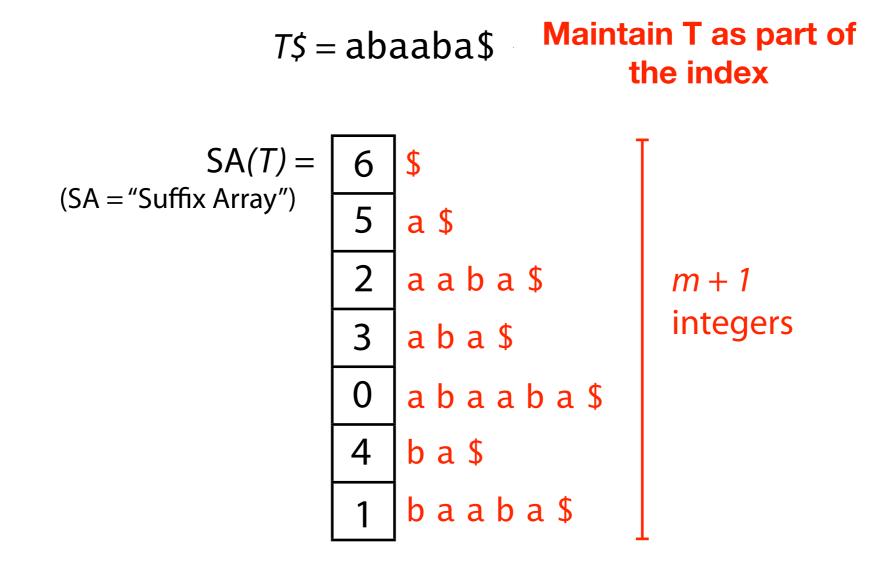
Full-text indexing: The Suffix Array



Suffix array



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

Another Example Suffix Array

```
s = cattcat$
```

- Idea: lexicographically sort all the suffixes.
 - Store the starting indices of the suffixes in an array.

```
0 cattcat$
1 attcat$
2 ttcat$
3 tcat$
4 cat$
5 at$
6 t$
7 $
```

```
sort the suffixes alphabetically

the indices just 
"come along for the ride"
```

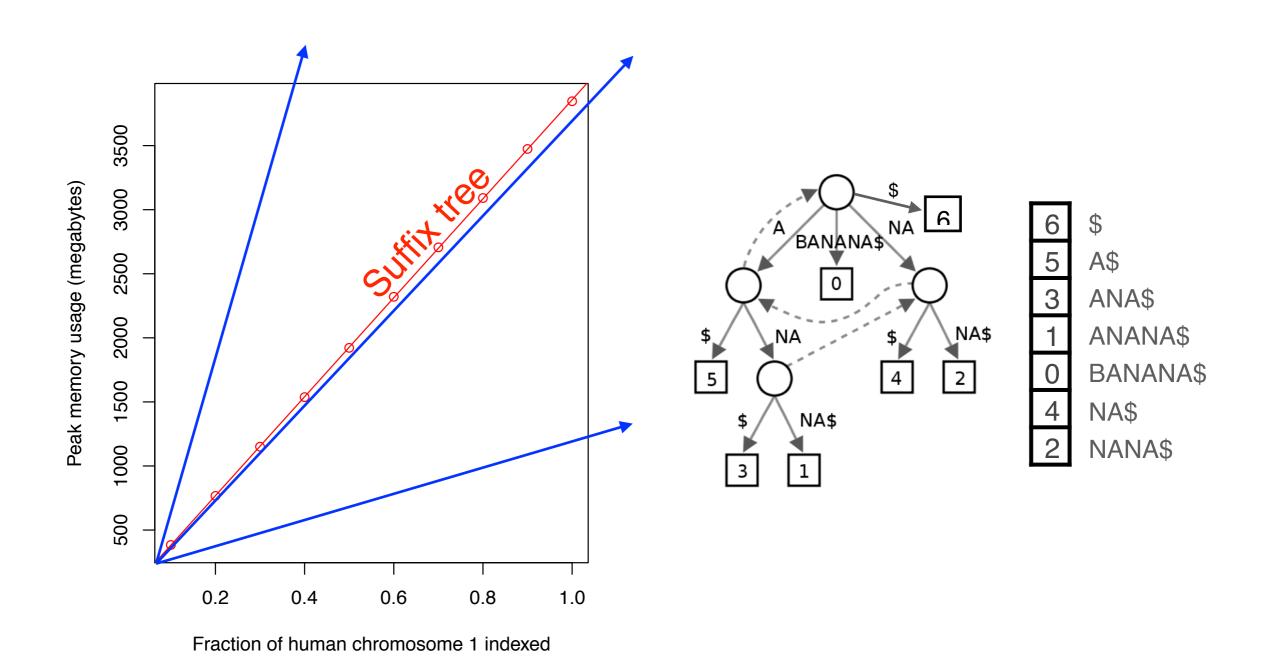
```
7 $
5 at$
4 cat$
0 cattcat$
6 t$
3 tcat$
2 ttcat$
```

index of suffix

suffix of s

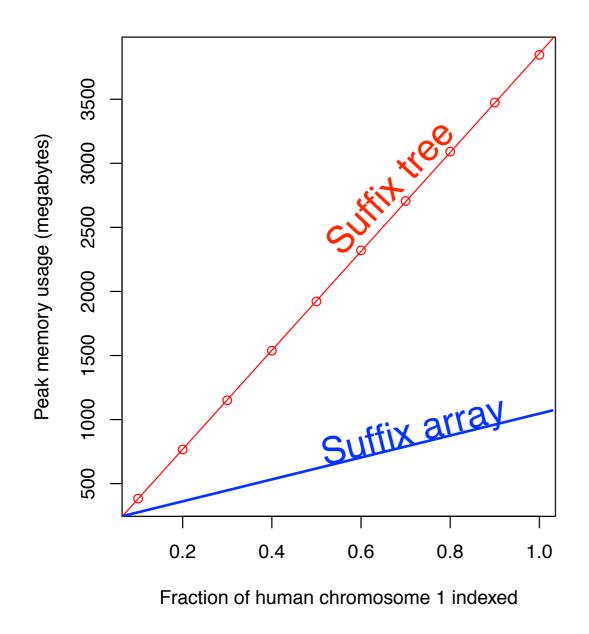
Suffix array

O(m) space, like suffix tree Is "constant factor" worse, better, same?



Suffix array

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



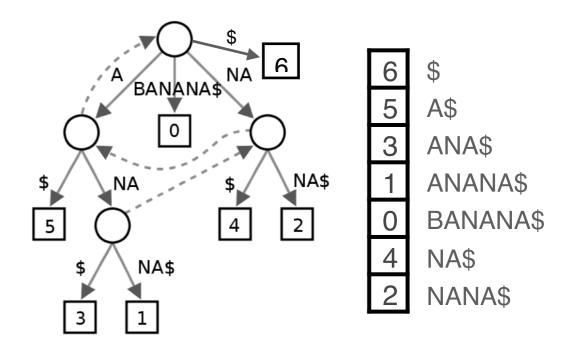


Table I. Performance Summary of the Construction Algorithms

Algorithm	Worst Case	Time	Memory
Prefix-Doubling			
MM [Manber and Myers 1993]	$O(n \log n)$	30	8n
LS [Larsson and Sadakane 1999]	$O(n \log n)$	3	8n
Recursive			
KA [Ko and Aluru 2003]	O(n)	2.5	7-10n
KS [Kärkkäinen and Sanders 2003]	O(n)	4.7	10-13n
KSPP [Kim et al. 2003]	O(n)	_	_
HSS [Hon et al. 2003]	O(n)	_	_
KJP [Kim et al. 2004]	$O(n \log \log n)$	3.5	13-16n
N [Na 2005]	O(n)	_	_
Induced Copying	_		
IT [Itoh and Tanaka 1999]	$O(n^2 \log n)$	6.5	5n
S [Seward 2000]	$O(n^2 \log n)$	3.5	5n
BK [Burkhardt and Kärkkäinen 2003]	$O(n \log n)$	3.5	5-6n
MF [Manzini and Ferragina 2004]	$O(n^2 \log n)$	1.7	5n
SS [Schürmann and Stoye 2005]	$O(n^2)$	1.8	9-10n
BB [Baron and Bresler 2005]	$O(n\sqrt{\log n})$	2.1	18n
M [Maniscalco and Puglisi 2007]	$O(n^{\frac{1}{2}}\log n)$	1.3	5-6n
MP [Maniscalco and Puglisi 2006]	$O(n^2 \log n)$	1	5-6n
Hybrid			
IT+KA	$O(n^2 \log n)$	4.8	5n
BK+IT+KA	$O(n \log n)$	2.3	5-6n
BK+S	$O(n \log n)$	2.8	5-6n
Suffix Tree	_		
K [Kurtz 1999]	$O(n\log\sigma)$	6.3	13–15n

Time is relative to MP, the fastest in our experiments. Memory is given in bytes including space required for the suffix array and input string and is the average space required in our experiments. Algorithms HSS and N are included, even though to our knowledge they have not been implemented. The time for algorithm MM is estimated from experiments in Larsson and Sadakane [1999].

