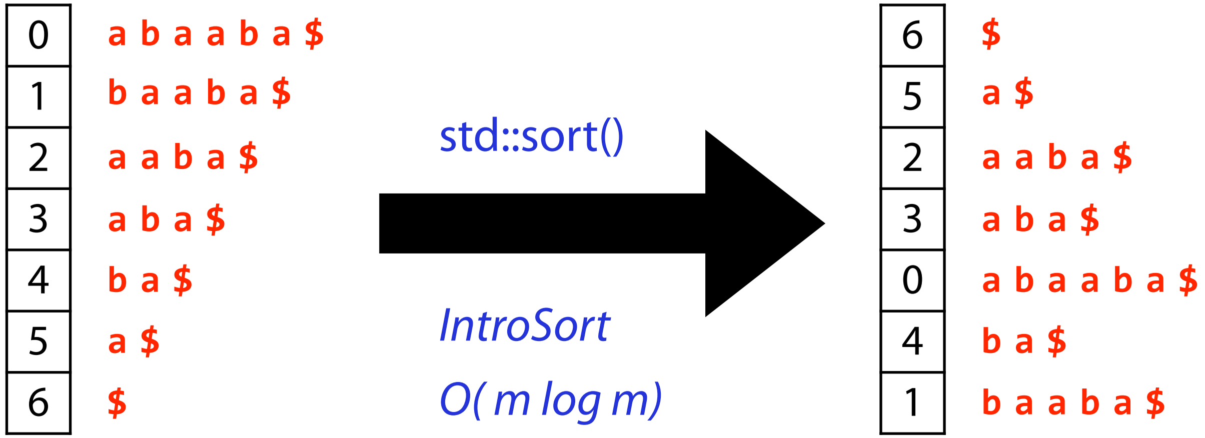
m suffixes

Output:

5
4
0
3
1
2

Suffix array: build by sorting (from array)

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



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	$

std::sort()

IntroSort

O(m 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 $

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.

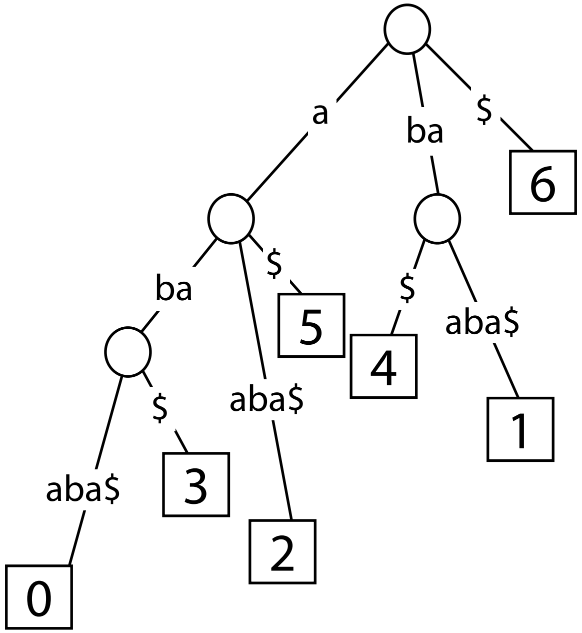
There exist several ***O*(*m*)** algorithms that *divide-and-conquer*

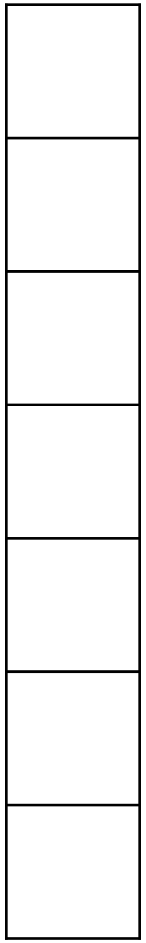
Kärkkäinen J, Sanders P. "Simple linear work suffix array construction." Automata, Languages and Programming (2003): 187-187.

