# CS 600.226: Data Structures Michael Schatz

Nov 14, 2016

Lecture 32: BWT



## HW8

## **Assignment 8: Competitive Spelling Bee**

Out on: November 2, 2018

Due by: November 9, 2018 before 10:00 pm

Collaboration: None

Grading:

Packaging 10%,

Style 10% (where applicable),

Testing 10% (where applicable),

Performance 30% (where applicable),

Functionality 40% (where applicable)

#### **Overview**

Your "one" task for this assignment is to take the simple spell checker we give you and to turn it into the fastest, most memory-efficient spell checker in the course, subject to the constraints detailed below. You are expected to do this by (once again) implementing the Map interface, this time using one of several hash table techniques (your choice, see below).

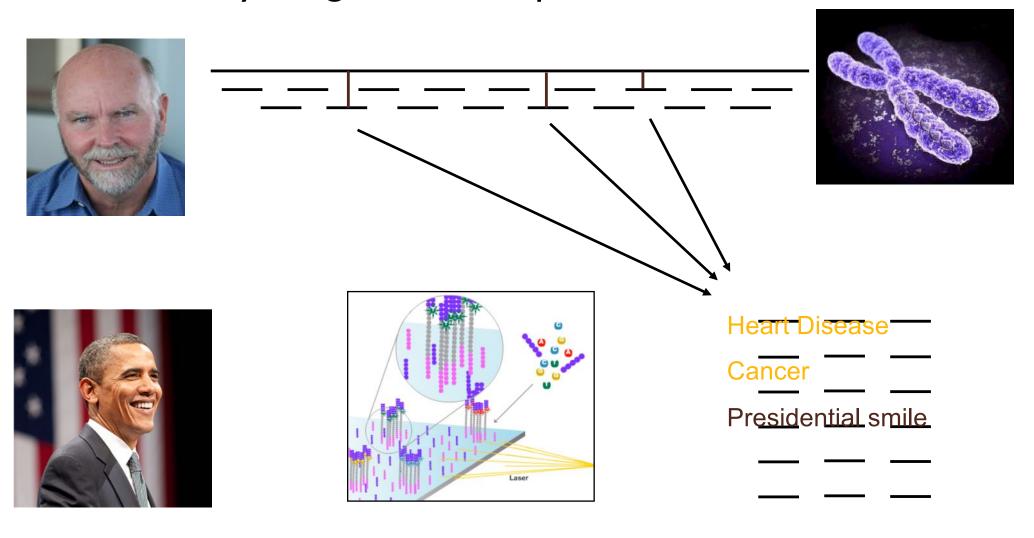


Remember: javac –Xlint:all & checkstyle \*.java & Junit & Jaybee BenchMarks

# Part I: Suffix Arrays

## Personal Genomics

How does your genome compare to the reference?



## Brute Force Analysis



- Brute Force:
  - At every possible offset in the genome:
    - Do all of the characters of the query match?
- Analysis
  - Simple, easy to understand

<ul><li>Genome length = n</li></ul>	[3B]
– Query length = m	[7]
<ul><li>Comparisons: (n-m+1) * m</li></ul>	[21B]

Overall runtime: O(nm)

[How long would it take if we double the genome size, read length?] [How long would it take if we double both?]

## Brute Force Reflections

## Why check every position?

- GATTACA can't possibly start at position 15

[WHY?]

I	2	3	4	5	6	7	8	9	10	П	12	13	14	15	•••
Т	G	Α	Т	Т	Α	С	Α	G	Α	Т	Т	Α	С	С	• • •
								G	Α	Т	Т	Α	С	Α	

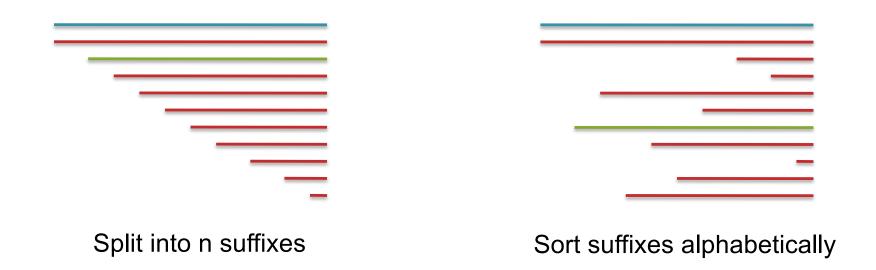
- Improve runtime to O(n + m)

[3B + 7]

- If we double both, it just takes twice as long
- Knuth-Morris-Pratt, 1977
- Boyer-Moyer, 1977, 1991
- For one-off scans, this is the best we can do (optimal performance)
  - We have to read every character of the genome, and every character of the query
  - For short queries, runtime is dominated by the length of the genome

## Suffix Arrays: Searching the Phone Book

- What if we need to check many queries?
  - We don't need to check every page of the phone book to find 'Schatz'
  - Sorting alphabetically lets us immediately skip 96% (25/26) of the book without any loss in accuracy
- Sorting the genome: Suffix Array (Manber & Myers, 1991)
  - Sort every suffix of the genome



[Challenge Question: How else could we split the genome?]

