

ALGORITHMS OF BIOINFORMATICS

Googling Genomes

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Outline

7 Googling Genomes

- 7.1 Range-Minimum Queries
- 7.2 RMQ – Sparse Table Solution
- 7.3 RMQ – Cartesian Trees
- 7.4 String Matching in Enhanced Suffix Array
- 7.5 The Burrows-Wheeler Transform
- 7.6 Inverting the BWT
- 7.7 Searching in the BWT

Recall Unit 6

Application 4: Longest Common Extensions

- We implicitly used a special case of a more general, versatile idea:

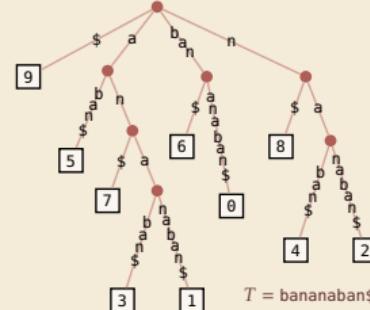
The **longest common extension (LCE)** data structure:

- **Given:** String $T[0..n]$
- **Goal:** Answer LCE queries, i.e.,
given positions i, j in T ,
how far can we read the same text from there?
formally: $\text{LCE}(i, j) = \max\{\ell : T[i..i + \ell] = T[j..j + \ell]\}$

↔ use suffix tree of T !

(length of) longest common prefix
of i th and j th suffix

- In \mathcal{T} : $\text{LCE}(i, j) = \text{LCP}(T_i, T_j) \rightsquigarrow$ same thing, different name!
 $=$ string depth of
lowest common ancestor (LCA) of
leaves $[i]$ and $[j]$



- in short: $\text{LCE}(i, j) = \text{LCP}(T_i, T_j) = \text{stringDepth}(\text{LCA}([i], [j]))$

Recall Unit 6

Efficient LCA

How to find lowest common ancestors?

- ▶ Could walk up the tree to find LCA $\rightsquigarrow \Theta(n)$ worst case 
- ▶ Could store all LCAs in big table $\rightsquigarrow \Theta(n^2)$ space and preprocessing 



Amazing result: Can compute data structure in $\Theta(n)$ time and space that finds any LCA in **constant(!) time**.

- ▶ a bit tricky to understand
- ▶ but a theoretical breakthrough
- ▶ and useful in practice



and suffix tree construction inside . . .

\rightsquigarrow for now, use $O(1)$ LCA as black box.

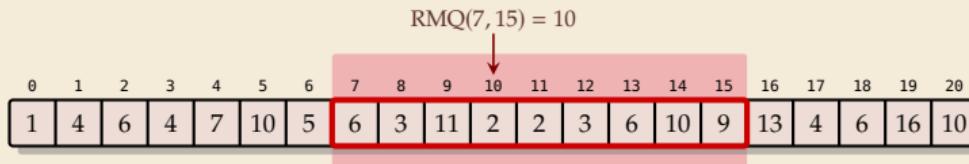
\rightsquigarrow After linear preprocessing (time & space), we can find LCEs in $O(1)$ time.

7.1 Range-Minimum Queries

Range-minimum queries (RMQ)

array/numbers don't change

- Given: Static array $A[0..n)$ of numbers
- Goal: Find minimum in a range;
 A known in advance and can be preprocessed



- Nitpicks:
 - Report *index* of minimum, not its value
 - Report *leftmost* position in case of ties

Finally: Longest common extensions

- In Unit 6: Left question open how to compute LCA in suffix trees
- But: Enhanced Suffix Array makes life easier!

$$\text{LCE}(i, j) = \text{LCP}[\text{RMQ}_{\text{LCP}}(\min\{R[i], R[j]\} + 1, \max\{R[i], R[j]\})]$$

Inverse suffix array: going left & right

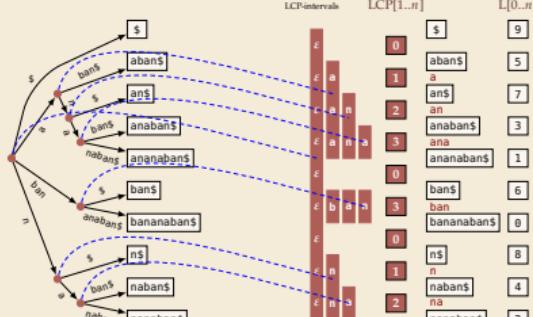
► to understand the fastest algorithm, it is helpful to define the *inverse suffix array*:

