

# 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:

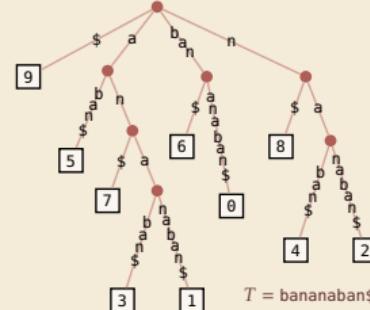
The **longest common extension (LCE)** data structure:

- **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  $[i]$  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.

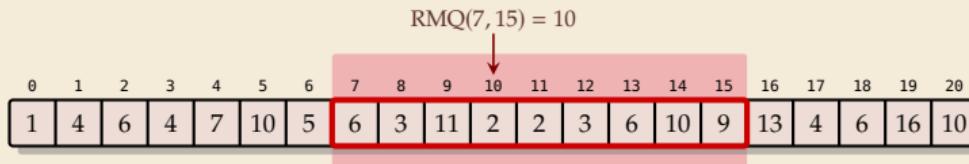
$\rightsquigarrow$  After linear preprocessing (time & space), we can find LCEs in  $O(1)$  time.

## 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

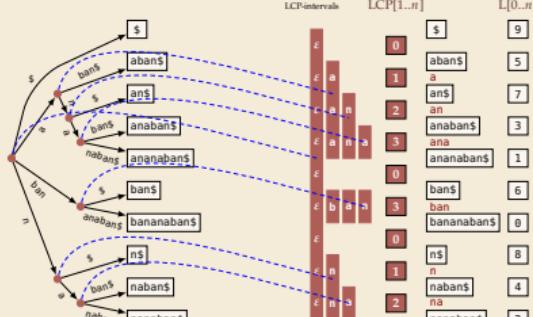
► to understand the fastest algorithm, it is helpful to define the *inverse suffix array*:

- $R[i] = r \iff L[r] = i$        $L = \text{leaf array}$
- $\iff$  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 <sup>th</sup>	bananaban\$		0	9	\$
1	4 <sup>th</sup>	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 <sup>th</sup>	\$		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!

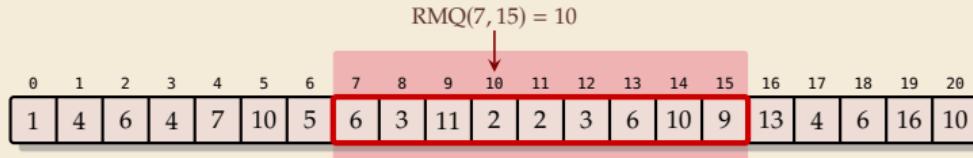
# Rules of the Game

- ▶ 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  
~~  $\langle O(1), O(n) \rangle$

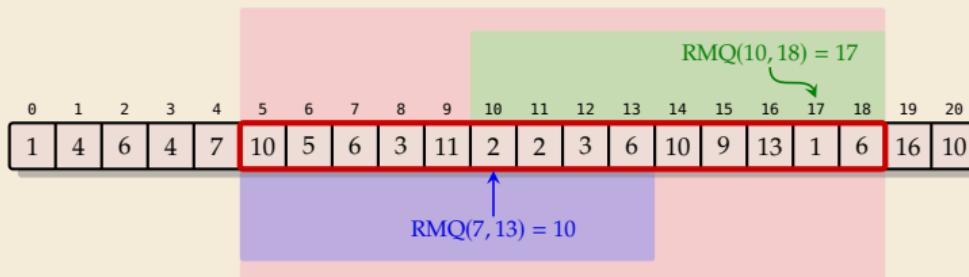
## 2. Precompute all

- ▶ 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?