- Strategy 2: Binary search
  - Compare to the middle, refine as higher or lower
- Searching for GATTACA
  - Lo = I; Hi = 15;



#	Sequence	Pos
_	ACAGATTACC	6
2	ACC	13
3	AGATTACC	8
4	ATTACAGATTACC	3
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6	C	15
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П	TACAGATTACC	5
12	TACC	12
13	TGATTACAGATTACC	I
14	TTACAGATTACC	4
15	TTACC	П



- Strategy 2: Binary search
  - Compare to the middle, refine as higher or lower
- Searching for GATTACA
  - Lo = I; Hi = 15; Mid = (1+15)/2 = 8
  - Middle = Suffix[8] = CC



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  - Lo = 9; Hi = 15;

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8	CC	14
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10	GATTACC	9
П	TACAGATTACC	5
12	TACC	12
	IACC	12

TGATTACAGATTACC...

TTACAGATTACC...

15 TTACC...

Pos

13

4

П

**S**equence

ACC...

ACAGATTACC...





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  - Middle = Suffix[8] = CC=> Higher: Lo = Mid + I
  - Lo = 9; Hi = 15; Mid = (9+15)/2 = 12
  - Middle = Suffix[12] = TACC

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  - Middle = Suffix[12] = TACC=> Lower: Hi = Mid I
  - Lo = 9; Hi = 11;





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  - Middle = Suffix[12] = TACC=> Lower: Hi = Mid I
  - Lo = 9; Hi = 11; Mid = (9+11)/2 = 10
  - Middle = Suffix[10] = GATTACC

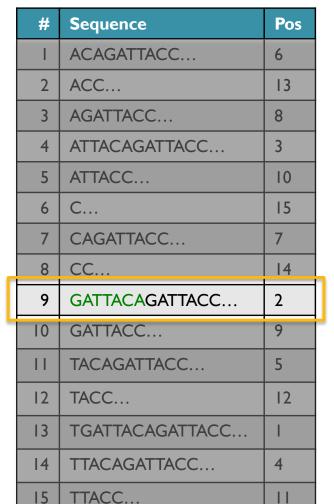
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  - Middle = Suffix[10] = GATTACC=> Lower: Hi = Mid I
  - Lo = 9; Hi = 9; Mid = (9+9)/2 = 9
  - Middle = Suffix[9] = GATTACA...=> Match at position 2!





## Binary Search Analysis

Binary Search

```
Initialize search range to entire list

mid = (hi+lo)/2; middle = suffix[mid]

if query matches middle: done

else if query < middle: pick low range

else if query > middle: pick hi range

Repeat until done or empty range
```

[WHEN?]

- Analysis
  - More complicated method
  - How many times do we repeat?
    - How many times can it cut the range in half?
    - Find smallest x such that:  $n/(2^x) \le 1$ ;  $x = \lg_2(n)$

[32]

- Total Runtime: O(m lg n)
  - More complicated, but much faster!
  - Looking up a query loops 32 times instead of 3B

[How long does it take to search 6B or 24B nucleotides?]



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Binary Search

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[32]

- Total Runtime: O(m lg n)
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Can be reduced to O(m + lg n) using an auxiliary data structure called the LCP array

## Suffix Array Construction

How can we store the suffix array?
 [How many characters are in all suffixes combined?]

$$S = 1 + 2 + 3 + \dots + n = \sum_{i=1}^{n} i = \frac{n(n+1)}{2} = O(n^2)$$

- Hopeless to explicitly store 4.5 billion billion characters
- Instead use implicit representation
  - Keep I copy of the genome, and a list of sorted offsets
  - Storing 3 billion offsets fits on a server (12GB)
- Searching the array is very fast, but it takes time to construct
  - This time will be amortized over many, many searches
  - Run it once "overnight" and save it away for all future queries