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

```
a $
  aaba$
  aba$
3
  abaaba$
0
  b a $
  baaba$
```

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

```
a $
  aaba$
  aba$
3
  abaaba$
0
  b a $
  baaba$
```

Is P a substring of T?

 For P to be a substring, it must be a prefix of ≥1 of T's suffixes 6

Pay attention to this observation!

Almost all full-text indices (definitely the ones we will learn about), work based on the observation that *every substring of T is a prefix of some suffix of T.* These indices then focus on how to *organize* suffixes of T in a manner amenable to efficient search.

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 $O(n \log m)$

a \$ aaba\$ aba\$ 3 abaaba\$ b a \$ baaba\$

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

† 'center' "right"

Notation: We'll use use SA[l] to refer to the suffix corresponding to suffix-array element l. We could write T[SA[l]:], but that's too verbose.

Throughout the search, invariant is maintained:

Y

Throughout search, invariant is maintained:

What do we do at each iteration?

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

If P < \text{SA}[c], either stop or let r = c and iterate

If P > \text{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 r
```

Longest Common Prefix

The longest common prefix of two strings s,t is simply the length of the prefix they share prior to the first difference (or the termination of either string).

S ACTTACAGACGACCCGAGAC

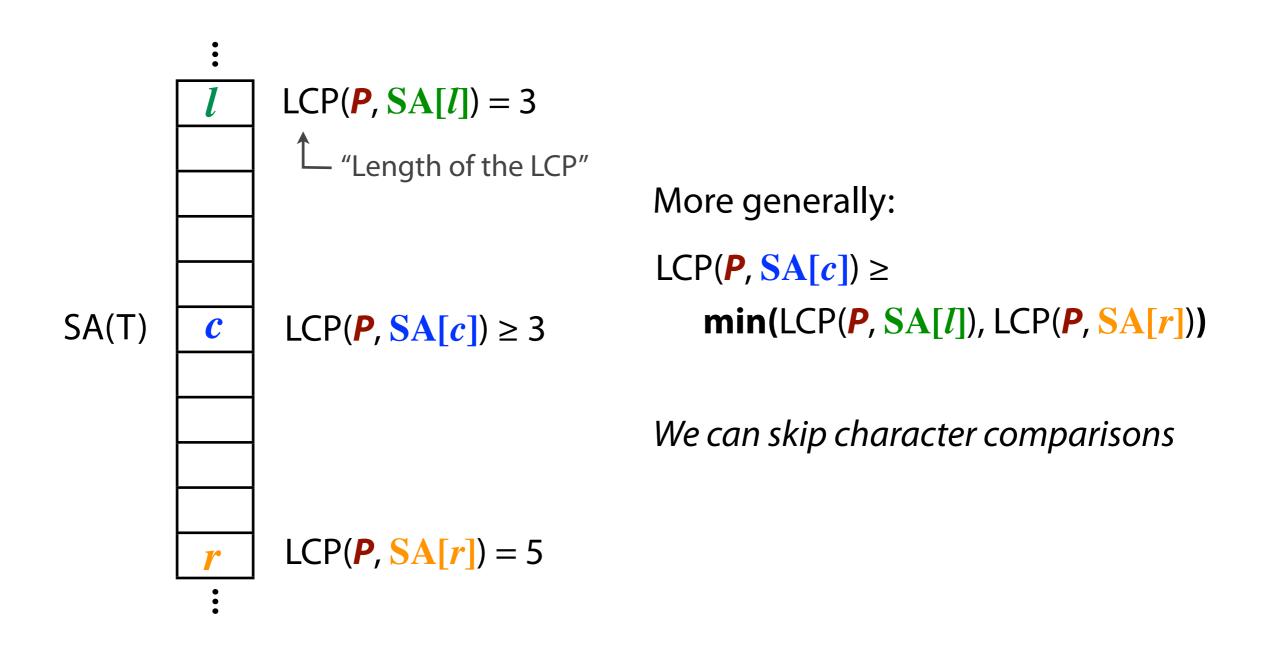
T ACTTACAGACGACGAGCTAGC

LCP(S,T) = ACTTACAGACGAC

|LCP(S,T)| = 13

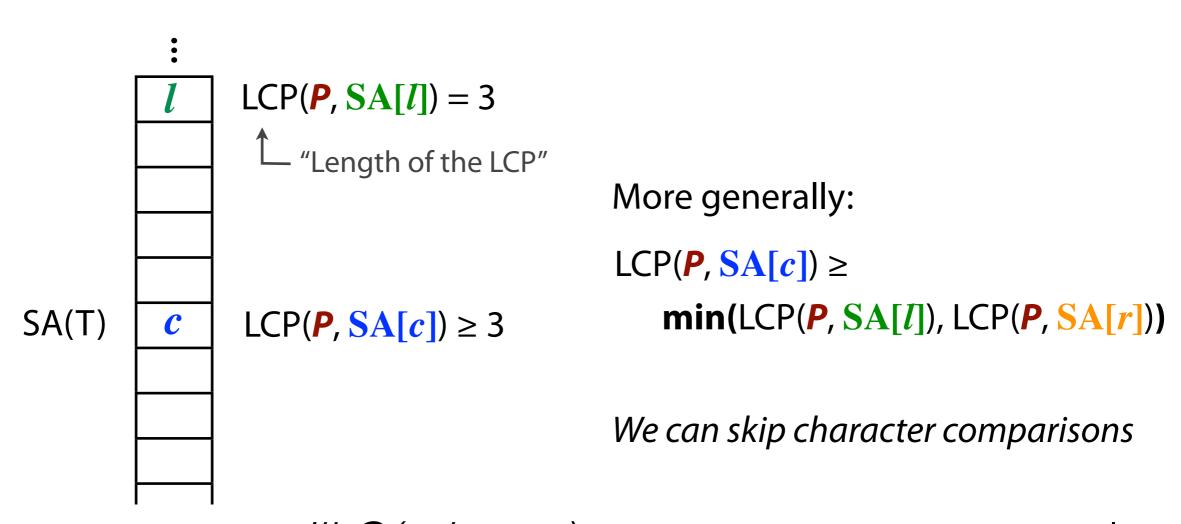
Below, to avoid extra notation, we will use LCP(S,T) as shorthand for |LCP(S,T)|

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