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

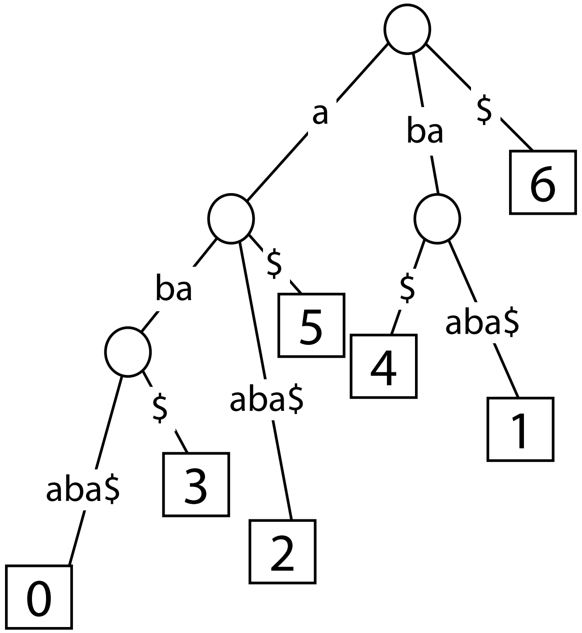
(a) Build suffix tree, (b) traverse in lexicographic order, (c) upon reaching leaf, append suffix to array





Suffix array: build by suffix tree

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



6	$
5	a$
2	aaba$
3	aba$
0	abaaba$
4	ba$
1	baaba$

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!

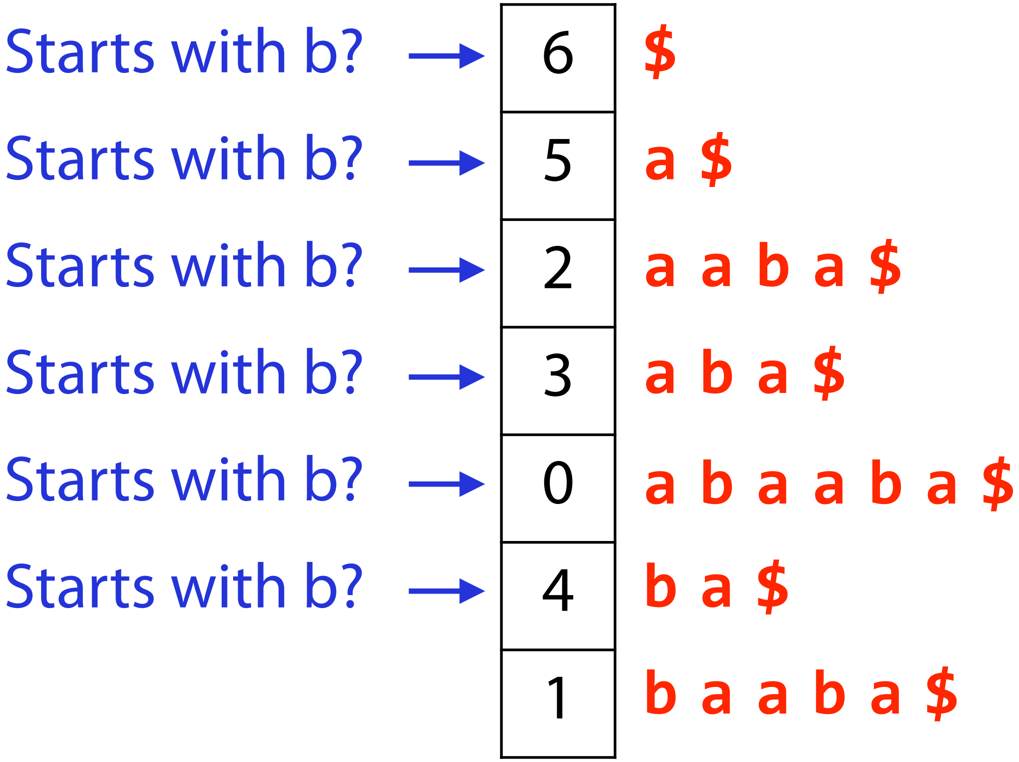
Challenge yourself: Try to build in O(m^2 log m) or better.

