

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 Random Access in BWT
- 7.8 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:

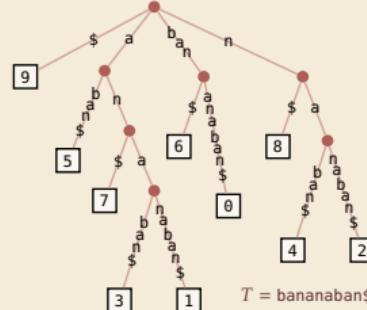
- **Given:** String $T[0..n]$
- **Goal:** Answer LCE queries, i. e.,
given positions i, j in T ,
how far can we read the same text from there?
formally: $\text{LCE}(i, j) = \max\{\ell : T[i..i + \ell] = T[j..j + \ell]\}$

↔ 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 \boxed{i} and \boxed{j}

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



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.

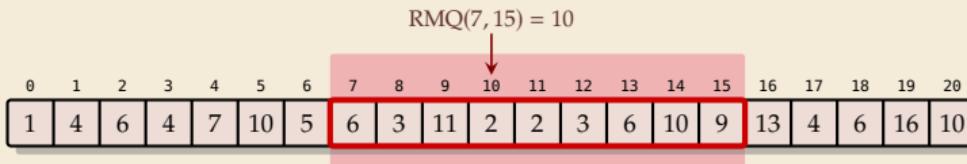
\rightsquigarrow After linear preprocessing (time & space), we can find LCEs in $O(1)$ time.

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

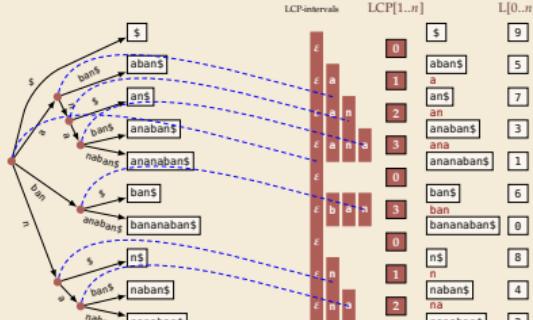
▶ to understand the fastest algorithm, it is helpful to define the *inverse suffix array*:

- ▶ $R[i] = r \iff L[r] = i$ $L = \text{leaf array}$
- ▶ there are r suffixes that come before T_i in sorted order
- ▶ 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 th	nanaban\$		2	7	an\$
3	3 th	anabans		3	3	anabans
4	8 th	naban\$		4	1	anabanans
5	1 th	aban\$		5	6	ban\$
6	5 th	ban\$		6	0	bananaban\$
7	2 th	an\$		7	8	n\$
8	7 th	n\$		8	4	naban\$
9	0 th	\$		9	2	nanaban\$

sort suffixes

LCP array and internal nodes



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

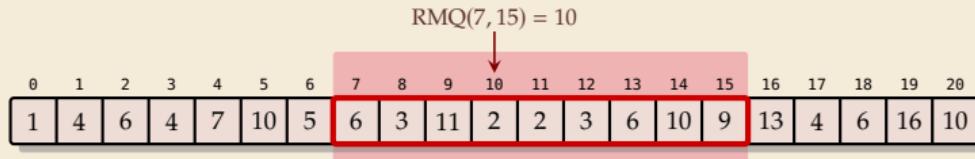
Rules of the Game

- ▶ 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

$\rightsquigarrow \langle O(1), O(n) \rangle$

2. Precompute all

- ▶ Precompute all answers in a big 2D array $M[0..n][0..n]$
- ▶ queries simple: $\text{RMQ}(i, j) = M[i][j]$

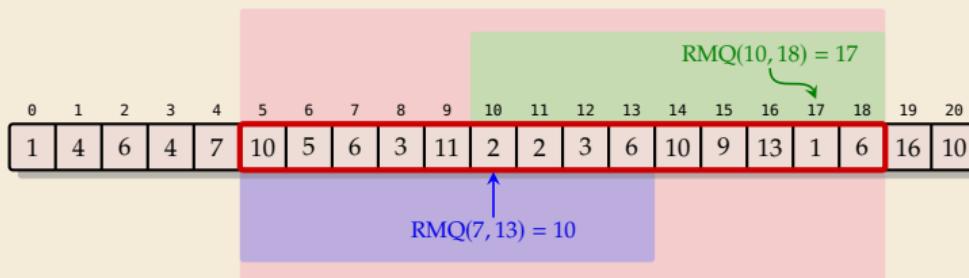
$\rightsquigarrow \langle O(n^3), O(1) \rangle$

- ▶ Preprocessing can reuse partial results $\rightsquigarrow \langle O(n^2), O(1) \rangle$

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?