7

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



worst case still O(n log m), but we're closer. worst case example $S=ac_{M-2}b$, P=c

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

Imagine we had pre-computed LCP(i,j) for all suffixes i and j in the original text T.

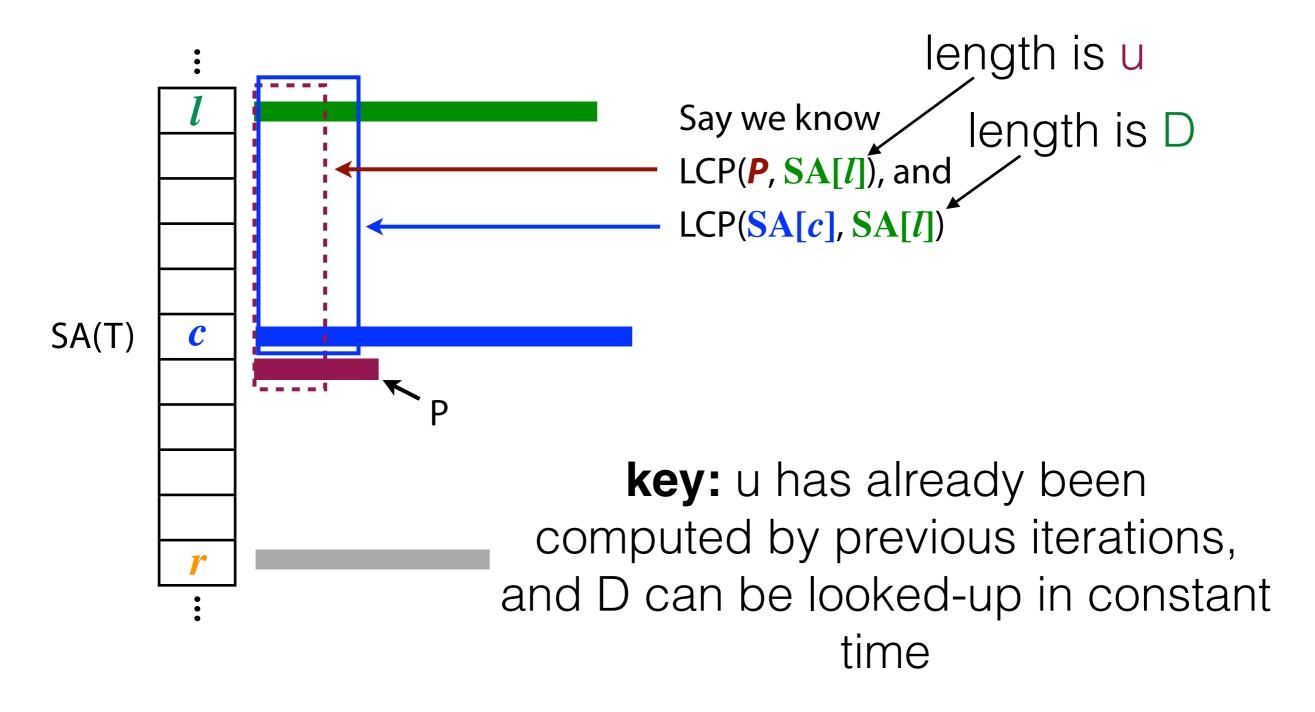
$$LCP(P, SA[c]) \ge 3$$

$$LCP(P, SA[r]) = 5$$

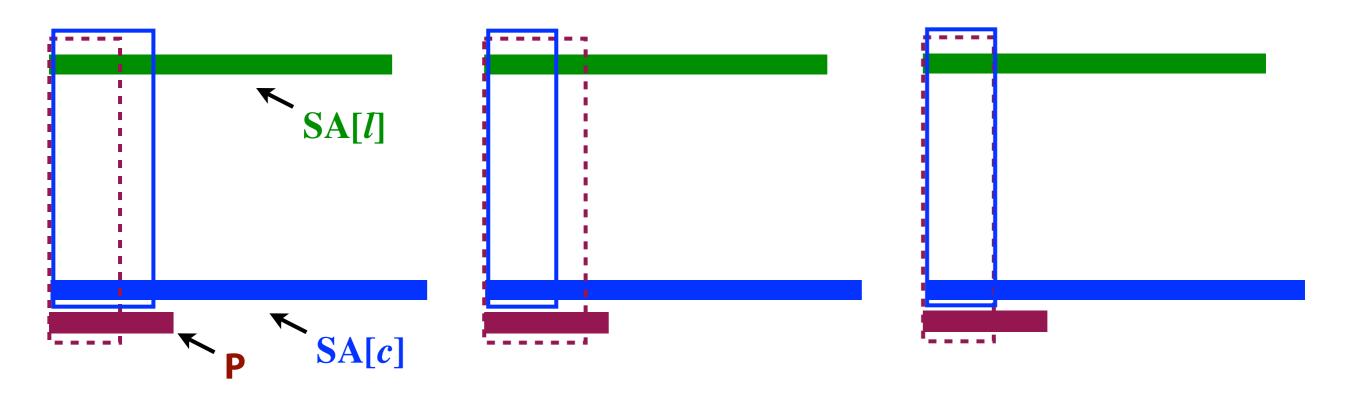
worst case still O(n log m), but we're closer.

Take an iteration of binary search:

Assume, wlog, that $D = LCP(SA[I], SA[c]) \ge D' = LCP(SA[c], SA[r])$ otherwise there are symmetric cases.



Three cases: or, if D' = LCP(P, SA[r]) is larger, 3 symmetric cases.



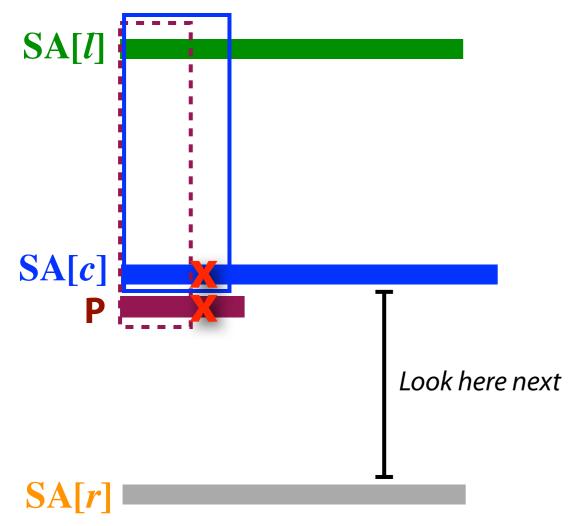
$$LCP(SA[c], SA[l]) >$$
 $LCP(P, SA[l])$

$$LCP(SA[c], SA[l]) =$$
 $LCP(P, SA[l])$

LCP(SA[c], SA[l]) >

Case 1:

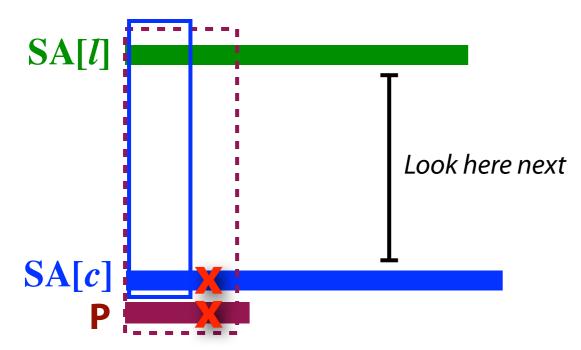
LCP(P, SA[l])



LCP(SA[c], SA[l]) >LCP(P, SA[l]) Next char of P after the LCP(P, SA[I]) must be *greater than* corresponding char of SA[c]

In this case, we compute LCP(P[u:], SA[c][u:]). c becomes our new I, and now we know the new LCP(P, SA[I]), b/c we just computed it!

Case 2: LCP(SA[c], SA[l]) < LCP(P, SA[l])



Next char of **SA**[*c*] after LCP(**SA**[*c*], **SA**[*l*]) must be *greater than* corresponding char of **P**

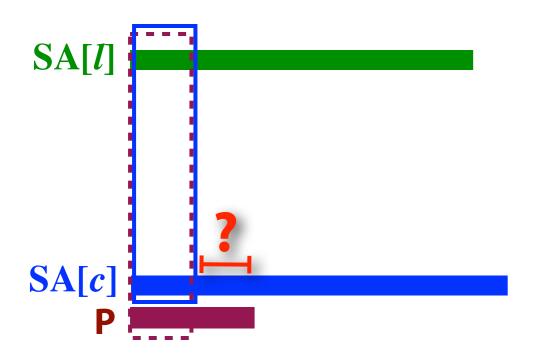
P < SA[c]

SA[r]

LCP(SA[c], SA[l]) < LCP(P, SA[l])

In this case, we compute LCP(P[u:], SA[c][u:]). c becomes our new r, and now we know the new LCP(P, SA[r]), b/c we just computed it!

Case 3:
$$LCP(SA[c], SA[l]) = LCP(P, SA[l])$$



Must do further character comparisons between P and SA[c]

Each such comparison either:

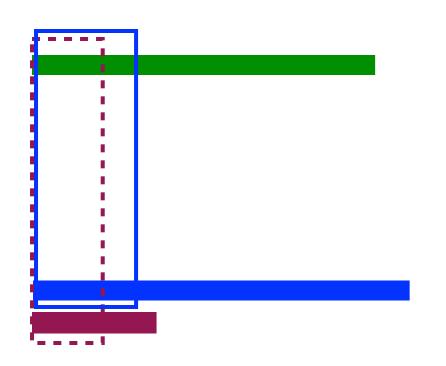
- (a) mismatches, leading to a bisection