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 $

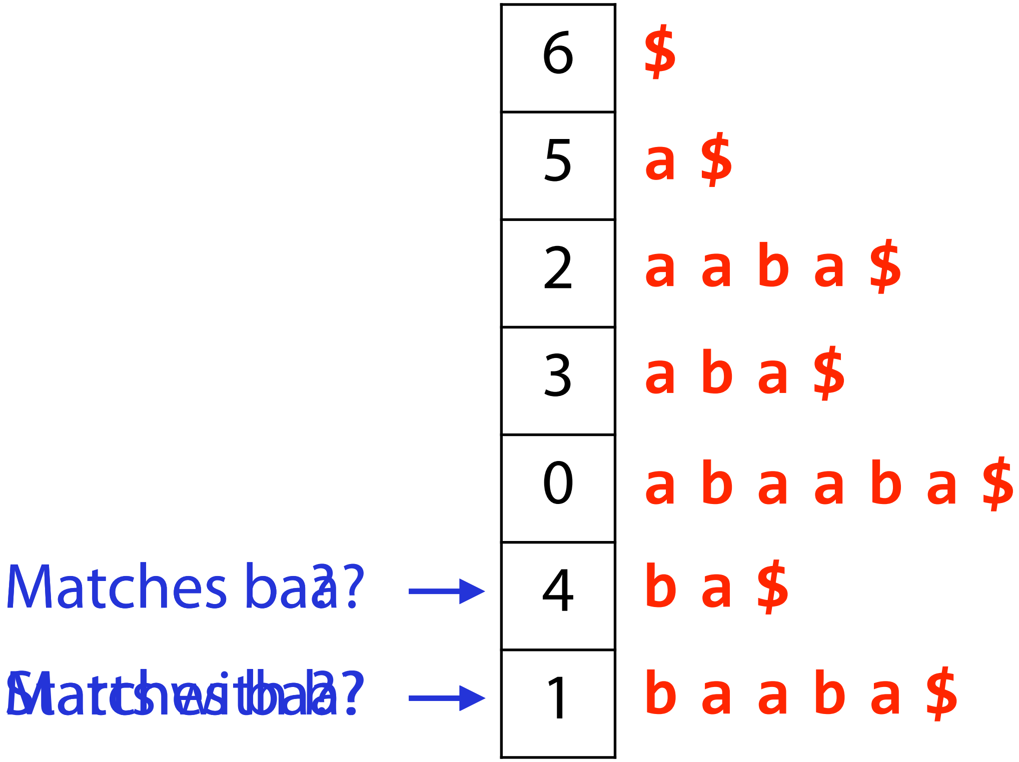
1 b a a b a $

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 $
4	b a $
1	b a a b a $

Matches baa? Matches ba? →

Starts with ba? Matches baa? →

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 $

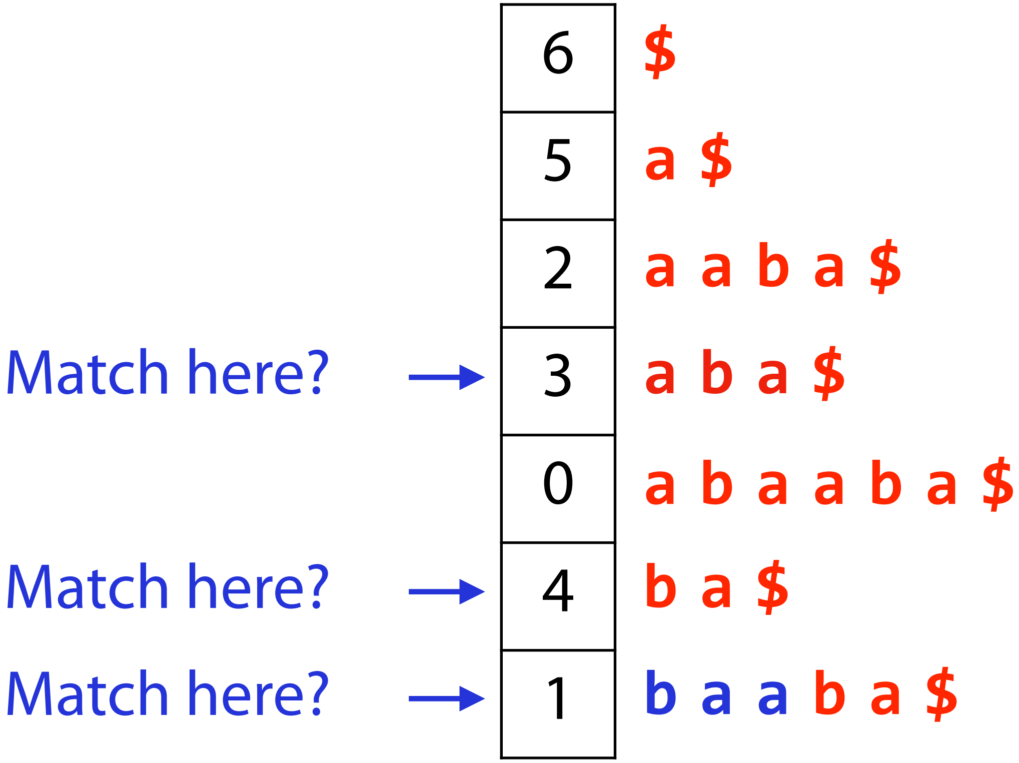
Return {1}

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 aaba$

Match here? → 3 aba$

0 abaaba$

Match here? → 4 ba$

Match here? → 1 baaba$

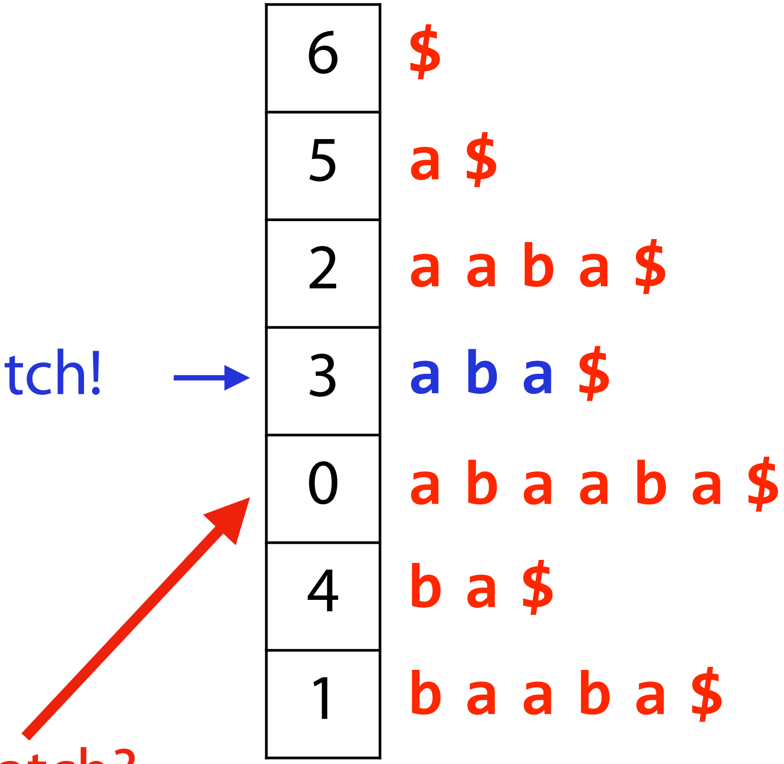
Return {1}

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!

Return {3}!

But what about our other match?

Searching a suffix array

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

1. Pick suffixes using binary search

2. Compare suffixes as normal

3. After match, check neighbors

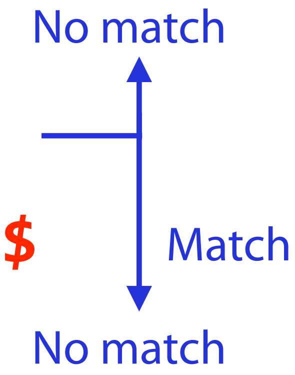
Assume we have k=m matches

What is our time complexity?

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 $



Return {0,3}

Searching a suffix array

How can we do better?