0		
ı	3	

3		

I	0	
ı	5	

14
----

9	

5		

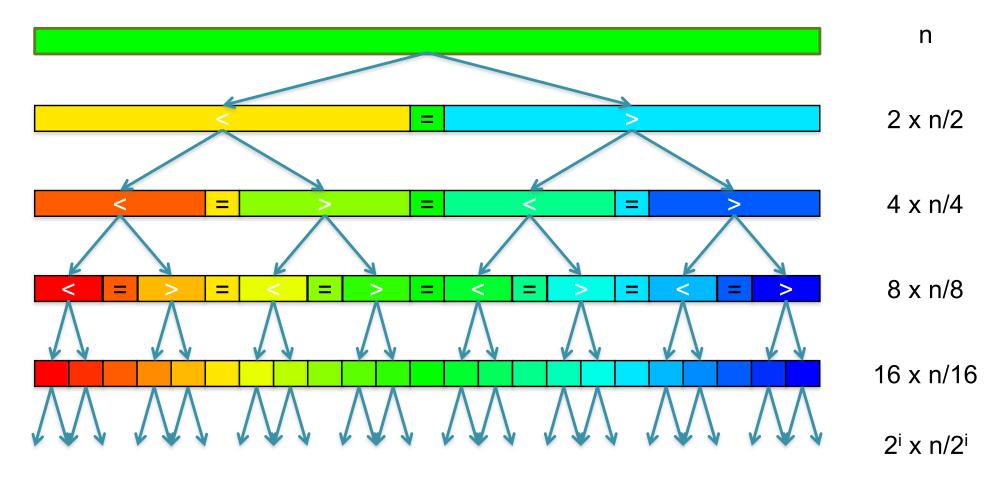


\_\_\_\_

П

## Divide and Conquer

- Selection sort is slow because it rescans the entire list for each element
  - How can we split up the unsorted list into independent ranges?
  - Hint I: Binary search splits up the problem into 2 independent ranges (hi/lo)
  - Hint 2: Assume we know the median value of a list



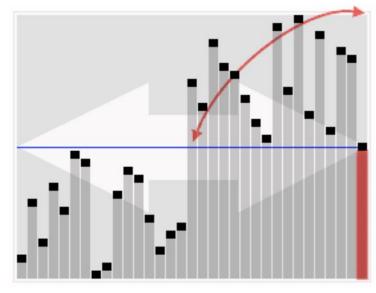
[How many times can we split a list in half?]

## QuickSort Analysis

```
QuickSort(Input: list of n numbers)
// see if we can quit
if (length(list)) <= 1): return list
```

```
// split list into lo & hi
pivot = median(list)
lo = {}; hi = {};
for (i = 1 to length(list))
if (list[i] < pivot): append(lo, list[i])
else: append(hi, list[i])</pre>
```

// recurse on sublists
return (append(QuickSort(lo), QuickSort(hi))



http://en.wikipedia.org/wiki/Quicksort

Analysis (Assume we can find the median in O(n))

$$T(n) = \begin{cases} O(1) & \text{if } n \le 1\\ O(n) + 2T(n/2) & \text{else} \end{cases}$$

$$T(n) = n + 2(\frac{n}{2}) + 4(\frac{n}{4}) + \dots + n(\frac{n}{n}) = \sum_{i=0}^{\lg(n)} \frac{2^{i}n}{2^{i}} = \sum_{i=0}^{\lg(n)} n = O(n \lg n)$$

## Implicit Suffix Comparison (I)

```
public class CompareSuffixes {
  // Compare two suffixes of text starting at s1 and s2
  // Return -1 if s1 is smaller, +1 if s2 is smaller
  public static int cmpSuffixes(String text, int s1, int s2) {
    if (s1 == s2) { return 0; }
    int d = 0;
    while ((s1 + d < text.length()) &&</pre>
           (s2 + d < text.length())) {
      char c1 = text.charAt(s1+d);
      char c2 = text.charAt(s2+d);
      if (c1 < c2) { return -1; }
      else if (c2 < c1) { return +1; }
      // else they are the same, keep going
      d++;
    // no differences through end of string
    // return shorter one, meaning having a bigger offset
    if (s1 < s2) { return +1; }
    return -1;
```

## Implicit Suffix Comparison (2)

```
public static void main(String [] args) {
    if (args.length < 3) {</pre>
      System.err.println("usage: CompareSuffixes text s1 s2\n");
     return;
    String text = args[0];
    int s1 = Integer.parseInt(args[1]);
    int s2 = Integer.parseInt(args[2]);
    // Show the suffixes for display purposes
    System.out.format("Comparing the suffixes of \"%s\"\n", text);
    System.out.format("s1 [%d]: \"%s\"\n", s1, text.substring(s1));
    System.out.format("s2 [%d]: \"%s\"\n", s2, text.substring(s2));
    int cmp = cmpSuffixes(text, s1, s2);
    System.out.println("Returned: " + cmp);
    if (cmp < 0) {
      System.out.format("s1 \"%s\" < s2 \"%s\"\n",
                        text.substring(s1),text.substring(s2));
    } else if (cmp > 0) {
      System.out.format("s2 \"%s\" < s1 \"%s\"\n",
                        text.substring(s2), text.substring(s1));
    } else {
      System.out.format("s1 \"%s\" == s2 \"%s\"\n",
                        text.substring(s1), text.substring(s2));
```