- (b) matches, in which case LCP(P, SA[c]) grows

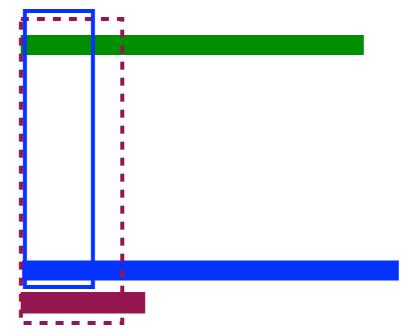
SA[r]

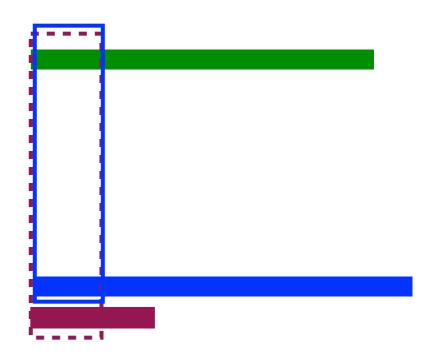
LCP(SA[c], SA[l]) = LCP(P, SA[l])

We improved binary search on suffix array from $O(n \log m)$ to $O(n + \log m)$ using information about Longest Common Prefixes (LCPs).

LCPs between *P* and suffixes of *T* computed during search, LCPs *among* suffixes of *T* computed *offline*







LCP(SA[c], SA[l]) >LCP(P, SA[l]) LCP(SA[c], SA[l]) < LCP(P, SA[l])

LCP(SA[c], SA[l]) = LCP(P, SA[l])

Bisect right!

Bisect left!

Compare some characters, then bisect!

Sketch of Running Time

Thm. Given the LCP(X,Y) values, searching for a string P in a suffix array of length m now takes $O(|P| + \log m)$ time.

In case 1 & 2, we make O(1) comparisons and bisect left or right — there are at most O(log m) bisections.

In case 3 we try to match characters starting at some offset between SA[c] and P. If they match, those characters will never be compared again, so there are at most O(IPI) such comparisons.

Mismatching characters may be compared more than once.

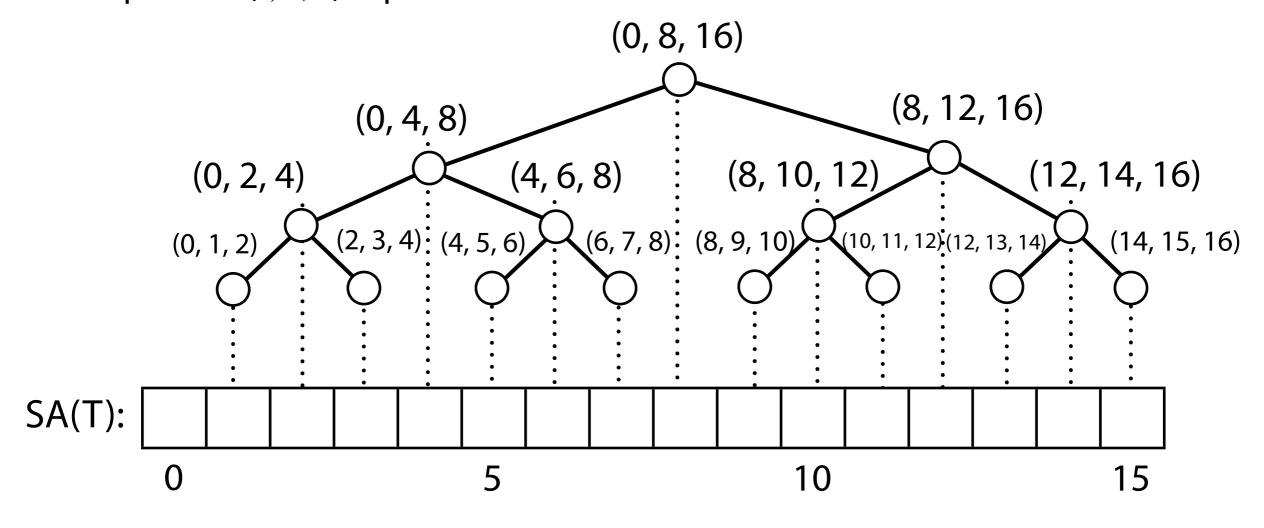
But there can be only 1 mismatch / bisection. There are O(log m) bisections, so there are at most O(log m) mismatches.

:. Total # of comparisons = $O(|P| + \log m)$.

How to pre-compute LCP

- To perform this "efficient" search, we must be able to look up LCP(SA[c], SA[I]) and LCP(SA[c], SA[r]).
- How can we pre-compute this information efficiently?
 - Which LCP values do we need (hint: not all of them)?
 - Given LCP for left and right sub-interval of a search, how can we compute LCP for the containing interval?

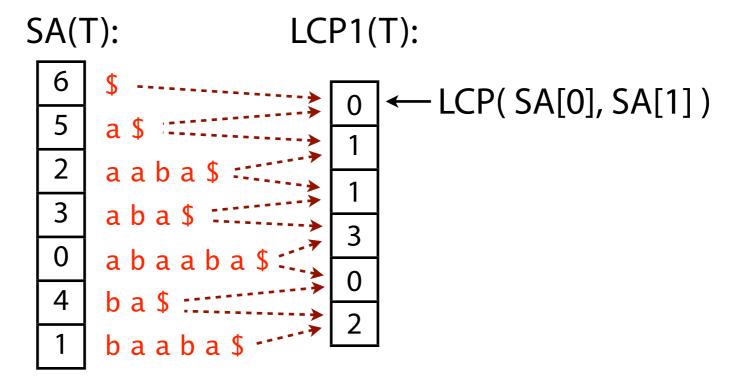
How to pre-calculate LCPs for every (l, c) and (c, r) pair in the search tree? Triples are (l, c, r) triples