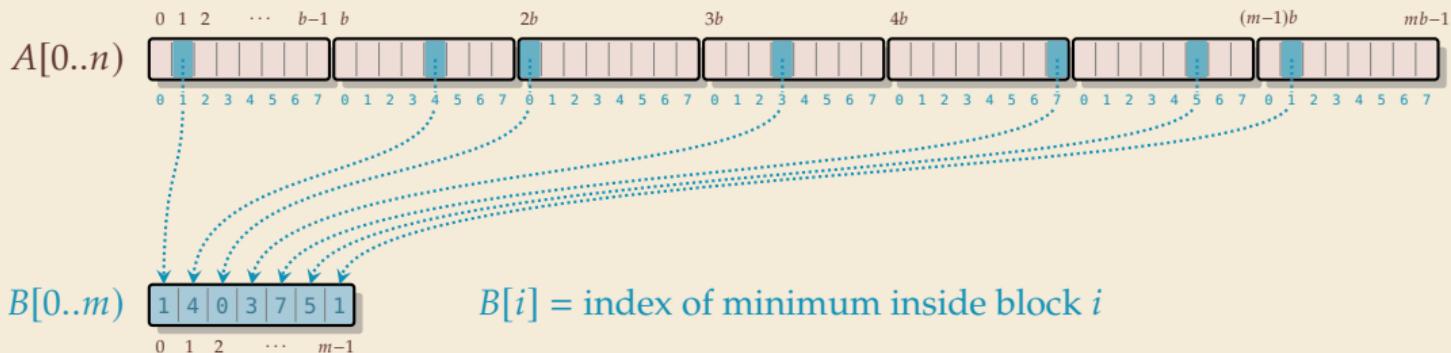


- Preprocessing can be done in  $O(n \log n)$  times
  - ~~~  $\langle O(n \log n), O(1) \rangle$  time solution!

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

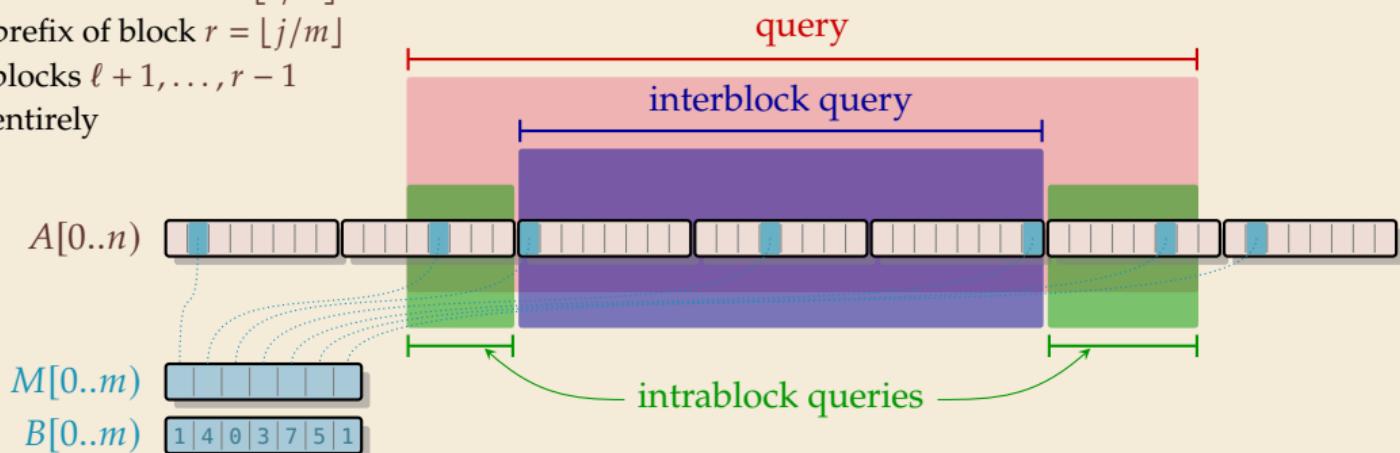


- ~~> Use sparse table solution for  $B$ .
- ~~> Can solve RMQs in  $B[0..m)$  in  $\langle O(n), O(1) \rangle$  time

# Query decomposition

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

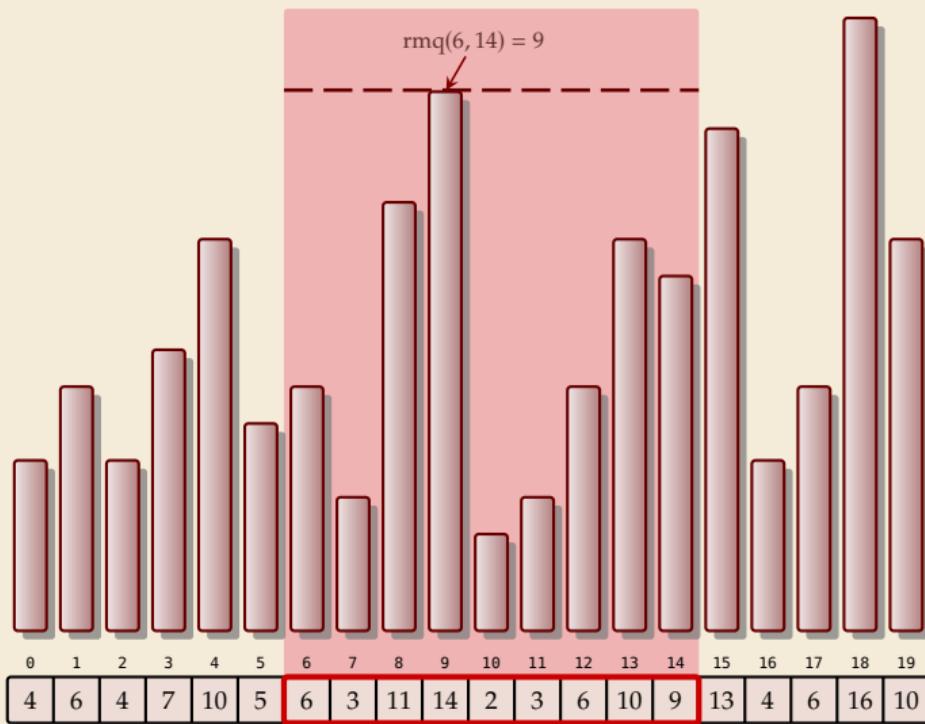