- $R[i] = r \iff L[r] = i$ $L = \text{leaf array}$
- \iff there are r suffixes that come before T_i in sorted order
- $\iff T_i$ has (0-based) *rank* r \rightsquigarrow call $R[0..n]$ the *rank array*

i	$R[i]$	T_i	right	r	$L[r]$	$T_{L[r]}$
0	6 th	bananaban\$		0	9	\$
1	4 th	ananaban\$	R[0] = 6	1	5	aban\$
2	9	nanaban\$		2	7	an\$
3	3	anabans		3	3	anabans
4	8	naban\$		4	1	anabanans
5	1	aban\$		5	6	ban\$
6	5	ban\$		6	0	bananaban\$
7	2	an\$		7	8	n\$
8	7	n\$		8	4	naban\$
9	0 th	\$		9	2	nanaban\$

sort suffixes

LCP array and internal nodes



\rightsquigarrow Leaf array $L[0..n]$ plus LCP array $LCP[1..n]$ encode full tree!

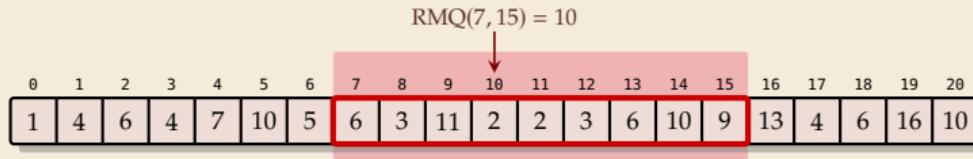
Rules of the Game

- ▶ For the following, consider RMQ on arbitrary arrays
- ▶ comparison-based \rightsquigarrow values don't matter, only relative order
- ▶ Two main quantities of interest:
 1. **Preprocessing time:** Running time $P(n)$ of the preprocessing step
 2. **Query time:** Running time $Q(n)$ of one query (using precomputed data)
- ▶ Write $\langle P(n), Q(n) \rangle$ **time solution** for short

RMQ Implications for LCE

- ▶ Recall: Can compute (inverse) suffix array and LCP array in $O(n)$ time
- $\rightsquigarrow \langle P(n), Q(n) \rangle$ time RMQ data structure implies
 $\langle P(n) + O(n), Q(n) \rangle$ time LCE data structure

Trivial Solutions



- ▶ Two easy solutions show extreme ends of scale:

1. Scan on demand

- ▶ no preprocessing at all
- ▶ answer $\text{RMQ}(i, j)$ by scanning through $A[i..j]$, keeping track of min
~~ $\langle O(1), O(n) \rangle$

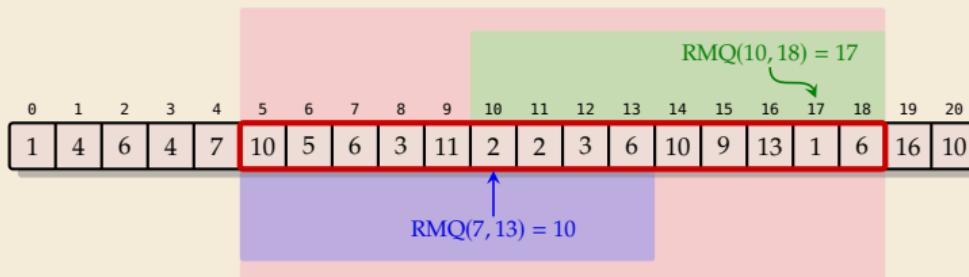
2. Precompute all

- ▶ Precompute all answers in a big 2D array $M[0..n][0..n]$
- ▶ queries simple: $\text{RMQ}(i, j) = M[i][j]$
~~ $\langle O(n^3), O(1) \rangle$
- ▶ Preprocessing can reuse partial results ~~ $\langle O(n^2), O(1) \rangle$

7.2 RMQ – Sparse Table Solution

Sparse Table

- Idea: Like “precompute-all”, but keep only *some* entries
- store $M[i][j]$ iff $\ell = j - i + 1$ is 2^k .
 - ~~~ $\leq n \cdot \lg n$ entries
 - ~~~ Can be stored as $M'[i][k]$
- How to answer queries?