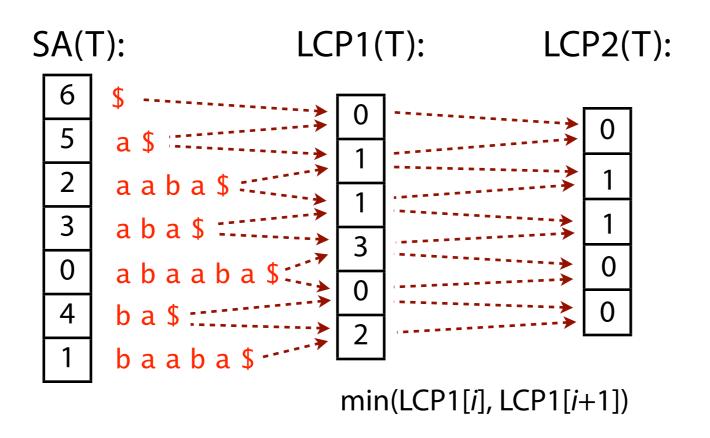
Example where m = 16 (incl. \$) # search tree nodes = m - 1

Suffix Array (SA) has *m* elements

Define LCP1 array with m - 1 elements such that LCP[i] = LCP(SA[i], SA[i+1])



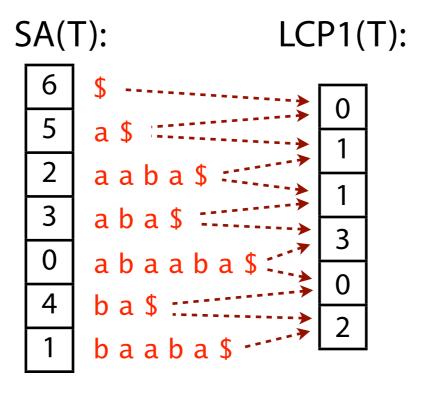
LCP2[i] = LCP(SA[i], SA[i+1], SA[i+2])

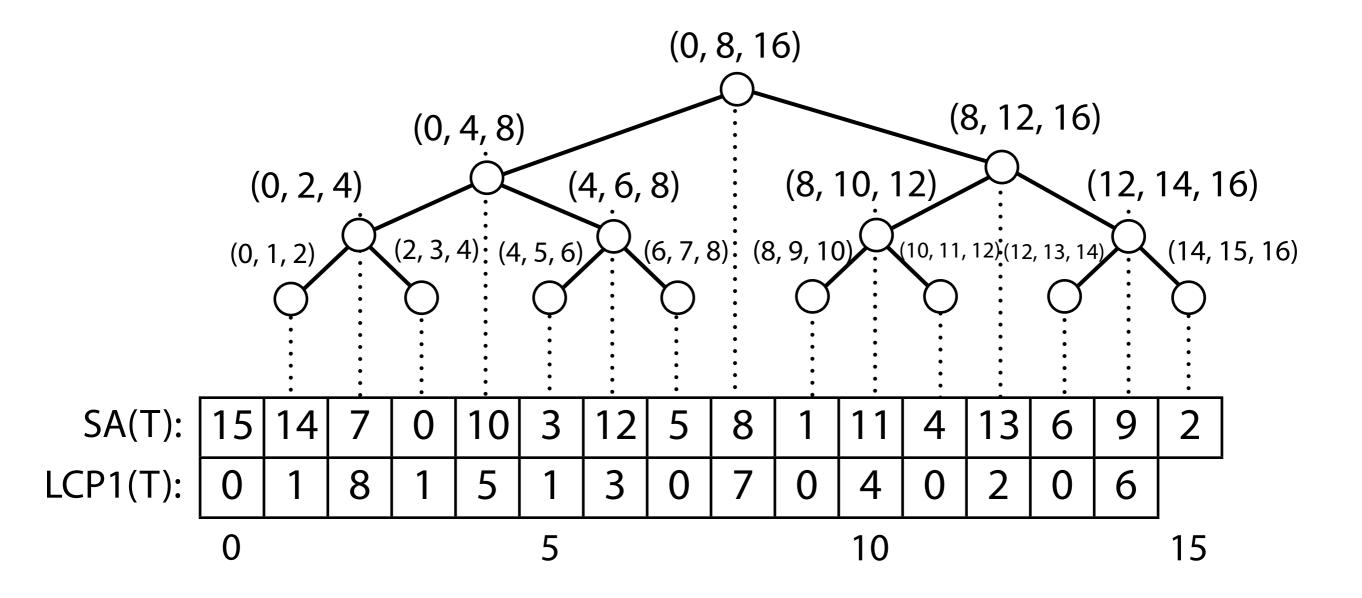


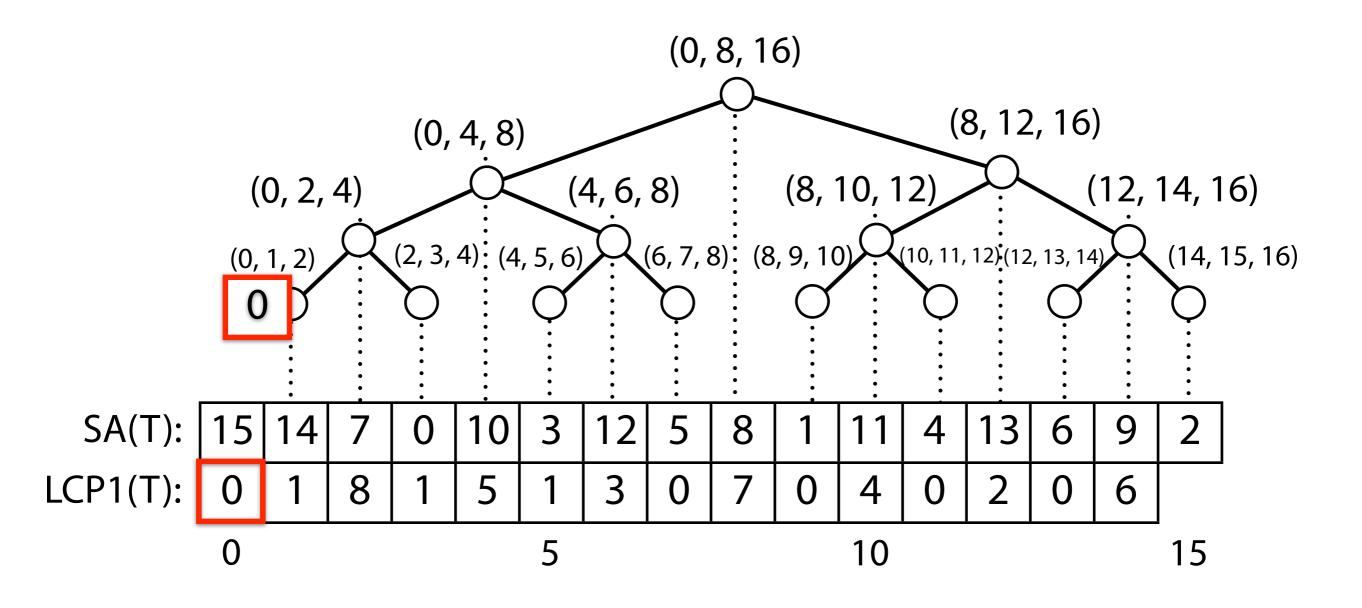
In fact, LCP of a range of consecutive suffixes in SA equals the minimum LCP1 among adjacent pairs in the range

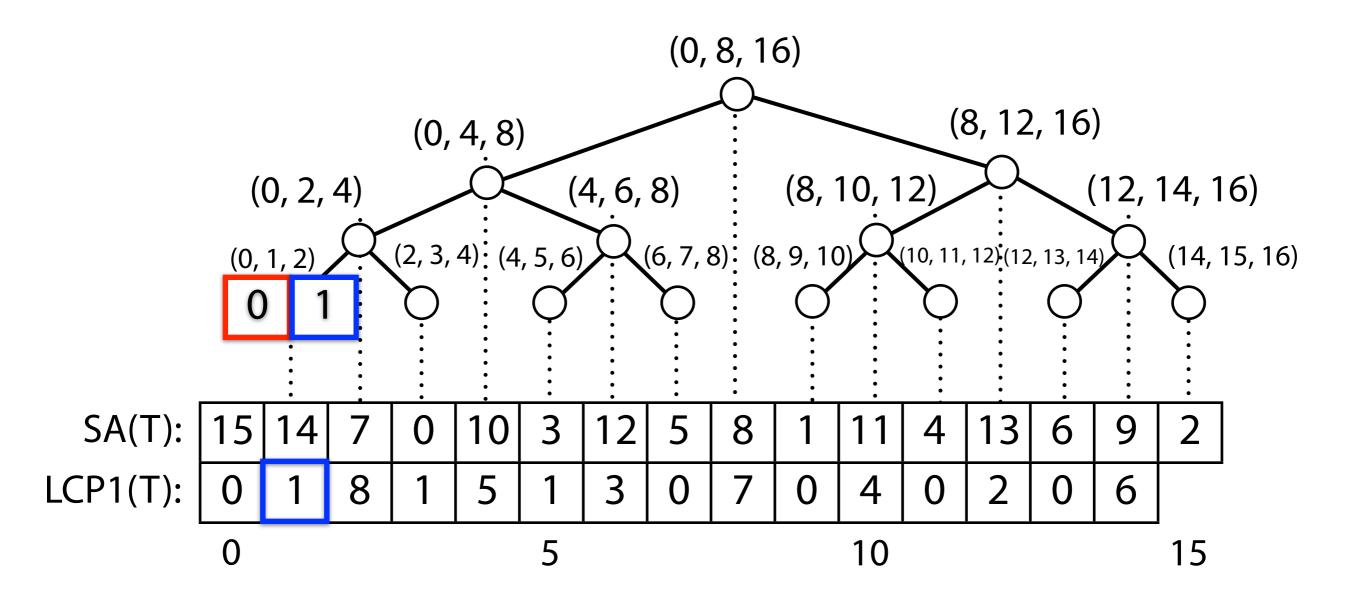
LCP1 is a building block for other useful LCPs

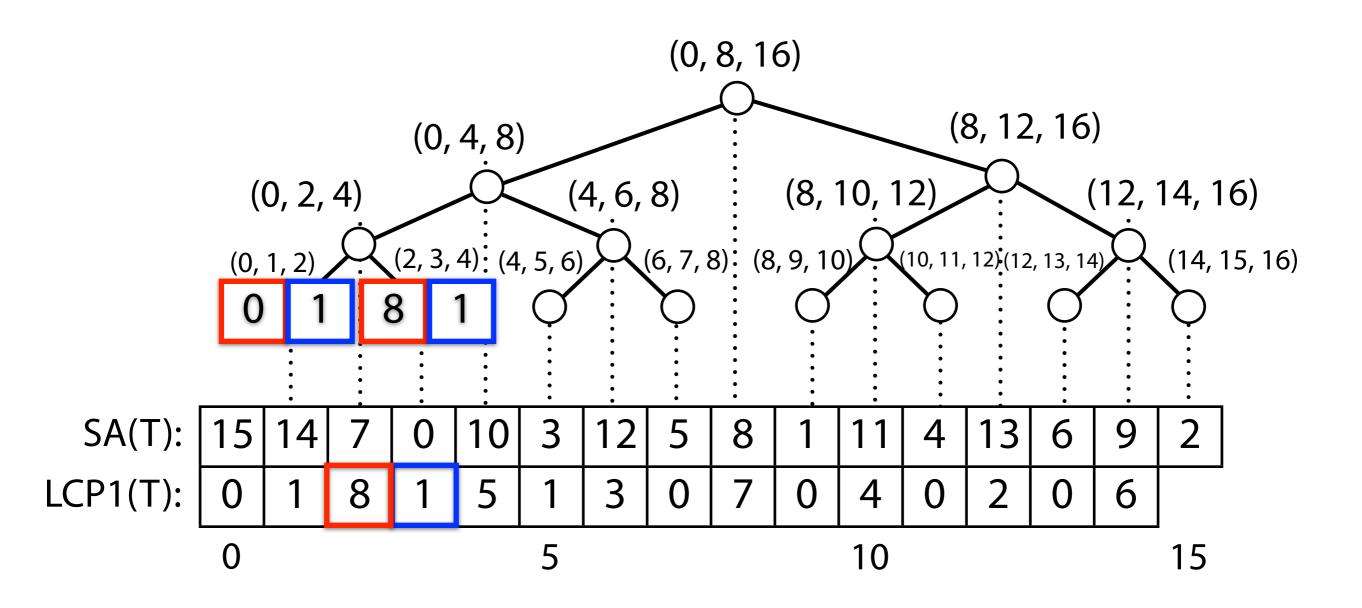
Good time to calculate LCP1 it is at the same time as we build the suffix array, since putting the suffixes in order involves breaking ties after common prefixes

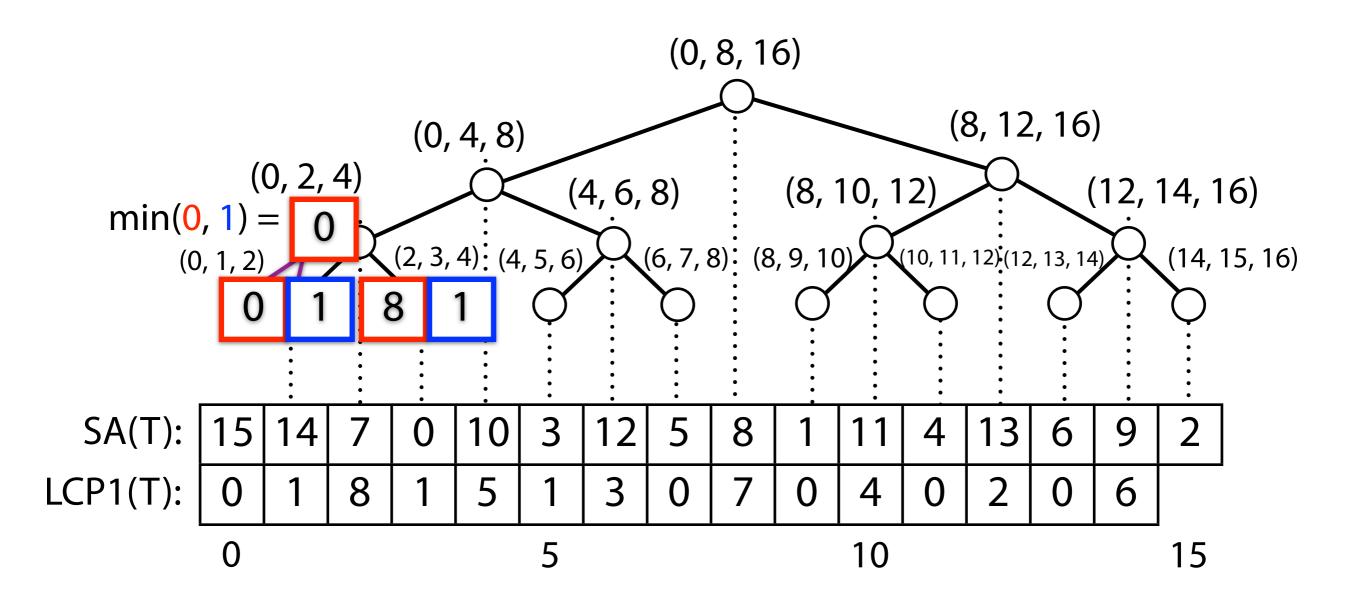


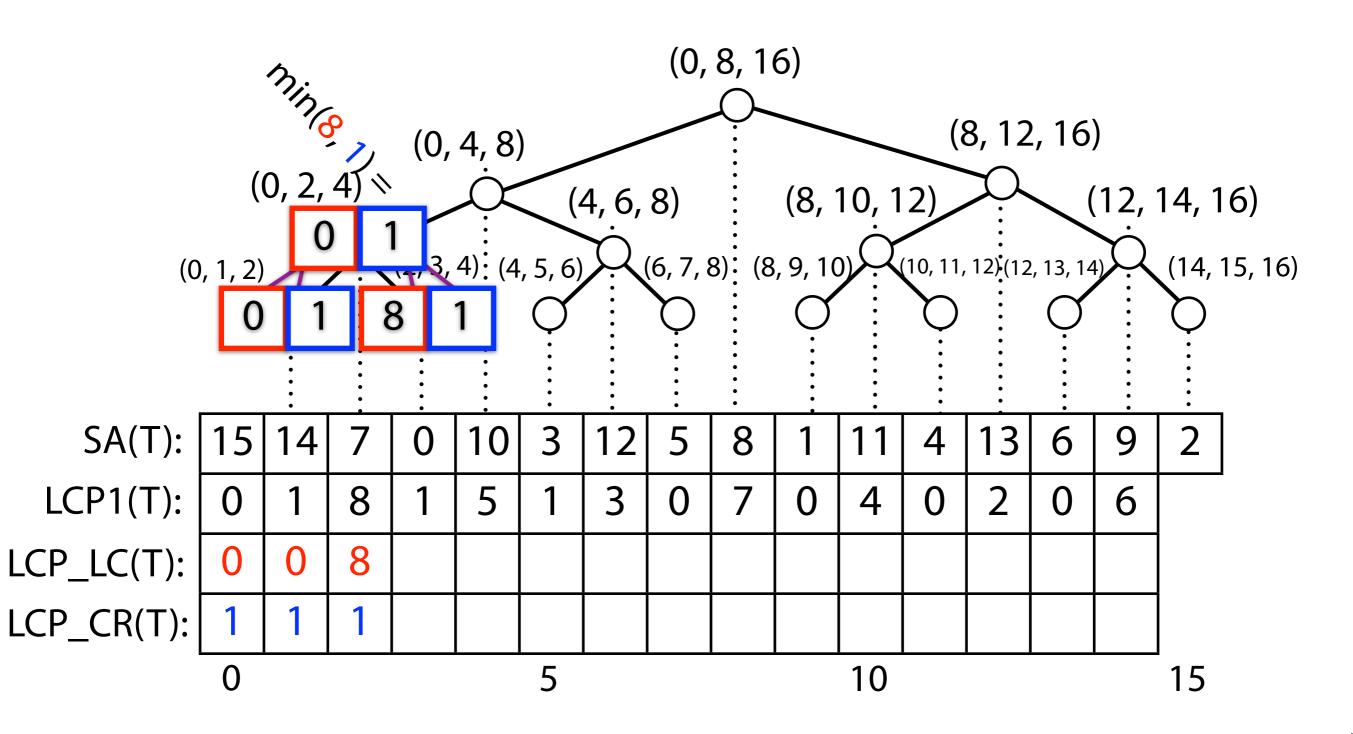




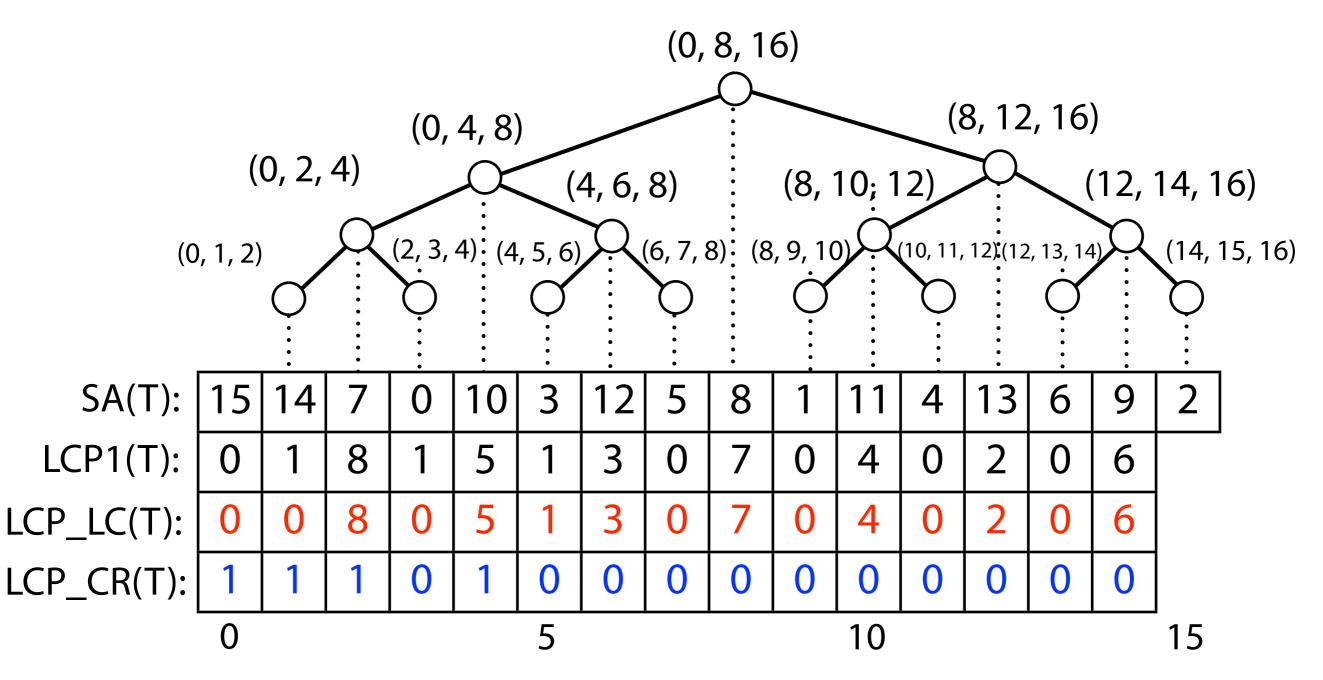








T = abracadabracada\$

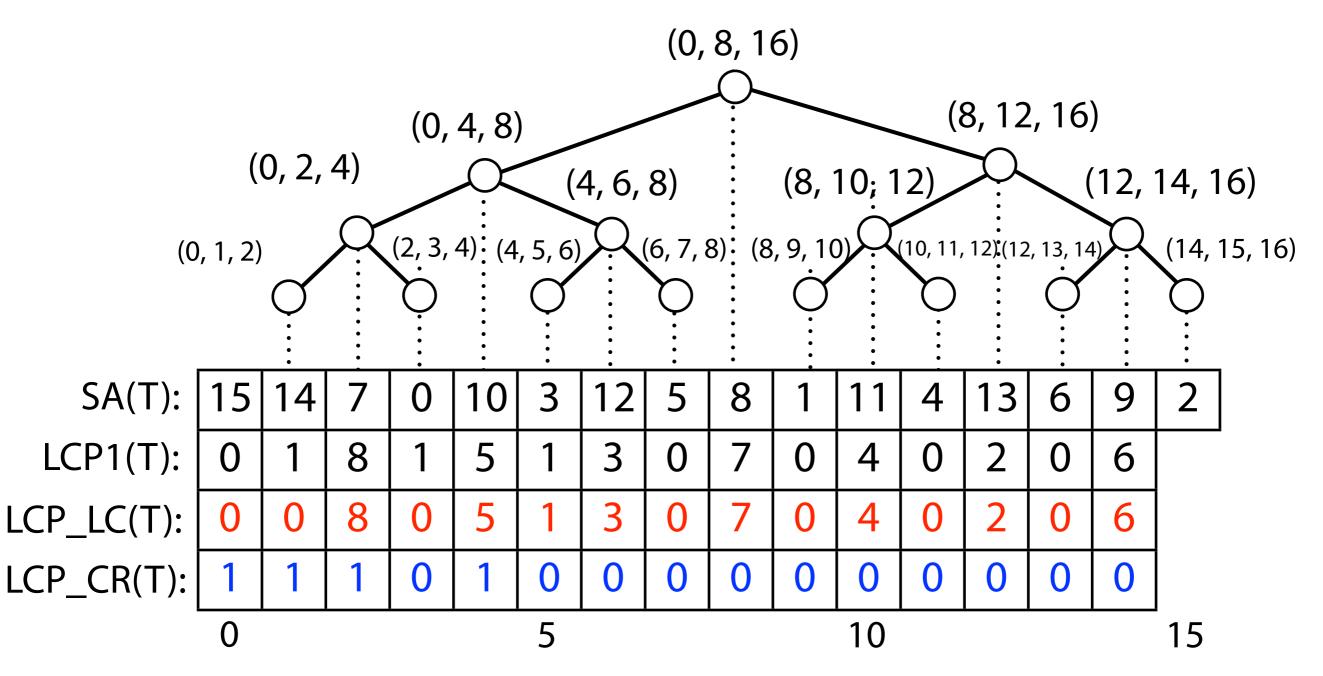


NOTE: These arrays are "shifted" by 1 — the value in LCP_LC corresponding to (0, 1, 2) is at LCP_LC[0], not LCP_LC[1]. So, to look up LCP(SA[I], SA[c]) we look at LCP_LC[c-1]

T = abracadabracada\$

Can be done in:

O(m) time and space



NOTE: These arrays are "shifted" by 1 — the value in LCP_LC corresponding to (0, 1, 2) is at LCP_LC[0], not LCP_LC[1]. So, to look up LCP(SA[I], SA[c]) we look at LCP_LC[c-1]

Suffix array: querying review

We saw 3 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 $O(n \log m)$, but it can be argued it's near $O(n + \log m)$ in practice.

Gusfield: "Simple Accelerant"

3. Binary search with skipping using all LCPs, including LCPs among T's suffixes. $O(n + \log m)$.

Gusfield: "Super Accelerant"