- suffix of block  $\ell = \lfloor i/m \rfloor$
- prefix of block  $r = \lfloor j/m \rfloor$
- blocks  $\ell + 1, \dots, r - 1$  entirely



- $\text{RMQ}_A(i, j) = \arg \min_{k \in K} A[k]$  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 ✓

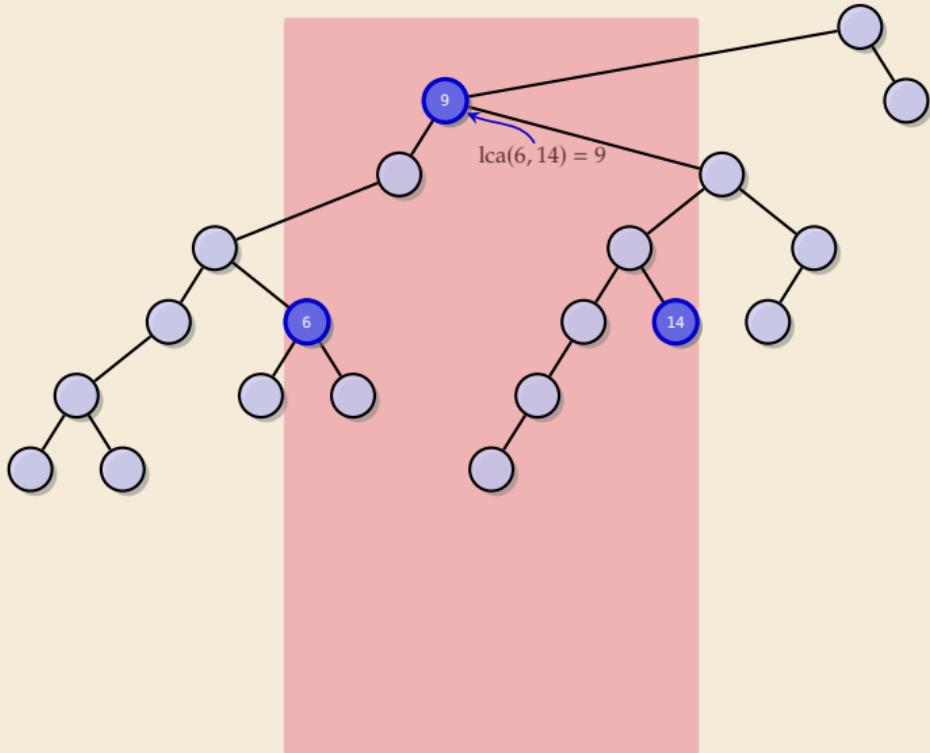
## 7.3 RMQ – Cartesian Trees

# RMQ & LCA



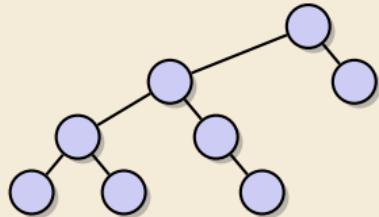
- ▶ Range-max queries on array  $A$ :  
 $\text{rmq}_A(i, j) = \arg \max_{i \leq k \leq j} A[k]$   
= index of max
- ▶ **Task:** Preprocess  $A$ ,  
then answer RMQs fast  
ideally constant time!

# 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:  $\lg n + 2$  *string* comparisons of string of length  $m$
- ~~~  $O(\log(n) \cdot m)$  character comparisons
- ▶ suffix tree could do  $O(m)$  total time (assuming constant  $\sigma$  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  $\ell_a$
- ▶ **Case 2:**  $\ell_a \neq \ell_b$ ; w.l.o.g.  $\boxed{\ell_a > \ell_b}$