1. Identify the *smallest* and *largest* matches to *P* w/ binary search

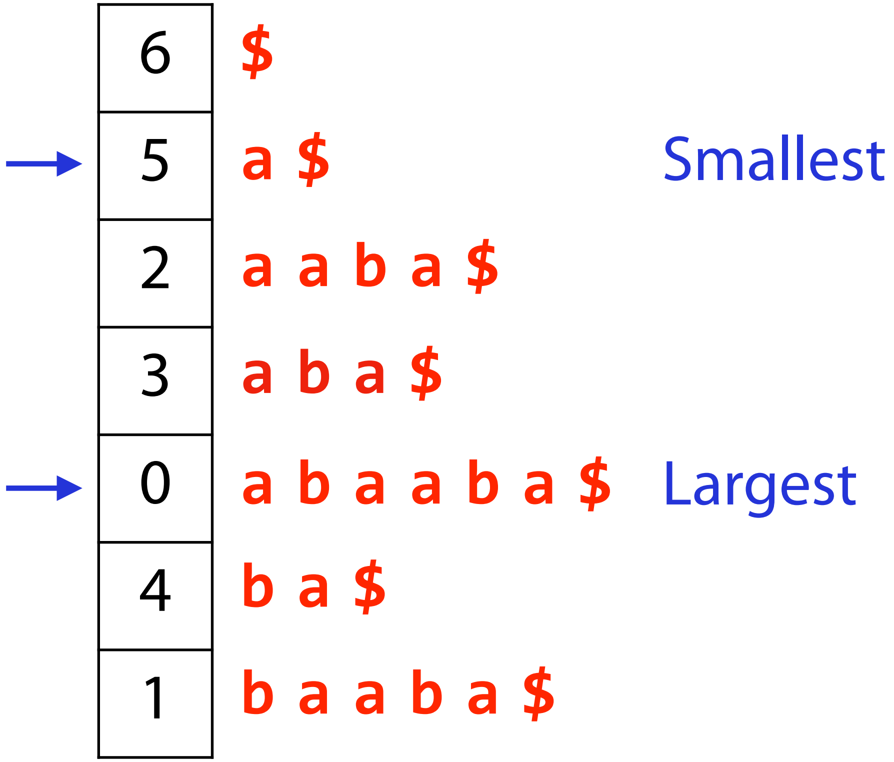
2. Return all values in that range!

Assume we have *k*=*m* matches

What is our time complexity?

T = abaaba$ *m* = |*T*|

P = a *n* = |*P*|



6	$	
5	a $	Smallest
2	a a b a $	
3	a b a $	
0	a b a a b a $	Largest
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

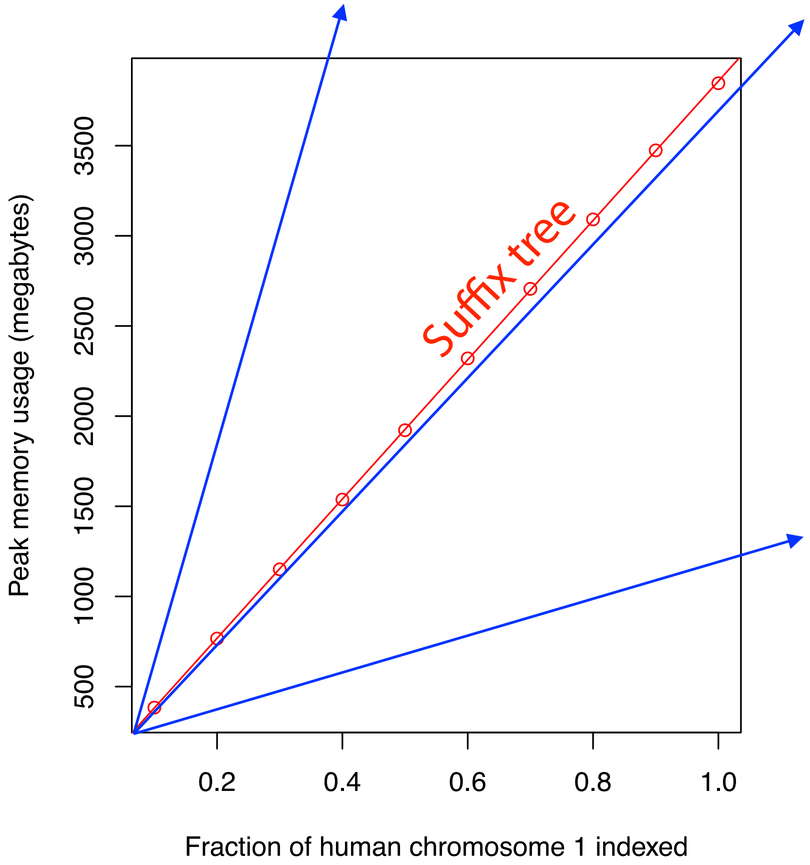
Be as efficient or inefficient as you like!