How much space do they require?

- 1. ~m integers (SA)
- 2. $\sim m$ integers (SA)
- 3. ~3*m* integers (SA, LCP_LC, LCP_CR)

Suffix array: performance comparison

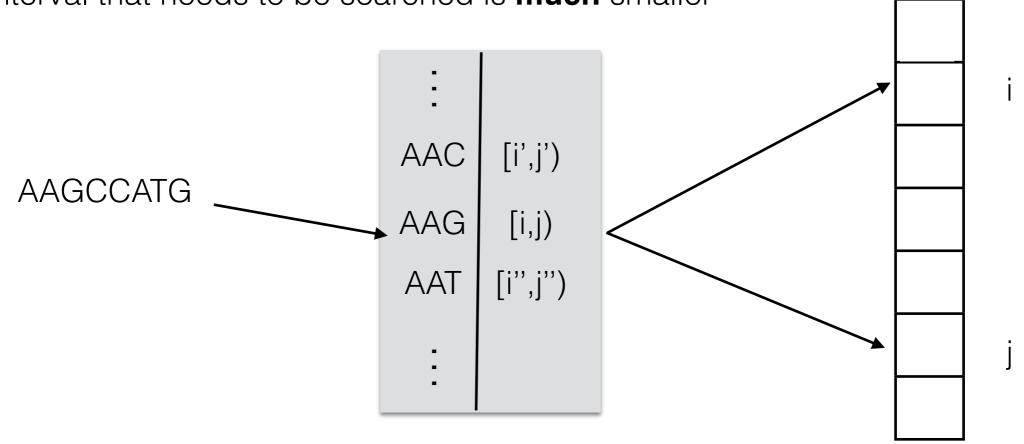
	Super accelerant	Simple accelerant	No accelerant	
python -O	68.78 s	69.80 s	102.71 s	
руру -О	5.37 s	5.21 s	8.74 s	
# character 99.5 M comparisons		117 M	235 M	

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

Another "practical" speedup

- Imagine you will never search for patterns of length
 k (e.g. 4-mers are non-informative in any moderately-sized genome)
- Consider the following "enhanced" suffix array:
 - Build a hash-table from k-mers to suffix array intervals. Now, any pattern of length k' > k must start with some hashed prefix of length k. Generally, the interval that needs to be searched is **much** smaller



Now, you only need to search the interval [i,j) — O(n * log(j-i)) time

Can provide considerable speedup

		dna	english	proteins	sources	xml
	m=16					
	$\overline{\mathrm{SA}}$	1.00	1.00	1.00	1.00	1.00
k=12	SA-LUT2	1.13	1.34	1.36	1.43	1.35
Linear	SA-LUT3	1.17	1.49	1.61	1.65	1.47
probing _	SA-hash	3.75	2.88	2.70	2.90	2.03
	$\overline{m=64}$					
Hash at	\overline{SA}	1.00	1.00	1.00	1.00	1.00
α =0.5	SA-LUT2	1.12	1.33	1.34	1.42	1.34
•	SA-LUT3	1.17	1.49	1.58	1.64	1.44
	SA-hash	3.81	2.87	2.62	2.75	1.79

Table 1. Speedups with regard to the search speed of the plain suffix array, for the five datasets and pattern lengths m = 16 and m = 64

Some other clever ideas#:

- Use a k-ary (B-tree) layout
- Use a lookup table where keys are concatenated Huffman codes of fixed bit length
- Use alternative strategy (doubling/galloping) to find the right SA boundary

Suffix array: sorting suffixes

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