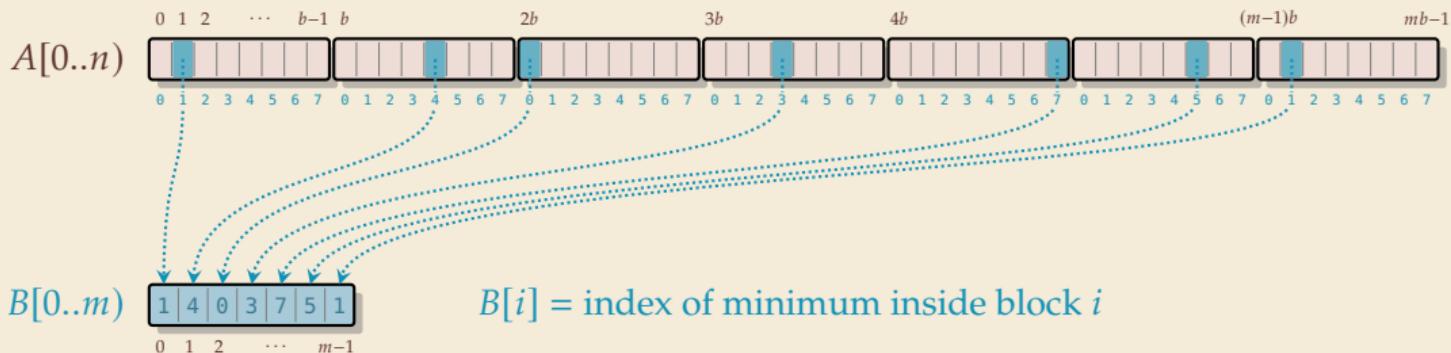


- Preprocessing can be done in $O(n \log n)$ times
 - ~~~ $\langle O(n \log n), O(1) \rangle$ time solution!

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 $m = \lceil n/b \rceil = O(n/\log n)$

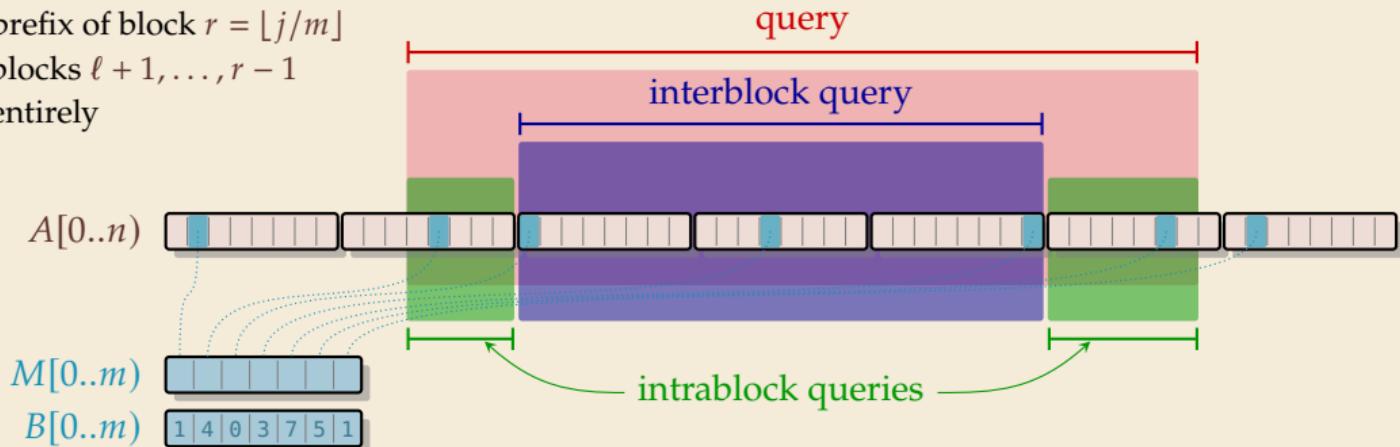


- ~~> Use sparse table solution for B .
- ~~> Can solve RMQs in $B[0..m)$ in $\langle O(n), O(1) \rangle$ time

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 $K =$

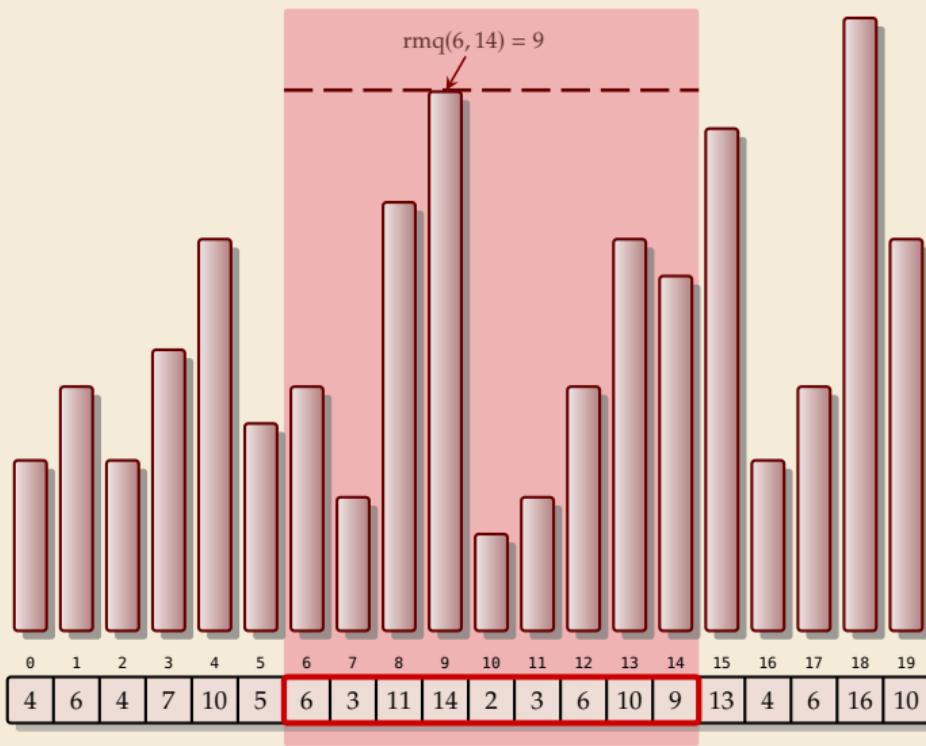
$$\left\{ \begin{array}{l} \text{RMQ}_{\text{block } \ell}(i - \ell b, (\ell + 1)b - 1), \\ b \cdot \text{RMQ}_M(\ell + 1, r - 1) + \\ B[\text{RMQ}_M(\ell + 1, r - 1)], \\ \text{RMQ}_{\text{block } r}(rb, j - rb) \end{array} \right\}$$

~ only 3 possible values to check

if intrablock and interblock queries known

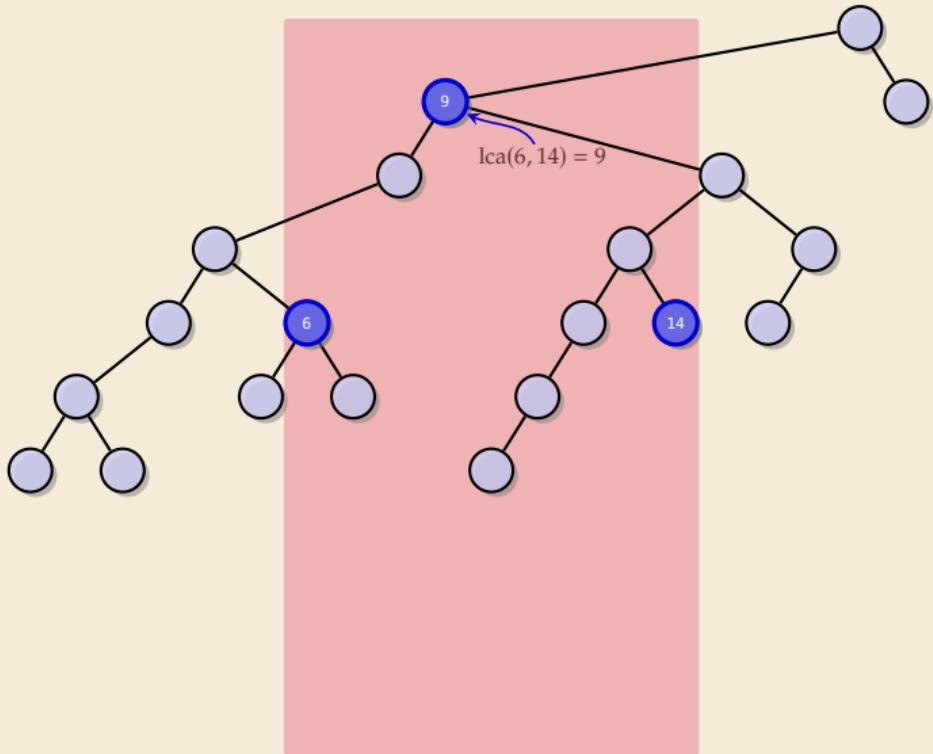
7.3 RMQ – Cartesian Trees

RMQ & LCA



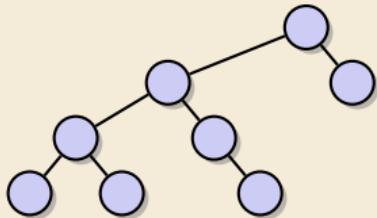
- ▶ Range-max queries on array A :
 $\text{rmq}_A(i, j) = \arg \max_{i \leq k \leq j} A[k]$
 $= \text{index of max}$
- ▶ **Task:** Preprocess A ,
then answer RMQs fast
ideally constant time!

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 $\leq 2^{2b} = 2^{\frac{1}{2} \lg n} = (2^{\lg n})^{1/2} = \sqrt{n}$

~~ 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: $\lg n + 2$ *string* comparisons of string of length m
- ~~ $O(\log(n) \cdot m)$ character comparisons
- ▶ suffix tree could do $O(m)$ total time (assuming constant σ or hashing for child links)
- ▶ surely, enhanced suffix arrays can do better than $O(m \log n)$ ☺

Idea: use LCP information to save character comparisons

- ▶ concretely: maintain LCP between lower/upper bound suffixes and P