## CompareSuffixes

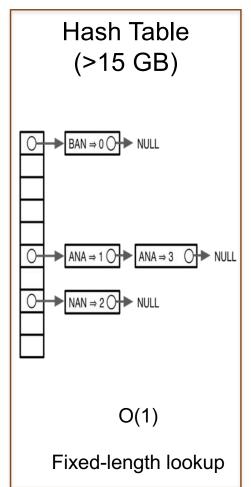
```
$ java CompareSuffixes MichaelSchatz 0 1
Comparing the suffixes of "MichaelSchatz"
s1 [0]: "MichaelSchatz"
s2 [1]: "ichaelSchatz"
Returned: -1
s1 "MichaelSchatz" < s2 "ichaelSchatz"</pre>
$ java CompareSuffixes MichaelSchatz 10 4
Comparing the suffixes of "MichaelSchatz"
s1 [10]: "atz"
s2 [4]: "aelSchatz"
Returned: 1
s2 "aelSchatz" < s1 "atz"</pre>
$ java CompareSuffixes AAAAAAAAA 0 9
Comparing the suffixes of "AAAAAAAAAAA"
s1 [0]: "AAAAAAAAAA"
s2 [9]: "AAA"
Returned: 1
s2 "AAA" < s1 "AAAAAAAAAAA
```

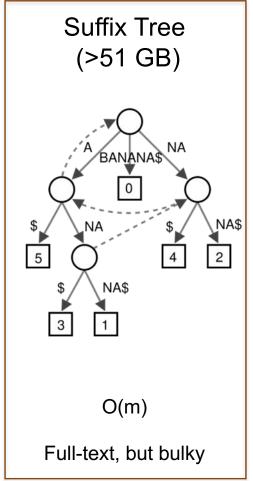
## Exact Matching Review & Overview

Where is GATTACA in the human genome?

**Brute Force** (3 GB) BANANA BAN ANA NAN ANA O(m \* n)Slow & Easy

Suffix Array (>15 GB) A\$ ANA\$ ANANA\$ BANANA\$ NA\$ NANA\$  $O(m + \lg n)$ Full-text index





\*\*\* These are general techniques applicable to any text search problem \*\*\*

## Part 2: Burrows Wheeler Transform

# Algorithmic challenge

How can we combine the speed of a suffix array O(m + lg(n)) (or even O(m)) with the size of a brute force analysis (n bytes)?

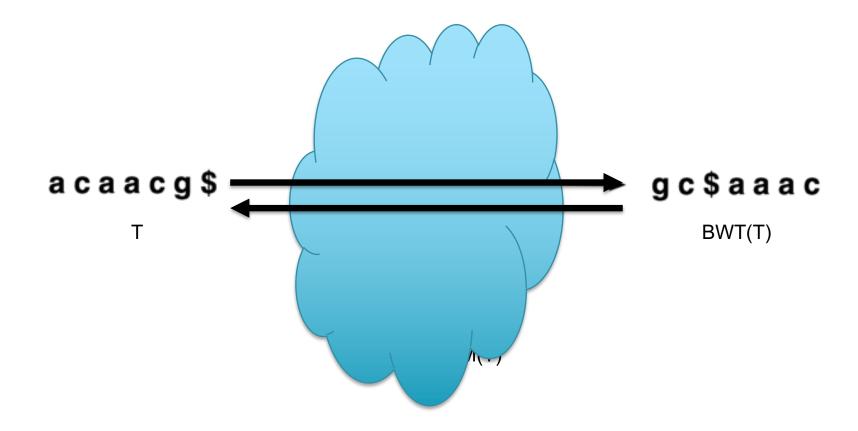
What would such an index look like?



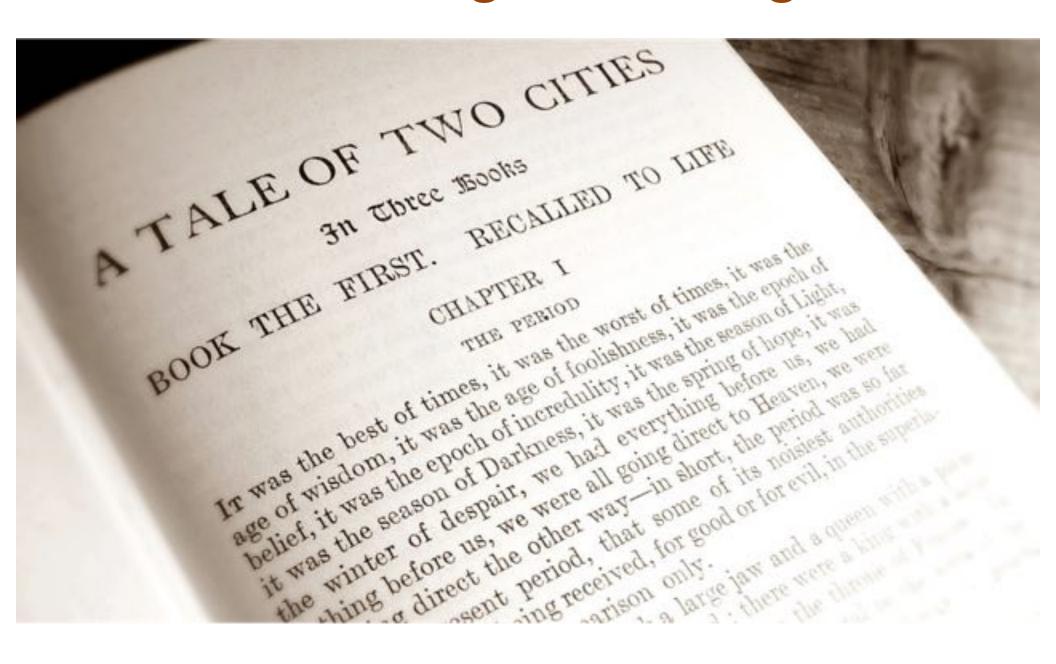
# Bowtie: Ultrafast and memory efficient alignment of short DNA sequences to the human genome