```
abaaba$
                        def quicksort(q):
                            lt, gt = [], []
     baaba$
                            if len(q) <= 1:
     aaba$
                               return q
                            for x in q[1:]:
     aba$
                               if x < q[0]: ←
     ba$
                                   lt.append(x)
                               else:
     a $
                                   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 $
```

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.

The Skew Algorithm (aka DC3)

Kärkkäinen & Sanders, 2003

Main idea: Divide suffixes into 3 groups:

- Those starting at positions i=0,3,6,9,... (i mod 3=0)
- Those starting at positions 1,4,7,10,... (i mod 3 = 1)
- Those starting at positions 2,5,8,11,... (i mod 3 = 2)
- For simplicity, assume text length is a multiple of 3 after padding with a special character.

$$T[0,n) = \texttt{y} \ \texttt{a} \ \texttt{b} \ \texttt{b} \ \texttt{a} \ \texttt{d} \ \texttt{a} \ \texttt{b} \ \texttt{b} \ \texttt{a} \ \texttt{d} \ \texttt{o} \ \texttt{o}$$

$$SA = (12, 1, 6, 4, 9, 3, 8, 2, 7, 5, 10, 11, 0)$$

Basic Outline:

- Recursively handle suffixes from the i mod 3 = 1 and i mod 3 = 2 groups.
- Merge the i mod 3 = 0 group at the end.

Step 0 — Constructing a sample

These are called the "sample suffixes"

Step 0: Construct a sample. For k = 0, 1, 2, define

$$B_k = \{i \in [0, n] \mid i \mod 3 = k\}.$$

Let $C = B_1 \cup B_2$ be the set of sample positions and S_C the set of sample suffixes.

Example. $B_1 = \{1, 4, 7, 10\}, B_2 = \{2, 5, 8, 11\}, \text{ i.e., } C = \{1, 4, 7, 10, 2, 5, 8, 11\}.$

Step 1: Sort sample suffixes. For k = 1, 2, construct the strings

$$R_k = [t_k t_{k+1} t_{k+2}][t_{k+3} t_{k+4} t_{k+5}] \dots [t_{\max B_k} t_{\max B_k + 1} t_{\max B_k + 2}]$$

whose characters are triples $[t_i t_{i+1} t_{i+2}]$. Note that the last character of R_k is always unique because $t_{\max B_k+2} = 0$. Let $R = R_1 \odot R_2$ be the concatenation of R_1 and R_2 . Then the (nonempty) suffixes of R correspond to the set S_C of sample suffixes: $[t_i t_{i+1} t_{i+2}][t_{i+3} t_{i+4} t_{i+5}] \dots$ corresponds to S_i . The correspondence is order preserving, i.e., by sorting the suffixes of R we get the order of the sample suffixes S_C .

$$Example. R = [abb][ada][bba][do0][bba][dab][bad][o00].$$

To sort the suffixes of R, first radix sort the characters of R and rename them with their ranks to obtain the string R'. If all characters are different, the order of characters gives directly the order of suffixes. Otherwise, sort the suffixes of R' using Algorithm DC3.

Example. R' = (1, 2, 4, 6, 4, 5, 3, 7) and $SA_{R'} = (8, 0, 1, 6, 4, 2, 5, 3, 7)$.

$$Example. R = [abb][ada][bba][do0][bba][dab][bad][o00].$$

Once the sample suffixes are sorted, assign a rank to each suffix. For $i \in C$, let $rank(S_i)$ denote the rank of S_i in the sample set S_C . Additionally, define $rank(S_{n+1}) = rank(S_{n+2}) = 0$. For $i \in B_0$, $rank(S_i)$ is undefined.