 $T[a..n] \leq_{\text{lex}} P \leq_{\text{lex}} T[b..n]$
 $\ell_a = \text{LCP}(T[a..n], P)$ and $\ell_b = \text{LCP}(T[b..n], P)$
- ▶ avoid comparing same characters again
- ▶ Note: with RMQ on LCP array can determine $\text{LCP}(T_i, T_j)$ for any $i, j \in [0..n]$

LCP Binary Search

- ▶ Input: $\ell_a = \text{LCP}(T_a, P)$
 $\ell_b = \text{LCP}(T_b, P)$
- $\rightsquigarrow \ell_m = \text{LCP}(T_m, P) \geq \min\{\ell_a, \ell_b\}$

- ▶ **Case 1:** $\ell_a = \ell_b$
Compare P and T_m starting at ℓ_a
- ▶ **Case 2:** $\ell_a \neq \ell_b$; w.l.o.g. $\ell_a > \ell_b$

▶ **Case 2a:** $\text{LCP}(T_a, T_m) > \ell_a$
 $P >_{\text{lex}} T_m$ w/o cmps!

▶ **Case 2b:** $\text{LCP}(T_a, T_m) < \ell_a$
 $P <_{\text{lex}} T_m$ w/o cmps!

▶ **Case 2c:** $\text{LCP}(T_a, T_m) = \ell_a$
Compare P and T_m from ℓ_a

- ▶ in each case, learn $\ell_m \rightsquigarrow$ invariant
- ▶ no redundant '='-comparisons

0: T_{20}	\$	
1: T_4	ahbansbananasman\$	
2: T_{18}	an\$	
3: T_{11}	$a \rightarrow$ ananasman\$	Case 2c
4: T_{13}	$m \rightarrow$ anasman\$	$P = \text{anarchy}$
5: T_1	annahbansbananasman\$	
6: T_7	$b \rightarrow$ ansbananasman\$	
7: T_{15}	asman\$	
8: T_{10}	bananasman\$	
9: T_6	bansbananasman\$	
10: T_0	hannahbansbananasman\$	
11: T_5	hbansbananasman\$	
12: T_{17}	man\$	
13: T_{19}	n\$	
14: T_3	nahbansbananasman\$	
15: T_{12}	nanasman\$	
16: T_{14}	nasman\$	
17: T_2	nnahbansbananasman\$	
18: T_8	nsbananasman\$	
19: T_9	sbananasman\$	
20: T_{16}	sman\$	

Enhanced Suffix Arrays – Update

- *Enhanced suffix array*: L , R and LCP array with RMQ support
- **Goal**: simulate any suffix tree operations
 - string matching in $O(m + \log n)$ time ✓
 - string depth of internal nodes = LCP values ✓
 - internal suffix tree node = LCP interval