Slides Courtesy of Ben Langmead

Reversible permutation of the characters in a text



A block sorting lossless data compression algorithm.



#### ref[614]:

It\_was\_the\_best\_of\_times,\_it\_was\_the\_worst\_of\_times,\_it\_was\_the\_age\_
of\_wisdom,\_it\_was\_the\_age\_of\_foolishness,\_it\_was\_the\_epoch\_of\_belief
,\_it\_was\_the\_epoch\_of\_incredulity,\_it\_was\_the\_season\_of\_Light,\_it\_wa
s\_the\_season\_of\_Darkness,\_it\_was\_the\_spring\_of\_hope,\_it\_was\_the\_wint
er\_of\_despair,\_we\_had\_everything\_before\_us,\_we\_had\_nothing\_before\_us
,\_we\_were\_all\_going\_direct\_to\_Heaven,\_we\_were\_all\_going\_direct\_the\_o
ther\_way\_-\_in\_short,\_the\_period\_was\_so\_far\_like\_the\_present\_period,\_
that\_some\_of\_its\_noisiest\_authorities\_insisted\_on\_its\_being\_received
,\_for\_good\_or\_for\_evil,\_in\_the\_superlative\_degree\_of\_comparison\_only.\$

#### Run Length Encoding:

- Replace a "run" of a character X with a single X followed by the length of the run
- GAAAAAAATTACA => GA8T2ACA (reverse is also easy to implement)
- If your text contains numbers, then you will need to use a (slightly) more sophisticated encoding

#### ref[614]:

It\_was\_the\_best\_of\_times,\_it\_was\_the\_worst\_of\_times,\_it\_was\_the\_age\_
of\_wisdom,\_it\_was\_the\_age\_of\_foolishness,\_it\_was\_the\_epoch\_of\_belief
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#### rle(ref)[614]:

It\_was\_the\_best\_of\_times,\_it\_was\_the\_worst\_of\_times,\_it\_was\_the\_age\_
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s\_the\_season\_of\_Darknes2,\_it\_was\_the\_spring\_of\_hope,\_it\_was\_the\_wint
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#### bwt[614]:

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#### rle(bwt)[464]:

.dlms2ftysesdtrsns\_y\_2\$\_yfofe4tg2sfefefg2e2drofr,12re2f-,fs,9nfrsdn2 hereghet2edndete2ge2nste2,s5t,es3ns2f2te2dt10r,4e3feh2\_2p\_2fpDw11e2h 1\_ew\_5eo2\_ne3oa2eo2\_4seph2r2hvh2w2egmgh7kr2w2h2s2Hr3vtr2ib2dbcbvs\_2t hw2p3vm2irdn2ib\_2eo12\_4e2n6a2i\_3ec2\_2t18s\_tsgltsLlvt2\_3h2o2re\_wr2ad2 wlors\_9r\_2lteiril2re\_oua2no2i2oeo4i3hki6o\_2ieitsp2ioi\_12g2nodsc\_s3\_g fhf\_f3hwh\_nsmo\_2ue2\_sio3ae4o2\_i2cgp2e2aoaeo2e2s2eu2teta11i\_2ei\_in\_2a 2ie\_e3rei\_hrs3nac2i2Ii7sn\_15oyoui\_2a\_i3ds\_2ai2ae2\_21tlar

#### bwt[614]:

```
.dlmssftysesdtrsns_y__$_yfofeeeetggsfefefggeedrofr,llreef-,fs,,,,,,,,,,,,,,nfrsdnnhereghettedndeteegeenstee,ssssst,esssnssffteedttttttttt,,,,,eeefehh__p__fpDwwwwwwwwwweehl_ew____eoo_neeeoaaeoo___sephhrrhvh hwwegmghhhhhhkrrwwhhssHrrrvtrribbdbcbvs__thwwpppvmmirdnnib__eoooooo oooooo__eennnnnaai__ecc__ttttttttttttttttttts_tsgltsLlvtt__hhoor e_wrraddwlors____r_lteirillre_ouaanooiioeooooiiihkiiiiio__iei tsppioi____ggnodsc_sss_gfhf_fffhwh_nsmo__uee_sioooaeeeeoo_ii cgppeeaoaeooeesseuutetaaaaaaaaaaai__ei_in__aaie_eeerei_hrsssnacciiIi iiiiiisn_____oyoui__a_iiids__aiiaee______tlar
```