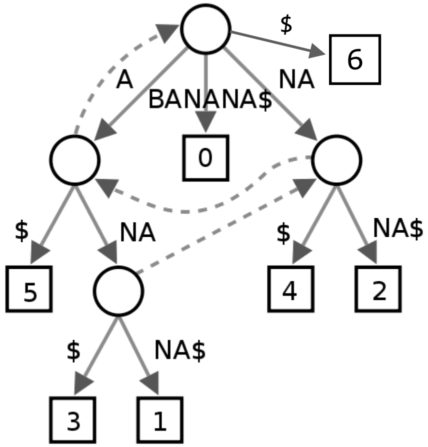
Challenge yourself: Try to search in $O(n \log m + k)$

Suffix tree vs suffix array: size

O(*m*) space, like suffix tree

Is “constant factor” worse, better, same?

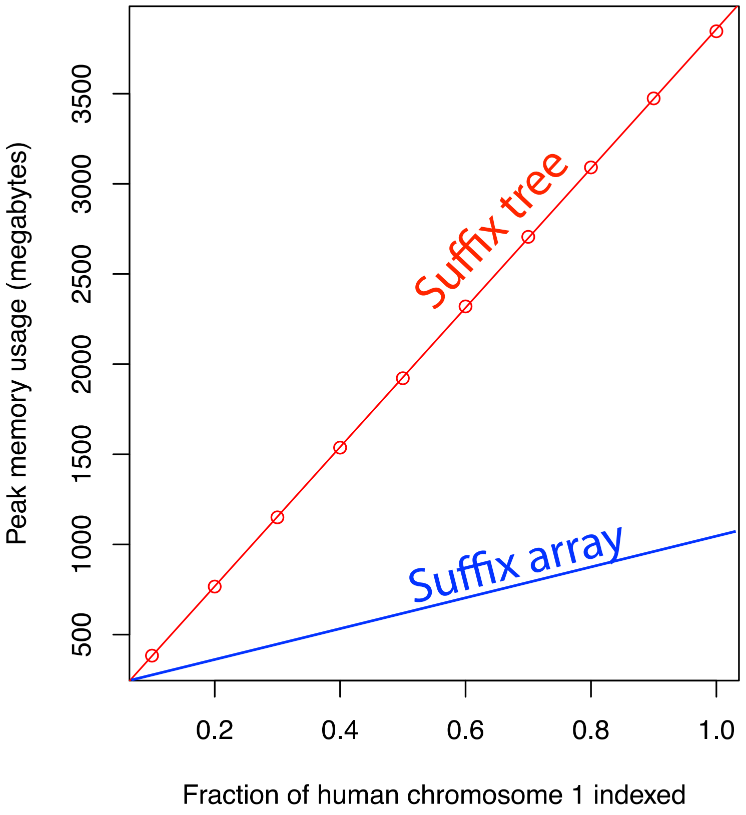


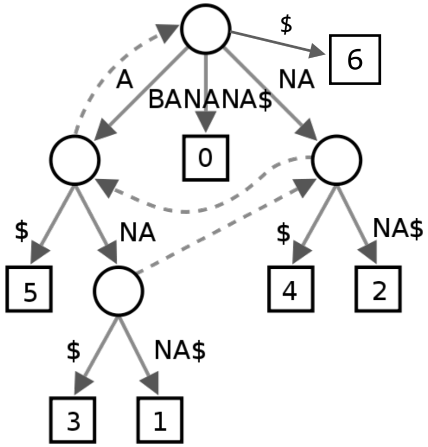


6	$
5	A$
3	ANA$
1	ANANA$
0	BANANA$
4	NA$
2	NANA$

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: size

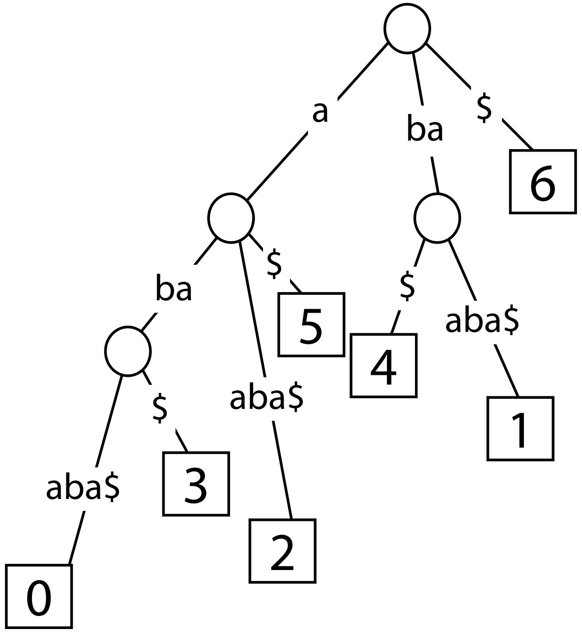
Suffix Array