 - ~~ storing information per node ✓
 - bottom-up traversal via enclosing LCP intervals ✓
 - longest common extension queries ✓
 - suffix links ✓

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

Towards Self-Indexes

- ▶ For large genomes or multiple-genome datasets, can't hold $T[0..n)$ in fast memory.
- ▶ An enhanced suffix array needs additional $\Theta(n)$ words of space.
- ~~> When reference genomes first became available, a major show stopper!
- ▶ But since string matching can reconstruct T , can't avoid storing T somehow!
- ▶ A *self-index* is a data structure that answers operations without access to T at query time
 - ▶ We get to decide *how* to store T ~~ might *compress* T (if compressible)
 - ▶ Known as "*encoding model*" in space-efficient data structures \uparrow genomes highly repetitive!
- ~~> **Key question:** *How to compress T while supporting random access and read mapping?*
"Computing over compressed data"

BWT – Definitions

$$T = \text{time}_\square \text{flies}_\square \text{quickly}_\square$$

$$\text{flies}_\square \text{quickly}_\square \text{time}_\square$$

- *cyclic shift* of a string:

- with end-of-word character $\$$

- ~~ can **recover** original string



- The Burrows-Wheeler Transform proceeds in three steps:

0. Append end-of-word character $\$$ to S .
1. Consider *all cyclic shifts* of S
2. Sort these strings lexicographically
3. B is the *list of trailing characters* (last column, top-down) of each string

BWT – Example

$S = \text{alf_eats_alfalfa\$}$

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

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

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_alfalfa
\$alf_eats_alfalfa