#### rle(bwt)[464]:

.dlms2ftysesdtrsns\_y\_2\$\_yfofe4tg2sfefefg2e2drofr,12re2f-,fs,9nfrsdn2 hereghet2edndete2ge2nste2,s5t,es3ns2f2te2dt10r,4e3feh2\_2p\_2fpDw11e2h 1\_ew\_5eo2\_ne3oa2eo2\_4seph2r2hvh2w2egmgh7kr2w2h2s2Hr3vtr2ib2dbcbvs\_2t hw2p3vm2irdn2ib\_2eo12\_4e2n6a2i\_3ec2\_2t18s\_tsgltsLlvt2\_3h2o2re\_wr2ad2 wlors\_9r\_2lteiril2re\_oua2no2i2oeo4i3hki6o\_2ieitsp2ioi\_12g2nodsc\_s3\_g fhf\_f3hwh\_nsmo\_2ue2\_sio3ae4o2\_i2cgp2e2aoaeo2e2s2eu2teta11i\_2ei\_in\_2a 2ie\_e3rei\_hrs3nac2i2Ii7sn\_15oyoui\_2a\_i3ds\_2ai2ae2\_21tlar

#### ref[614]:

It\_was\_the\_best\_of\_times,\_it\_was\_the\_worst\_of\_times,\_it\_was\_the\_age\_
of\_wisdom,\_it\_was\_the\_age\_of\_foolishness,\_it\_was\_the\_epoch\_of\_belief
,\_it\_was\_the\_epoch\_of\_incredulity,\_it\_was\_the\_season\_of\_Light,\_it\_wa
s\_the\_season\_of\_Darkness,\_it\_was\_the\_spring\_of\_hope,\_it\_was\_the\_wint
er\_of\_despair,\_we\_had\_everything\_before\_us,\_we\_had\_nothing\_before\_us
,\_we\_were\_all\_going\_direct\_to\_Heaven,\_we\_were\_all\_going\_direct\_the\_o
ther\_way\_-\_in\_short,\_the\_period\_was\_so\_far\_like\_the\_present\_period,\_
that\_some\_of\_its\_noisiest\_authorities\_insisted\_on\_its\_being\_received
,\_for\_good\_or\_for\_evil,\_in\_the\_superlative\_degree\_of\_comparison\_only.\$

#### rle(bwt)[464]:

.dlms2ftysesdtrsns\_y\_2\$\_yfofe4tg2sfefefg2e2drofr,l2re2f-,fs,9nfrsdn2 hereghet2edndete2ge2nste2,s5t,es3ns2f2te2dt10r,4e3feh2\_2p\_2fpDw11e2h l\_ew\_5eo2\_ne3oa2eo2\_4seph2r2hvh2w2egmgh7kr2w2h2s2Hr3vtr2ib2dbcbvs\_2t hw2p3vm2irdn2ib\_2eo12\_4e2n6a2i\_3ec2\_2t18s\_tsgltsLlvt2\_3h2o2re\_wr2ad2 wlors\_9r\_2lteiril2re\_oua2no2i2oeo4i3hki6o\_2ieitsp2ioi\_12g2nodsc\_s3\_g fhf\_f3hwh\_nsmo\_2ue2\_sio3ae4o2\_i2cgp2e2aoaeo2e2s2eu2teta11i\_2ei\_in\_2a 2ie\_e3rei\_hrs3nac2i2Ii7sn\_15oyoui\_2a\_i3ds\_2ai2ae2\_21tlar

#### ref[614]:

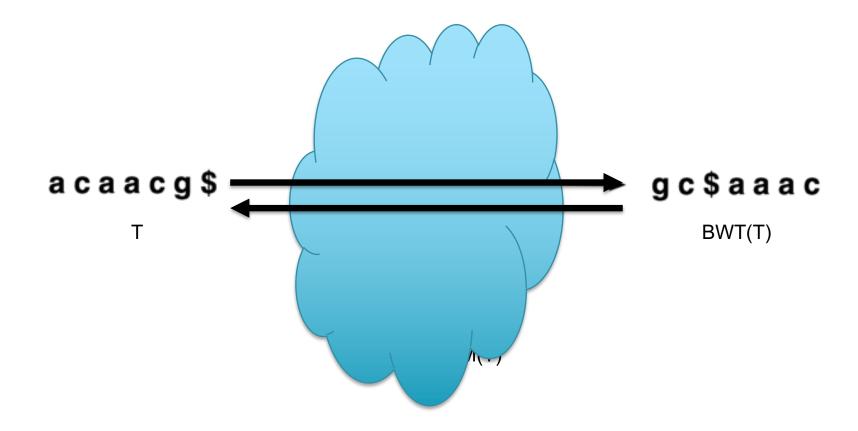
It\_was\_the\_best\_of\_times,\_it\_was\_the\_worst\_of\_times,\_it\_was\_the\_age\_
of\_wisdom,\_it\_was\_the\_age\_of\_foolishness,\_it\_was\_the\_epoch\_of\_belief
,\_it\_was\_the\_epoch\_of\_incredulity,\_it\_was\_the\_season\_of\_Light,\_it\_wa
s\_the\_season\_of\_Darkness,\_it\_was\_the\_spring\_of\_hope,\_it\_was\_the\_wint
er\_of\_despair,\_we\_had\_everything\_before\_us,\_we\_had\_nothing\_before\_us
,\_we\_were\_all\_going\_direct\_to\_Heaven,\_we\_were\_all\_going\_direct\_the\_o
ther\_way\_-\_in\_short,\_the\_period\_was\_so\_far\_like\_the\_present\_period,\_
that\_some\_of\_its\_noisiest\_authorities\_insisted\_on\_its\_being\_received
,\_for\_good\_or\_for\_evil,\_in\_the\_superlative\_degree\_of\_comparison\_only.\$