- ▶ **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  $\ell_a$

- ▶ 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      ↗ genomes highly repetitive!
- ~~ **Key question:** How to compress  $T$  while supporting random access and read mapping?  
"Computing over compressed data"

## BWT – Definitions

*T = time<sub>H</sub> flies<sub>H</sub> quickly<sub>H</sub>*

flies quickly time

- *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\$b  
alfa\$alf\_eats\_alf**f**  
alfalfa\$alf\_eats\_alf**e**  
ats\_alfalfa\$alf\_e**e**  
eats\_alfalfa\$alf\_e**f**  
f\_eats\_alfalfa\$al**f**  
fa\$alf\_eats\_alfal**f**  
falfa\$alf\_eats\_alf**a**  
lf\_eats\_alfalfa\$al**f**  
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   | lfalfa\$alf_eats     | s 8  |
| 2   | eats_alfalfa\$al     | f 3  |
| 3   | a\$alf_eats_alfal    | f 15 |
| 4   | lf_eats_alfalfa\$    | 0    |
| 5   | alfa\$alf_eats_alf   | f 12 |
| 6   | lfalfa\$alf_eats     | s 9  |
| 7   | ats_alfalfa\$alf_e   | e 5  |
| 8   | eats_alfalfa\$alf    | f 4  |
| 9   | f_eats_alfalfa\$al   | l 2  |
| 10  | fa\$alf_eats_alfal   | l 14 |
| 11  | falfa\$alf_eats_alf  | l 11 |
| 12  | lf_eats_alfalfa\$al  | a 1  |
| 13  | lfa\$alf_eats_alf    | a 13 |
| 14  | lfalfa\$alf_eats_alf | a 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  
,\_havent,\_has,\_what\$\_have,\_had,\_hadnt,\_h  
\_havent,\_has,\_what\$\_have,\_had,\_hadnt,\_h  
\_hadnt,\_hasnt,\_havent,\_has,\_what\$\_have,\_h  
\_adnt,\_hasnt,\_havent,\_has,\_what\$\_have,\_h  
\_adnt,\_hasnt,\_havent,\_has,\_what\$\_have,\_had  
\_as,\_what\$\_have,\_had,\_hadnt,\_hasnt,\_havent  
,\_havent,\_has,\_what\$\_have,\_had,\_hadnt,\_h  
\_at\$\_have,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_w  
\_h  
\_ave,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what\$\_h  
\_avent,\_has,\_what\$\_have,\_had,\_hadnt,\_hasnt,\_h  
\_d,\_hadnt,\_hasnt,\_havent,\_has,\_what\$\_have,\_h  
\_adnt,\_hasnt,\_havent,\_has,\_what\$\_have,\_had  
\_e,\_hadnt,\_hasnt,\_havent,\_has,\_what\$\_have  
\_ent,\_has,\_what\$\_have,\_had,\_hadnt,\_hasnt,\_h  
\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what\$\_have  
,\_hadnt,\_hasnt,\_havent,\_has,\_what\$\_have,\_had  
\_has,\_what\$\_have,\_had,\_hadnt,\_hasnt,\_havent  
,\_havent,\_has,\_what\$\_have,\_had,\_hadnt,\_h  
\_hat\$\_have,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_w  
\_have,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what\$\_  
\_havent,\_has,\_what\$\_have,\_had,\_hadnt,\_hasnt  
\_nt,\_has,\_what\$\_have,\_had,\_hadnt,\_hasnt,\_h  
\_avent,\_hasnt,\_havent,\_has,\_what\$\_have,\_had  
\_h  
\_adnt,\_havent,\_has,\_what\$\_have,\_had,\_hadnt,\_h  
\_as,\_what\$\_have,\_had,\_hadnt,\_hasnt,\_h  
\_snt,\_havent,\_has,\_what\$\_have,\_had,\_hadnt,\_h  
\_t\$\_have,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_wh  
\_t,\_has,\_what\$\_have,\_had,\_hadnt,\_hasnt,\_h  
\_avent,\_hasnt,\_havent,\_has,\_what\$\_have,\_had  
\_h  
\_adnt,\_havent,\_has,\_what\$\_have,\_had,\_hadnt,\_h  
\_ve,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what\$\_h  
\_avent,\_has,\_what\$\_have,\_had,\_hadnt,\_hasnt,\_h  
\_what\$\_have,\_had,\_hadnt,\_h  
\_asnt,\_havent,\_has,\_what\$\_have,\_had,\_hadnt,\_h  
\_t\$\_have,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_wh  
\_t,\_has,\_what\$\_have,\_had,\_hadnt,\_hasnt,\_h  
\_avent,\_hasnt,\_havent,\_has,\_what\$\_have,\_had  
\_h  
\_adnt,\_havent,\_has,\_what\$\_have,\_had,\_hadnt,\_h  
\_ve,\_had,\_hadnt,\_hasnt,\_havent,\_has,\_what\$\_h  
\_avent,\_has,\_what\$\_have,\_had,\_hadnt,\_hasnt,\_h  
\_what\$\_have,\_had,\_hadnt,\_h

*T = have, had, hadn't, hasn't, haven't, has, what*

*B = t e d t t t s h h h h h h h h h a a v v v v v v v w \$ .. e d s a a a n n n a a ..*