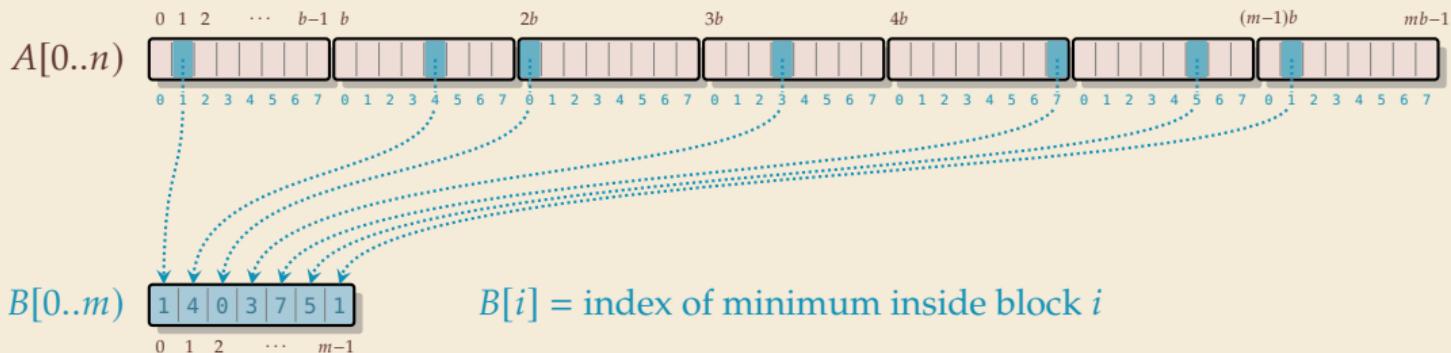


- Preprocessing can be done in $O(n \log n)$ times
 - ~~~ $\langle O(n \log n), O(1) \rangle$ time solution!

1. Find k with $\ell/2 \leq 2^k \leq \ell$
2. Cover range $[i..j]$ by
 2^k positions right from i and
 2^k positions left from j
3. $\text{RMQ}(i, j) = \arg \min\{A[\text{rmq}_1], A[\text{rmq}_2]\}$
with $\text{rmq}_1 = \text{RMQ}(i, i+2^k-1)$
 $\text{rmq}_2 = \text{RMQ}(j-2^k+1, j)$

Bootstrapping

- We know a $\langle O(n \log n), O(1) \rangle$ time solution
- If we use that for $m = \Theta(n/\log n)$ elements, $O(m \log m) = O(n)!$
- Break A into blocks of $b = O(\log n)$ numbers
- Create array of block minima $B[0..m)$ for $m = \lceil n/b \rceil = O(n/\log n)$

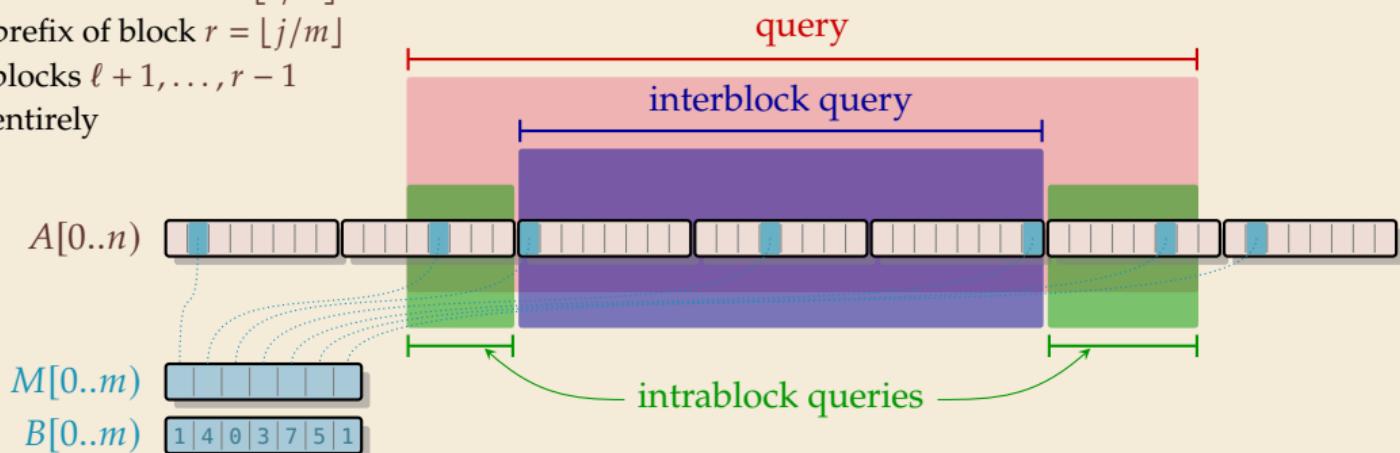


- ~~> Use sparse table solution for B .
- ~~> Can solve RMQs in $B[0..m)$ in $\langle O(n), O(1) \rangle$ time

Query decomposition

- Query $\text{RMQ}_A(i, j)$ covers

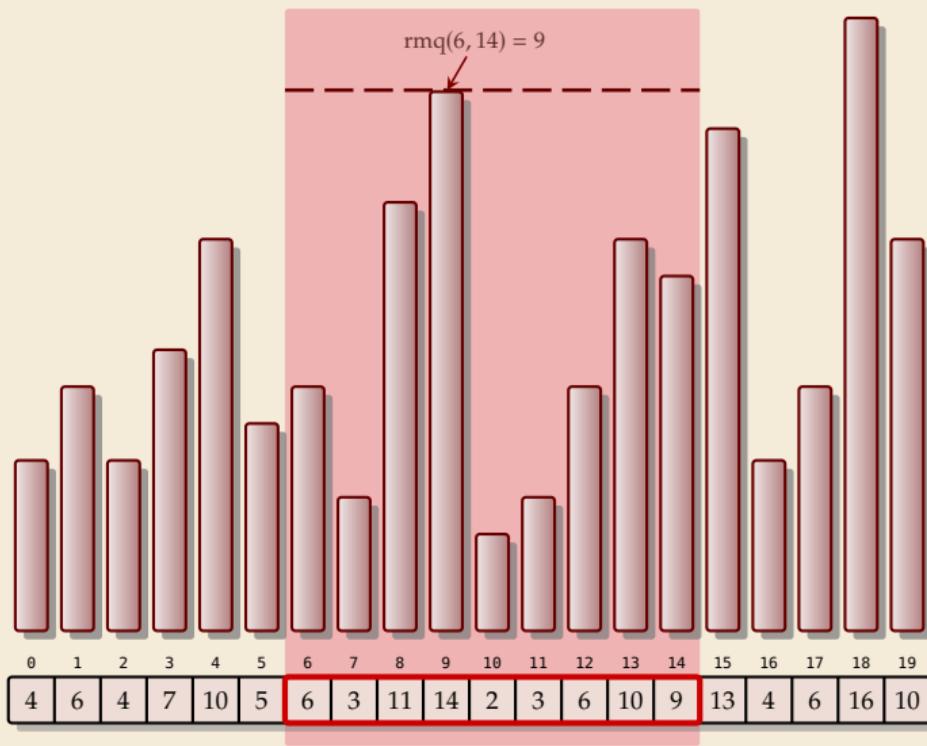
- suffix of block $\ell = \lfloor i/m \rfloor$
- prefix of block $r = \lfloor j/m \rfloor$
- blocks $\ell + 1, \dots, r - 1$ entirely



- $\text{RMQ}_A(i, j) = \arg \min_{k \in K} A[k]$ with $K = \left\{ \begin{array}{l} \text{RMQ}_{\text{block } \ell}(i - \ell b, (\ell + 1)b - 1), \\ b \cdot \text{RMQ}_M(\ell + 1, r - 1) + \\ B[\text{RMQ}_M(\ell + 1, r - 1)], \\ \text{RMQ}_{\text{block } r}(rb, j - rb) \end{array} \right\}$
- ~~ only 3 possible values to check
if intrablock and interblock queries known ✓

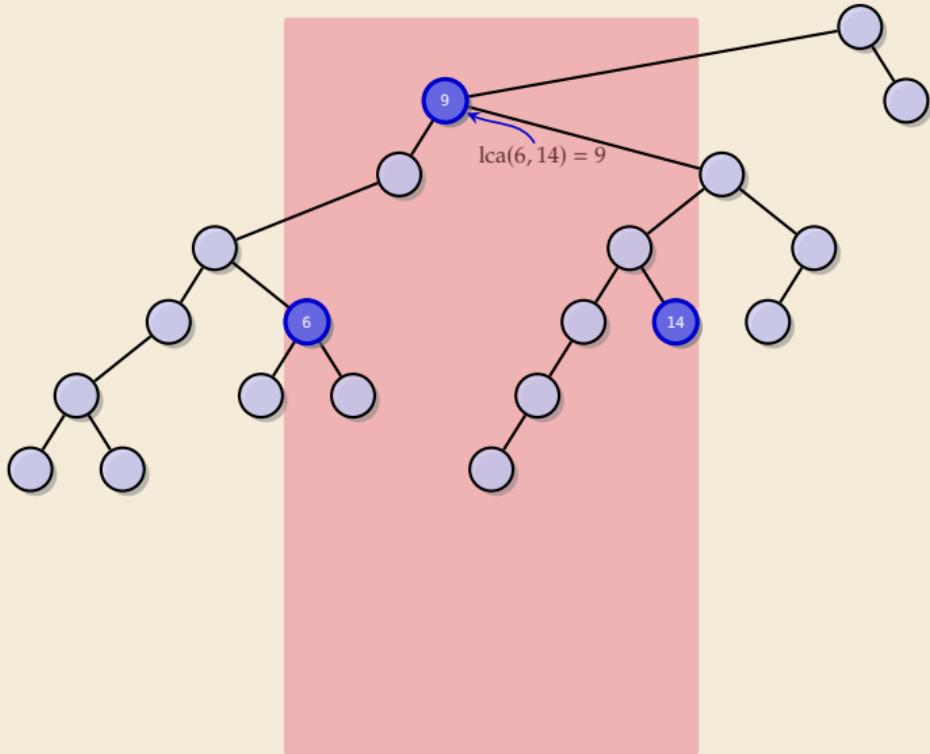
7.3 RMQ – Cartesian Trees

RMQ & LCA



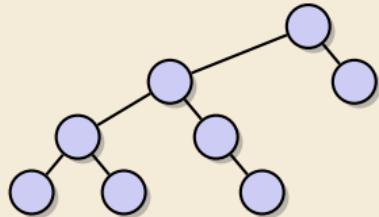
- ▶ Range-max queries on array A :
 $\text{rmq}_A(i, j) = \arg \max_{i \leq k \leq j} A[k]$
= index of max
- ▶ **Task:** Preprocess A ,
then answer RMQs fast
ideally constant time!