#### rle(bwt)[464]:

.dlms2ftysesdtrsns\_y\_2\$\_yfofe4tg2sfefefg2e2drofr,l2re2f-,fs,9nfrsdn2hereghet2edndete2ge2nste2,s5t,es3ns2f2te2dt10r,4e3feh2\_2p\_2fpDw11e2hl\_ew\_5eo2\_ne3oa2eo2\_4seph2r2hvh2w2egmgh7kr2w2h2s2Hr3vtr2ib2dbcbvs\_2thw2p3vm2irdn2ib\_2eo12\_4e2n6a2i\_3ec2\_2t18s\_tsgltsLlvt2\_3h2o2re\_wr2ad2wlors\_9r\_2lteiril2re\_oua2no2i2oeo4i3hki6o\_2ieitsp2ioi\_12g2nodsc\_s3\_gfhf\_f3hwh\_nsmo\_2ue2\_sio3ae4o2\_i2cgp2e2aoaeo2e2s2eu2teta11i\_2ei\_in\_2a2ie\_e3rei\_Saved 614-464 = 150 bytes (24%) with zero loss of information!

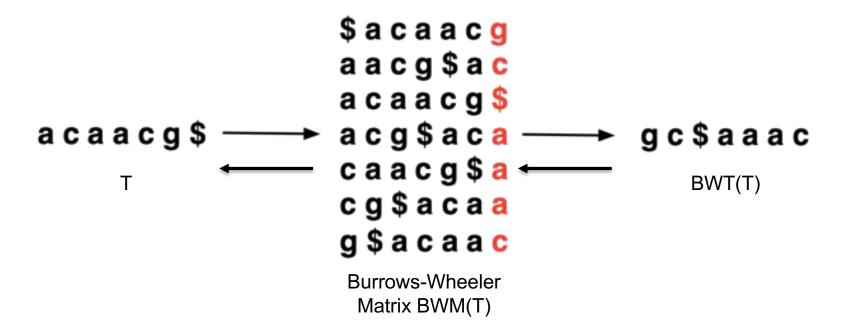
Common to save 50% to 90% on real world files with bzip2

Reversible permutation of the characters in a text



A block sorting lossless data compression algorithm.

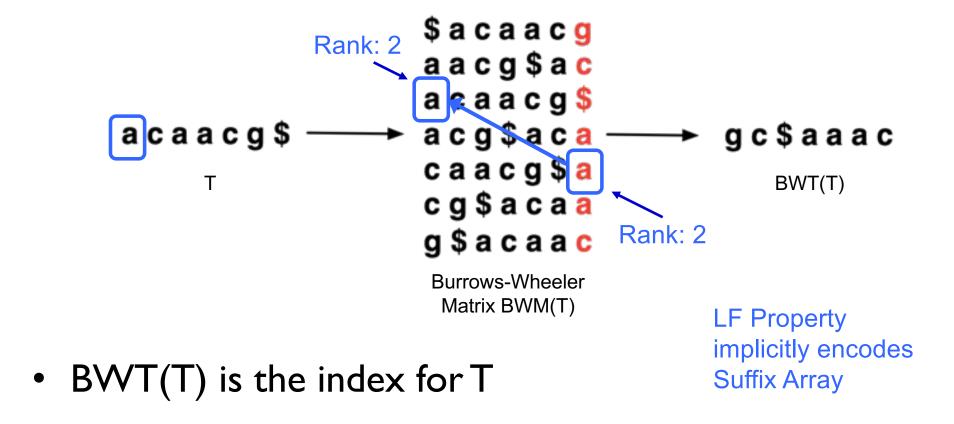
Reversible permutation of the characters in a text