~~~  
sort

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

# 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  $L$
- more direct methods now also available

| $r$ | $\downarrow L[r]$    |    |
|-----|----------------------|----|
| 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    | 13 |
| 14  | lfalfa\$alf_eats_a   | 10 |
| 15  | s_alfalfa\$alf_eat   | 7  |
| 16  | ts_alfalfa\$alf_ea   | 6  |

# BWT – Properties

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

## Why does BWT help for compression?

- sorting *groups* characters *by what follows*
  - Example: lf always preceded by a
  - more generally: BWT can be partitioned into letters following a given context

(formally: low higher-order empirical entropy)

- ~~ If  $S$  allows predicting symbols from context,  $B$  has locally low entropy of characters.
  - that makes MTF (move-to-front) transformation effective!
  - ~~ use in compression pipeline for bzip2:  
BTW → MTF → RLE → Huffman

## A Bigger Example

\_have,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what  
\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what\$have  
\_hadnt,\_hasnt,\_havent,\_has,\_what\$have,\_had  
\_has,\_what\$have,\_had,\_hadnt,\_hasnt,\_havent  
\_hasnt,\_havent,\_has,\_what\$have,\_had,\_hadnt  
\_havent,\_has,\_what\$have,\_had,\_hadnt,\_hasnt  
\_hadnt,\_hasnt,\_havent,\_has,\_what\$have,\_had  
\_hadnt,\_hasnt,\_havent,\_has,\_what\$have,\_had  
\_hasnt,\_havent,\_has,\_what\$have,\_had,\_hadnt  
\_at\$have,\_had,\_hadnt,\_hasnt,\_havent,\_has  
\_have,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what\$  
\_havent,\_has,\_what\$have,\_had,\_hadnt,\_hasnt  
\_d,\_hadnt,\_hasnt,\_havent,\_has,\_what\$have,\_ha  
\_dnt,\_hasnt,\_havent,\_has,\_what\$have,\_had,\_ha  
\_e,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what\$ha  
\_ent,\_has,\_what\$have,\_had,\_hadnt,\_hasnt,\_ha  
\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what\$have  
\_hadnt,\_hasnt,\_havent,\_has,\_what\$have,\_had  
\_has,\_what\$have,\_had,\_hadnt,\_hasnt,\_havent  
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\_had\$have,\_had,\_hadnt,\_hasnt,\_havent,\_has  
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\_havent,\_has,\_what\$have,\_had,\_hadnt,\_hasnt  
\_nt,\_has,\_what\$have,\_had,\_hadnt,\_hasnt,\_hav  
\_nt,\_hasnt,\_havent,\_has,\_what\$have,\_had,\_had  
\_nt,\_havent,\_has,\_what\$have,\_had,\_hadnt,\_has  
\_s,\_what\$have,\_had,\_hadnt,\_hasnt,\_havent,\_ha  
\_snt,\_havent,\_has,\_what\$have,\_had,\_hadnt,\_ha  
\_t\$have,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_wha  
\_t,\_hasnt,\_havent,\_has,\_what\$have,\_had,\_hadn  
\_t,\_havent,\_has,\_what\$have,\_had,\_hadnt,\_has  
\_ve,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what\$ha  
\_vent,\_has,\_what\$have,\_had,\_hadnt,\_hasnt,\_ha  
\_what\$have,\_had,\_hadnt,\_hasnt,\_havent,\_has

*B = tedtttshhhhhhhhaavv.....w\$..edsaaannnaa..*

# Run-length BWT Compression

- ▶ amazingly, just run-length compressing the BWT is already powerful!
- ▶  $r$  = number of runs in BWT

## Example:

$S = \text{alf\_eats\_alfalfa\$}$

$B = \text{asfff\$f\_e\_lllaata}$

$RL(B) = [a] [s] [f] [\$] [f] [u] [e] [u] [l] [a] [t] [a]$

$\rightsquigarrow r = |RL(B)| = 12; n = 17$

## Larger Example:

$S = \text{have\_had\_hadnt\_hasnt\_havent\_has\_what\$}$

$B = \text{tedtttshhhhhhaavv\_w\$\_edsaaannnaa\_}$

$\rightsquigarrow r = 19; n = 36$

- ▶ Indeed:  $r = O(z \log^2(n))$ ,  $z$  number of LZ77 phrases

proven in 2019 (!)