RMQ & LCA



- ▶ **Range-max queries** on array A :
 $\text{rmq}_A(i, j) = \arg \max_{i \leq k \leq j} A[k]$
 $= \text{index of max}$
- ▶ **Task:** Preprocess A ,
then answer RMQs fast
ideally constant time!
- ▶ **Cartesian tree:** (cf. *treap*)
construct binary tree by
sweeping line down
- ▶ $\text{rmq}(i, j)$ = inorder of
lowest common ancestor (LCA)
of i th and j th node in inorder

Counting binary trees



- ▶ Given the Cartesian tree,
all RMQ answers are determined
and vice versa!

- ▶ How many different Cartesian trees are there for arrays of length n ?

- ▶ known result: *Catalan numbers* $\frac{1}{n+1} \binom{2n}{n}$

- ▶ easy to see: $\leq 2^{2n}$

~~ many arrays will give rise to the same Cartesian tree

Can we exploit that?

Intrablock queries

~~ It remains to solve the **intrablock** queries!

► Want $\langle O(n), O(1) \rangle$ time overall

must include preprocessing for all $m = \left\lceil \frac{n}{b} \right\rceil = \Theta\left(\frac{n}{\log n}\right)$ blocks!

► Choose $b = \left\lceil \frac{1}{4} \lg n \right\rceil$

► many blocks, but just b numbers long

~~ Cartesian tree of b elements can be encoded using $2b = \frac{1}{2} \lg n$ bits

~~ # different Cartesian trees is $\leq 2^{2b} = 2^{\frac{1}{2} \lg n} = \left(2^{\lg n}\right)^{1/2} = \sqrt{n}$

~~ many *equivalent* blocks!

~~ Recall: *Exhaustive-Tabulation Technique*:

1. represent each subproblem by storing its *type* (here: encoding of Cartesian tree)
2. *enumerate* all possible subproblem types and their solutions
3. use type as index in a large *lookup table*

Exhaustive Tabulation

1. For each block, compute $2b$ bit representation of Cartesian tree
 - ▶ can be done in linear time
2. Compute large lookup table

Block type	i	j	$\text{RMQ}(i, j)$
\vdots			
\vdots			

- ▶ $\leq \sqrt{n}$ block types