# Run-length BWT Compression

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

**Example:**

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

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

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

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

**Larger Example:**

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

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

$\rightsquigarrow r = 19; n = 36$

- ▶ 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:**

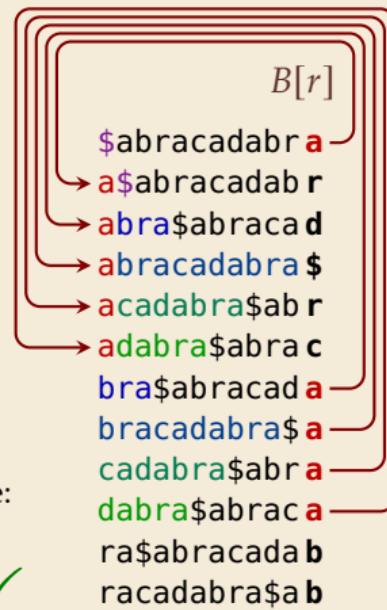
$B = \text{ard\$rcaaaabb}$

$S = \text{abracadabra\$}$

|    | $D$     | 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
  - (i) char in *first* column of *current row*
  - (ii) 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.

$\text{rank}_c(T[0..n], i) = \# \text{occurrences of } c$

$$\begin{aligned} \blacktriangleright \text{rank}_c(T[0..n], i) &= |T[0..i]|_c \\ &= \#c \text{ in first } i \text{ characters of } T \end{aligned}$$

$$\begin{aligned} \blacktriangleright \text{select}_c(T[0..n], r) &= \min\{j : |T[0..j]|_c \geq r\} \cup \{n\} \\ &= \text{index of } r\text{th } c \text{ in } T, (r = 1, 2, \dots) \end{aligned}$$

## 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  $B$  =  $\text{select}_c(B, r)$

| $T[0..9]$                    | 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 |
| rank <sub>a</sub> ( $T, i$ ) | 0 | 0 | 1 | 1 | 2 | 2 | 3 | 3 | 4 |
| rank <sub>b</sub> ( $T, i$ ) | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 2 |
| rank <sub>n</sub> ( $T, i$ ) | 0 | 0 | 0 | 1 | 1 | 2 | 2 | 2 | 3 |

| select <sub>a</sub> ( $T, r$ ) | / | 1 | 3 | 5 | 7 | 9 | 9 | 9 | 9 |
|--------------------------------|---|---|---|---|---|---|---|---|---|
| select <sub>b</sub> ( $T, r$ ) | / | 0 | 6 | 9 | 9 | 9 | 9 | 9 | 9 |
| select <sub>n</sub> ( $T, r$ ) | / | 2 | 4 | 8 | 9 | 9 | 9 | 9 | 9 |

| sort( $T$ )       | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|-------------------|---|---|---|---|---|---|---|---|---|
| a a a a b b n n n | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |

$$O[0..\sigma] = [0, 4, 6, 9]$$

# 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!)* ↗ 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 ↗ 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  $R[0..n]$  ↗ may need to go back  $t$  characters for access  
↗  $O((\ell + t) \log \sigma)$  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 n   | 0: (\$, 6)       |
| 1   | 4 <sup>th</sup> | ananaban\$b |        | 5   | 1          | aban\$bana n   | 1: (a, 5)        |
| 2   | 9 <sup>th</sup> | nanaban\$ba |        | 7   | 2          | an\$banana b   | 2: (a, 7)        |
| 3   | 3 <sup>th</sup> | anaban\$ban |        | 3   | 3          | ana\$ban\$ba n | 3: (a, 8)        |
| 4   | 8 <sup>th</sup> | naban\$bana |        | 1   | 4          | anana\$ban\$ b | 4: (a, 9)        |
| 5   | 1 <sup>th</sup> | aban\$banan |        | 6   | 5          | ban\$banan a   | 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 a   | 7: (n, 0)        |
| 8   | 7 <sup>th</sup> | n\$bananaba |        | 4   | 8          | naban\$ban a   | 8: (n, 1)        |
| 9   | 0 <sup>th</sup> | \$bananaban |        | 2   | 9          | nanaban\$ba n  | 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?



Navarro: *Indexing Highly Repetitive String Collections, Part II: Compressed Indexes*, ACM Comp. Surv. 2021