Kempa, Kociumaka: *Resolution of the Burrows-Wheeler Transform Conjecture*, CACM 2022

## 7.6 Inverting the BWT

# Inverse BWT

- Great, can compute BWT efficiently and it helps compression. *But can we get  $T$  back?*

- “Magic” solution:

1. Create array  $D[0..n]$  of pairs:  
 $D[r] = (B[r], r)$ .

2. Sort  $D$  stably with respect to *first entry*.

3. Use  $D$  as linked list with (char, next entry)

**Example:**

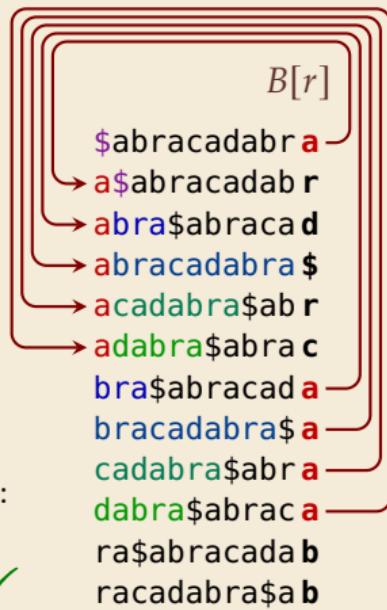
$B = \text{ard\$rcaaaabb}$

$S = \text{abracadabra\$}$

|    | $D$     | sorted $D$ |
|----|---------|------------|
|    |         | char next  |
| 0  | (a, 0)  | 0 (\$, 3)  |
| 1  | (r, 1)  | 1 (a, 0)   |
| 2  | (d, 2)  | 2 (a, 6)   |
| 3  | (\$, 3) | 3 (a, 7)   |
| 4  | (r, 4)  | 4 (a, 8)   |
| 5  | (c, 5)  | 5 (a, 9)   |
| 6  | (a, 6)  | 6 (b, 10)  |
| 7  | (a, 7)  | 7 (b, 11)  |
| 8  | (a, 8)  | 8 (c, 5)   |
| 9  | (a, 9)  | 9 (d, 2)   |
| 10 | (b, 10) | 10 (r, 1)  |
| 11 | (b, 11) | 11 (r, 4)  |

# Inverse BWT – The magic revealed

- ▶ Inverse BWT very easy to compute:
  - ▶ only sort individual characters in  $B$  (not suffixes)
    - ~~  $O(n)$  with counting sort
- ▶ but why does this work!?
- ▶ decode char by char
  - ▶ can find unique \$ ~~ starting row
- ▶ to get next char, we need
  - char in *first* column of *current row*
  - find row with that char's copy in BWT
    - ~~ then we can walk through and decode
- ▶ for (i): first col = chars of  $B$  in sorted order ✓
- ▶ for (ii): relative order of same character stays same:  
 $i$ th a in first column =  $i$ th a in BWT
  - ~~ stably sorting  $(B[r], r)$  by first entry enough ✓



# Random Access Decoding

Can similarly output **any substring**  $T[i..i + \ell]$  if we know inverse suffix array:

Simply do  $\ell$  steps of the inverse BWT starting at  $r = R[i - 1]$ !

| $i$ | $R[i]$          | $T_i$       | $r$ | $L[r]$ | $T_{L[r]}$   | $B[r]$  | $D$        | $\text{sort}(D)$ |
|-----|-----------------|-------------|-----|--------|--------------|---------|------------|------------------|
| 0   | 6 <sup>th</sup> | bananaban\$ | 0   | 9      | \$bananaba n | (n, 0)  | 0: (\$, 6) |                  |
| 1   | 4 <sup>th</sup> | ananaban\$b | 1   | 5      | aban\$bana n | (n, 1)  | 1: (a, 5)  |                  |
| 2   | 9 <sup>th</sup> | nanaban\$ba | 2   | 7      | an\$banana b | (b, 2)  | 2: (a, 7)  |                  |
| 3   | 3 <sup>th</sup> | anaban\$ban | 3   | 3      | anaban\$ba n | (n, 3)  | 3: (a, 8)  |                  |
| 4   | 8 <sup>th</sup> | naban\$bana | 4   | 1      | ananaban\$ b | (b, 4)  | 4: (a, 9)  |                  |
| 5   | 1 <sup>th</sup> | aban\$banan | 5   | 6      | ban\$banan a | (a, 5)  | 5: (b, 2)  |                  |
| 6   | 5 <sup>th</sup> | ban\$banana | 6   | 0      | bananaban \$ | (\$, 6) | 6: (b, 4)  |                  |
| 7   | 2 <sup>th</sup> | an\$bananab | 7   | 8      | n\$bananab a | (a, 7)  | 7: (n, 0)  |                  |
| 8   | 7 <sup>th</sup> | n\$bananaba | 8   | 4      | naban\$ban a | (a, 8)  | 8: (n, 1)  |                  |
| 9   | 0 <sup>th</sup> | \$bananaban | 9   | 2      | nanaban\$b a | (a, 9)  | 9: (n, 3)  |                  |