- ▶ $\leq b^2$ combinations for i and j
- $\rightsquigarrow \Theta(\sqrt{n} \cdot \log^2 n)$ rows
- ▶ each row can be computed in $O(\log n)$ time
- \rightsquigarrow overall preprocessing: $O(n)$ time!

RMQ Discussion

- ▶ $\langle O(n), O(1) \rangle$ time solution for RMQ
 - ~~ $\langle O(n), O(1) \rangle$ time solution for LCE in strings!

 optimal preprocessing and query time!

 a bit complicated

7.4 String Matching in Enhanced Suffix Array

Binary searching the suffix array

Recall: Can solve the string matching problem by binary searching $P[0..m]$ in $L[0..n]$

- ▶ worst-case cost: $O(\log(n) \cdot m)$ character comparisons
- ~~> use LCP information to speed up string comparisons
- ▶ with RMQ on LCP array can determine lcp with middle

Conclusion

- ▶ (*Enhanced*) *Suffix Arrays* are the modern version of suffix trees
 - ▶ directly simulate suffix tree operations on L and LCP arrays

👎 can be harder to reason about

👍 can support same algorithms as suffix trees

👍 but use much less space

👍 simple(r) linear-time construction

Outlook:

- ▶ enhanced suffix arrays still need original text T to work
- ▶ a *self-index* avoids that
 - ▶ can store T in *compressed* form **and** support operations like string matching

7.5 The Burrows-Wheeler Transform

Digression: Recall BWT

Burrows-Wheeler Transform

1. Take all cyclic shifts of S
2. Sort cyclic shifts
3. Extract last column

$S = \text{alf_eats_alfalfa\$}$

$B = \text{asff\$f_e_lllaaata}$

alf_eats_alfalfa\$
lf_eats_alfalfa\$a
f_eats_alfalfa\$al
_eats_alfalfa\$alf
eats_alfalfa\$alf_
ats_alfalfa\$alf_e
ts_alfalfa\$alf_ea
s_alfalfa\$alf_eat
_alfalfa\$alf_eats
alfalfa\$alf_eats_
lfalfa\$alf_eats_a
falfa\$alf_eats_al
alfa\$alf_eats_alf
lfa\$alf_eats_alfa
fa\$alf_eats_alfal
a\$alf_eats_alfalf
\$alf_eats_alfalfa