BWT(T) is the index for T

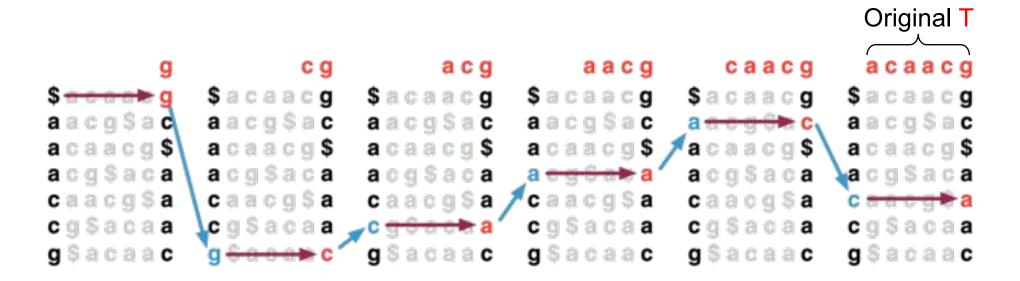
A block sorting lossless data compression algorithm.

Reversible permutation of the characters in a text



A block sorting lossless data compression algorithm.

- Recreating T from BWT(T)
  - Start in the first row and apply LF repeatedly, accumulating predecessors along the way



## **BWT Exact Matching**

LFc(r, c) does the same thing as LF(r) but it ignores r's actual final character and "pretends" it's c:

```
$ a c a a c g

a a c g $ a c

a c a a c g $

a c g $ a c a

c a a c g $ a g

c a a c g $ a g

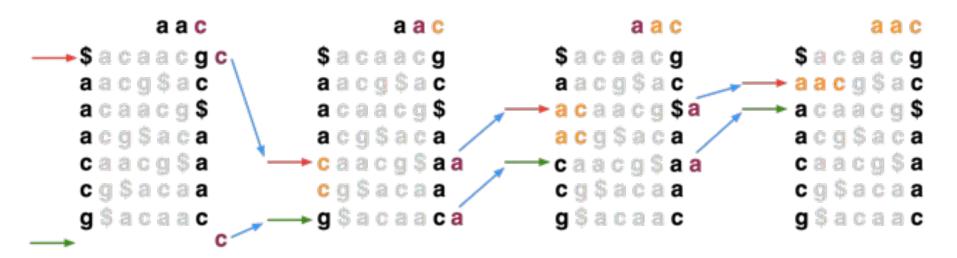
c g $ a c a a

Rank: 2
```

# **BWT Exact Matching**

 Start with a range, (top, bot) encompassing all rows and repeatedly apply LFc:

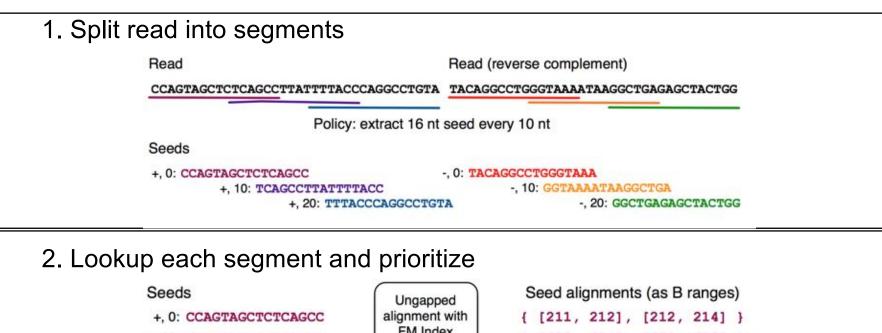
```
top = LFc(top, qc); bot = LFc(bot, qc)
qc = the next character to the left in the query
```



Ferragina P, Manzini G: Opportunistic data structures with applications. FOCS. IEEE Computer Society; 2000.

[Search for TTA this BWT string: ACTGA\$TTA]

# Algorithm Overview



```
+, 0: CCAGTAGCTCTCAGCC
+, 10: TCAGCCTTATTTTACC
+, 20: TTTACCCAGGCCTGTA
-, 0: TACAGGCCTGGGTAAA
-, 10: GGTAAAATAAGGCTGA
-, 20: GGCTGAGAGCTACTGG

Ungapped
alignment with
FM Index
{ [211, 212], [212, 214] }
{ [653, 654], [651, 653] }

{ [684, 685] }

{ [684, 685] }

{ [624, 625] }
```

3. Evaluate end-to-end match

```
Extension candidates
                                         SAM alignments
                          SIMD dynamic
                                                 chr12
                                                          1936
                          programming
SA:684, chr12:1955
                            aligner
SA:624, chr2:462
                                              CCAGTAGCTCTCAGCCTTATTTTACCCAGGCCTGTA
SA:211: chr4:762
                                                              XG:1:0
SA:213: chr12:1935
                                             NM: i:0
                                                      MD:Z:36 YT:Z:UU
SA:652: chr12:1945
                                             YM: i:0
                                                         (Langmead & Salzberg, 2012)
```

## Next Steps

- I. Reflect on the magic and power of Suffix Arrays and the BWT!
- I. Assignment 8 due Friday November 16 @ 10pm