*sort suffixes*

Decoding only needs access to

1.  $i$ th char  $c$  of  $\text{sort}(T) = \text{sort}(B)$
2. *position* of (that copy of)  $c$  in  $B$

↝ If we have that, can skip sorting / storing all of  $D$ !

## 7.7 Random Access in BWT

# Rank & Select on Sequences

Recall: Decoding only needs access to

1.  $i$ th char  $c$  of  $\text{sort}(T) = \text{sort}(B)$
2. *position* of (that copy of)  $c$  in  $B$

Both can be supported using  
rank/select on sequences.

rank/select on sequences.  $\quad \# \text{occurrences of } c$

- ▶  $\text{rank}_c(T[0..n], i) = |T[0..i]|_c \quad \text{#} \downarrow$   
 $= \#c \text{ in first } i \text{ characters of } T$
- ▶  $\text{select}_c(T[0..n], r)$   
 $= \min \{j : |T[0..j]|_c \geq r\} \cup \{n\}$   
 $= \text{index of } r\text{th } c \text{ in } T, (r = 1, 2, \dots)$

|                       |                     |
|-----------------------|---------------------|
| $T[0..9]$             | 0 1 2 3 4 5 6 7 8   |
|                       | b a n a n a b a n   |
|                       | 0 1 2 3 4 5 6 7 8 9 |
| $\text{rank}_a(T, i)$ | 0 0 1 1 2 2 3 3 4 4 |
| $\text{rank}_b(T, i)$ | 0 1 1 1 1 1 1 2 2 2 |
| $\text{rank}_n(T, i)$ | 0 0 0 1 1 2 2 2 2 3 |

|                         |                     |
|-------------------------|---------------------|
| $\text{select}_a(T, r)$ | / 1 3 5 7 9 9 9 9 9 |
| $\text{select}_b(T, r)$ | / 0 6 9 9 9 9 9 9 9 |
| $\text{select}_n(T, r)$ | / 2 4 8 9 9 9 9 9 9 |

|                  |                   |
|------------------|-------------------|
| $\text{sort}(T)$ | 0 1 2 3 4 5 6 7 8 |
|                  | a a a a b b n n n |
| $O[0..9]$        | [0, 4, 6, 9]      |

## Random Access in BWT

- ▶ store offsets  $O[c] = \sum_{c'=0}^{c-1} |B|_{c'}$  for  $c \in \Sigma$
- ▶  $i$ th char of  $\text{sort}(B)$  = unique  $c$  for which  $O[c] \leq i < O[c + 1]$
- ▶ position of  $r$ th  $c$  in  $B$  =  $\text{select}_c(B, r)$

# Wavelet Trees

The **Wavelet Trees** for a  $T \in [0..n]$  over  $\Sigma = [0..\sigma]$



- ▶ supports access to  $T[i]$  in  $O(\log \sigma)$  time,
- ▶  $\text{rank}_c(T, i)$  and  $\text{select}_c(T, r)$  in  $O(\log \sigma)$  time, and
- ▶ occupies  $\sim n \lg \sigma$  bits of space. *(Further compression possible!)*  $\rightsquigarrow$  Advanced Data Structures
- ▶ The generalized  $\sigma\text{-rank}_c(T, i) = \text{rank}_c(T, i) + \sum_{c' < c} |T|_{c'}$  is also supported in  $O(\log \sigma)$  time

Storing  $B[0..n]$  as a wavelet tree  $\rightsquigarrow$  reconstruct  $\ell$  chars from  $T$  in  $O(\ell \log \sigma)$  time

e.g.,  $t = \lg n$

*if starting position known*

Storing **every  $t$ th entry** of  $R[0..n]$   $\rightsquigarrow$  may need to go back  $t$  characters for access  
 $\rightsquigarrow O((\ell + t) \log \sigma)$  time for decode  
using  $\sim n \lg n/t$  extra bits of space

## Locally decodable BWT

- ▶ no longer need to store  $T[0..n]$ !
- ▶ compressible (e.g., Wavelet trees with compressed bitvectors)

## 7.8 Searching in the BWT

# Backwards Search

Recall how the sorted suffixes in a suffix array  $L[0..n]$  made **string matching** very easy.