~~~  
sort

↓  
BWT  
\$alf\_eats\_alfalfa**a**  
**alfalfa\$alf\_eat**s****  
**\_eats\_alfalfa\$al**f****  
**a\$alf\_eats\_alfal**f****  
**alf\_eats\_alfalfa**\$****  
**alfa\$alf\_eats\_alf**f****  
**alfalfa\$alf\_eats**u****  
**ats\_alfalfa\$alfe**  
**eats\_alfalfa\$alfe**  
**f\_eats\_alfalfa\$al**l****  
**fa\$alf\_eats\_alfal**l****  
**falfa\$alf\_eats\_alf**l****  
**lf\_eats\_alfalfa\$**a****  
**lfa\$alf\_eats\_alf**a****  
**lfalfa\$alf\_eats\_u**a****  
**s\_alfalfa\$alf\_eat**t****  
**ts\_alfalfa\$alf\_ea**

# Digression: Computing the BWT

How can we compute the BWT of a text efficiently?

- ▶ cyclic shifts  $S \hat{=} \text{suffixes of } S$ 
  - ▶ comparing cyclic shifts stops at first \$
  - ▶ for comparisons, anything after \$ irrelevant!
- ▶ BWT is essentially suffix sorting!
  - ▶  $B[i] = S[L[i] - 1]$
  - ▶ where  $L[i] = 0, B[i] = \$$
- ~~ Can compute  $B$  in  $O(n)$  time from  $L$

| $r$ | $\downarrow L[r]$    |    |
|-----|----------------------|----|
| 0   | \$alf_eats_alfalfa\$ | 16 |
| 1   | _alfalfa\$alf_eats\$ | 8  |
| 2   | _eats_alfalfa\$alf   | 3  |
| 3   | a\$alf_eats_alfalf   | 15 |
| 4   | alf_eats_alfalfa\$   | 0  |
| 5   | alfa\$alf_eats_alf   | 12 |
| 6   | alfalfa\$alf_eats_   | 9  |
| 7   | ats_alfalfa\$alf_e   | 5  |
| 8   | eats_alfalfa\$alf_   | 4  |
| 9   | f_eats_alfalfa\$al   | 2  |
| 10  | fa\$alf_eats_alfal   | 14 |
| 11  | falfa\$alf_eats_ al  | 11 |
| 12  | lf_eats_alfalfa\$ a  | 1  |
| 13  | lfa\$alf_eats_alf a  | 13 |
| 14  | lfalfa\$alf_eats_a   | 10 |
| 15  | s_alfalfa\$alf_eat   | 7  |
| 16  | ts_alfalfa\$alf_ea   | 6  |

## 7.6 Inverting the BWT



## 7.7 Searching in the BWT