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 $

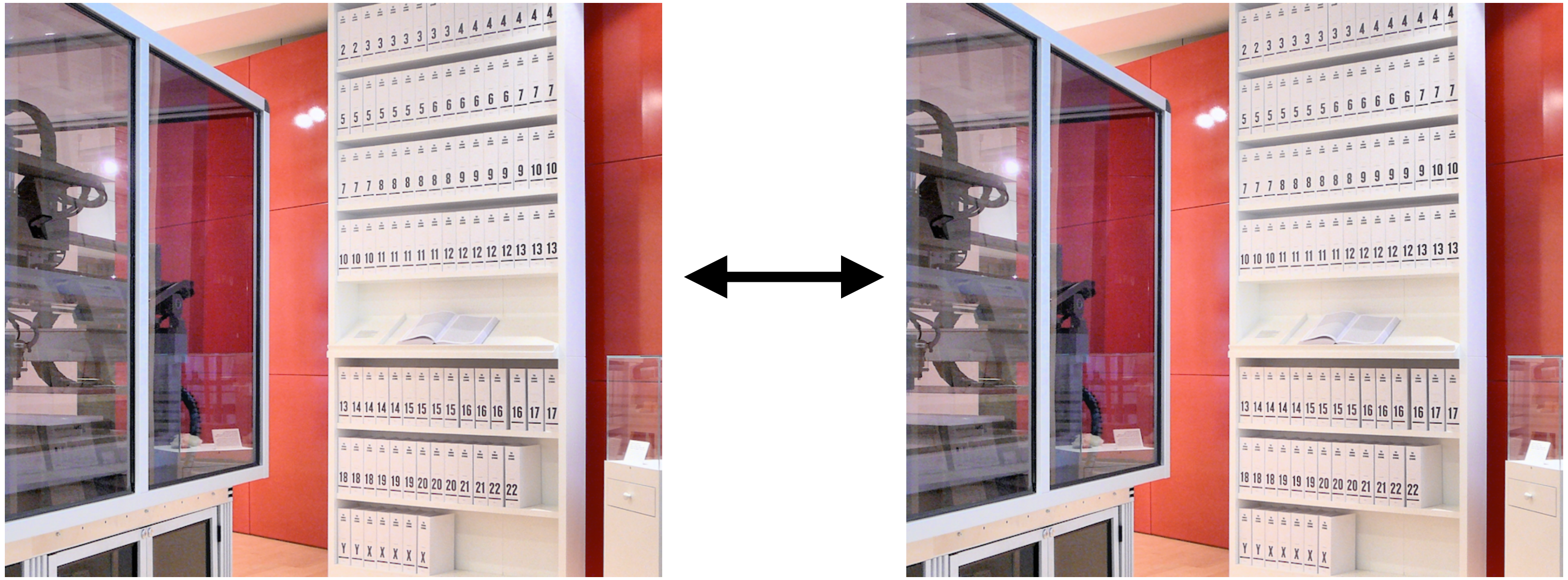
Suffix Tree

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.

Delcher, Arthur L., et al. "Fast algorithms for large-scale genome alignment and comparison." *Nucleic Acids Research* 30.11 (2002): 2478-2483.

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

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

~ 4,000 citations

http://mummer.sourceforge.net