- ▶ Simply binary search the pattern  $P[0..m]$  in  $L$ !
  - ~~ all occurrences must form interval

With wavelet tree BWT, we can replace binary search by **backwards radix search**!

- ▶ use  $\text{sort}(B)$  to locate interval for **last** character  $P[m - 1]$
- ▶ use one step of inverse BWT to narrow down on  $P[m - 2..m)$ , repeat.

| $i$ | $R[i]$          | $T_i$       | $L[r]$ | $r$ | $T_{L[r]}$          | $B[r]$   | $\text{sort}(D)$ |
|-----|-----------------|-------------|--------|-----|---------------------|----------|------------------|
| 0   | 6 <sup>th</sup> | bananaban\$ | 9      | 0   | \$bananaba          | <b>n</b> | 0: (\$, 6)       |
| 1   | 4 <sup>th</sup> | ananaban\$b | 5      | 1   | aban\$bana          | <b>n</b> | 1: (a, 5)        |
| 2   | 9 <sup>th</sup> | nanaban\$ba | 7      | 2   | an\$banana          | <b>b</b> | 2: (a, 7)        |
| 3   | 3 <sup>th</sup> | anaban\$ban | 3      | 3   | <b>ana</b> ban\$ba  | <b>n</b> | 3: (a, 8)        |
| 4   | 8 <sup>th</sup> | naban\$bana | 1      | 4   | <b>ana</b> aban\$ba | <b>n</b> | 4: (a, 9)        |
| 5   | 1 <sup>th</sup> | aban\$banan | 6      | 5   | ban\$banan          | <b>a</b> | 5: (b, 2)        |
| 6   | 5 <sup>th</sup> | ban\$banana | 0      | 6   | bananaban           | \$       | 6: (b, 4)        |
| 7   | 2 <sup>th</sup> | an\$bananab | 8      | 7   | n\$bananab          | <b>a</b> | 7: (n, 0)        |
| 8   | 7 <sup>th</sup> | n\$bananaba | 4      | 8   | naban\$ban          | <b>a</b> | 8: (n, 1)        |
| 9   | 0 <sup>th</sup> | \$bananaban | 2      | 9   | nanaban\$ba         | <b>n</b> | 9: (n, 3)        |

$P = \text{ana}$

# Backwards Search – Code

Recall total rank operation supported by wavelet trees

$$\sigma\text{-rank}_c(B, i) = |B[0..i]|_c + \sum_{c' < c} |B|_{c'}$$

---

```
1 procedure backwardSearch( $B[0..n]$ ,  $P[0..m]$ )
2   //  $B[0..n]$  given as wavelet tree
3   // returns range  $[s..e]$  of ranks for suffixes starting with  $P$ 
4    $c := P[m - 1]$ 
5    $s := \sigma\text{-rank}_c(B, 0)$ 
6    $e := \sigma\text{-rank}_c(B, n)$ 
7   for  $j := m - 2, m - 3, \dots, 0$ 
8     if  $s \geq e$  break // no matches
9      $c := P[j]$ 
10     $s := \sigma\text{-rank}_c(B, s)$ 
11     $e := \sigma\text{-rank}_c(B, e)$ 
12  return  $[s..e]$ 
```

---

# Locating Matches

- ▶ Backwards Search finds interval  $[s..e)$  such that
$$P[0..m) = T[L[r] .. L[r]+m) \text{ iff } r \in [s..e)$$
- ~~ still need suffix array  $L[0..n]$  to locate matches!
- ▶ but can detect and count occurrences even without  $L$

## Sampled Suffix Array

- ▶ As for inverse suffix array, can store  $L[r]$  only for every  $t$ th starting index  $i$  in  $T$ , i.e., only store entries for ranks  $r$  with  $L[r] \equiv 0 \pmod{t}$
- ~~  $O(n \log n/t)$  bits of extra space
- ~~ Need to continue backwards search for at most  $t$  extra characters to locate match
- ~~ String matching in  $O(m \log \sigma + occ \cdot t \log \sigma)$  time

*Wavelet-tree BWT + Sampled Suffix Array = FM Index*



Ferragina, Manzini: Indexing compressed text, JACM 2005

# FM-Index Discussion

- ▶ FM-Index is one of first *compressed self-indexes*
- ▶ can represent text using  $\sim \mathcal{H}_k(T)n$  bits of space  
 $\mathcal{H}_k(T) = k$ th order empirical entropy
- ▶ still widely used, e. g., as basis of *bowtie2* read alignment tool



Langmead, Salzberg: *Fast gapped-read alignment with Bowtie 2*, Nature Methods 2012

## Ongoing research

- ▶ Reduce space for very repetitive strings (collection of genomes)
  - e. g., *r*-index
- ▶ full support of suffix tree functionality with little extra space?