```
Example. \ \ rank(S_i) \ \ \bot \ 1 \ 4 \ \bot \ 2 \ 6 \ \bot \ 5 \ 3 \ \bot \ 7 \ 8 \ \bot \ 0 \ 0
```

Once the sample suffixes are sorted, assign a rank to each suffix. For $i \in C$, let $rank(S_i)$ denote the rank of S_i in the sample set S_C . Additionally, define $rank(S_{n+1}) = rank(S_{n+2}) = 0$. For $i \in B_0$, $rank(S_i)$ is undefined.

$$i$$
 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 $Example. \ rank(S_i) \perp 1 \ 4 \ \perp \ 2 \ 6 \ \perp \ 5 \ 3 \ \perp \ 7 \ 8 \ \perp \ 0 \ 0$

$$T[0,n) = \mathtt{y} \ \mathtt{a} \ \mathtt{b} \ \mathtt{b} \ \mathtt{a} \ \mathtt{d} \ \mathtt{a} \ \mathtt{b} \ \mathtt{b} \ \mathtt{a} \ \mathtt{d} \ \mathtt{o}$$

$$Example. \ R = [abb][ada][bba][do0][bba][dab][bad][o00].$$

$$i$$
 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 $Example. \ rank(S_i) \ \perp \ 1 \ 4 \ \perp \ 2 \ 6 \ \perp \ 5 \ 3 \ \perp \ 7 \ 8 \ \perp \ 0 \ 0$

Once the sample suffixes are sorted, assign a rank to each suffix. For $i \in C$, let $rank(S_i)$ denote the rank of S_i in the sample set S_C . Additionally, define $rank(S_{n+1}) = rank(S_{n+2}) = 0$. For $i \in B_0$, $rank(S_i)$ is undefined.

$$i$$
 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 $Example. \ rank(S_i) \perp 1 \ 4 \ \perp \ 2 \ 6 \ \perp \ 5 \ 3 \ \perp \ 7 \ 8 \ \perp \ 0 \ 0$

Note: After only 1 level of recursion, these suffixes would be "tied"

$$Example. \ R = [abb][ada][bba][do0][bba][dab][bad][o00].$$

The resolved ranks here represent what we'd get after a second level of recursion.

$$T[0,n) = \mathtt{y} \ \mathtt{a} \ \mathtt{b} \ \mathtt{b} \ \mathtt{a} \ \mathtt{d} \ \mathtt{a} \ \mathtt{b} \ \mathtt{b} \ \mathtt{a} \ \mathtt{d} \ \mathtt{o}$$

$$Example. \ R = [abb][ada][bba][do0][bba][dab][bad][o00].$$

$$R_2 = [247][463][474][638]$$

These suffixes were tied at the previous level, but here, we can resolve them. The *lexical renaming* allows us to compare longer and longer suffixes of the text.

Step 2 — Sorting the non-sample suffixes

Step 2: Sort nonsample suffixes. Represent each nonsample suffix $S_i \in S_{B_0}$ with the pair $(t_i, rank(S_{i+1}))$. Note that $rank(S_{i+1})$ is always defined for $i \in B_0$. Clearly we have, for all $i, j \in B_0$,

$$S_i \leq S_j \iff (t_i, rank(S_{i+1})) \leq (t_j, rank(S_{j+1})).$$

The pairs $(t_i, rank(S_{i+1}))$ are then radix sorted.

Example. $S_{12} < S_6 < S_9 < S_3 < S_0$ because (0,0) < (a,5) < (a,7) < (b,2) < (y,1).

Step 2 — Sorting the non-sample suffixes

Step 3: Merge. The two sorted sets of suffixes are merged using a standard comparison-based merging. To compare suffix $S_i \in S_C$ with $S_j \in S_{B_0}$, we distinguish two cases:

$$i \in B_{1}: \qquad S_{i} \leq S_{j} \iff (t_{i}, rank(S_{i+1})) \leq (t_{j}, rank(S_{j+1}))$$

$$i \in B_{2}: \qquad S_{i} \leq S_{j} \iff (t_{i}, t_{i+1}, rank(S_{i+2})) \leq (t_{j}, t_{j+1}, rank(S_{j+2}))$$

$$S_{1} \leq S_{2} \leq S_{3} \leq S_{3} \leq S_{4} \leq S_{5} \leq S_{5$$

Note that the ranks are defined in all cases.

Example. $S_1 < S_6$ because (a, 4) < (a, 5) and $S_3 < S_8$ because (b, a, 6) < (b, a, 7).

Running Time

$$T(n) = O(n) + T(2n/3)$$
time to sort and array in recursive calls is 2/3rds the size of starting array

Solves to T(n) = O(n):

- Expand big-O notation: $T(n) \le cn + T(2n/3)$ for some c.
- Guess: $T(n) \leq 3cn$
- Induction step: assume that is true for all i < n.
- $T(n) \le cn + 3c(2n/3) = cn + 2cn = 3cn \square$