Exact String Matching and searching for SNPs (2)
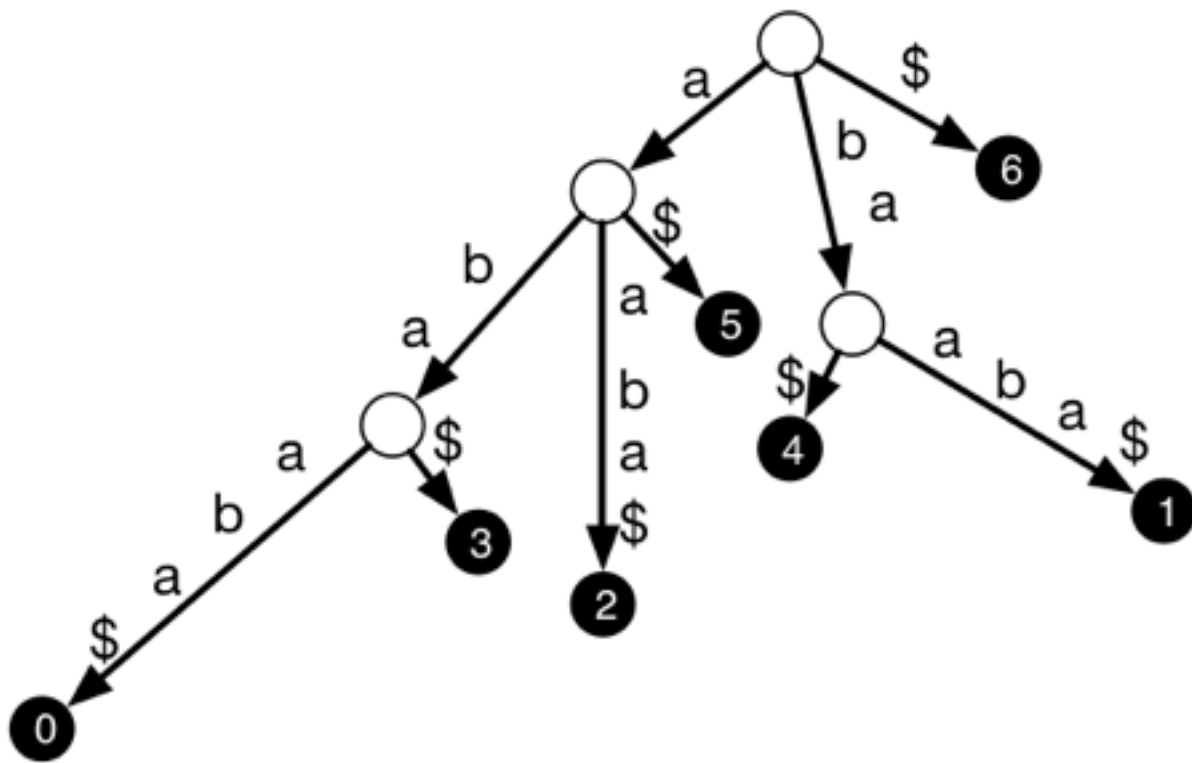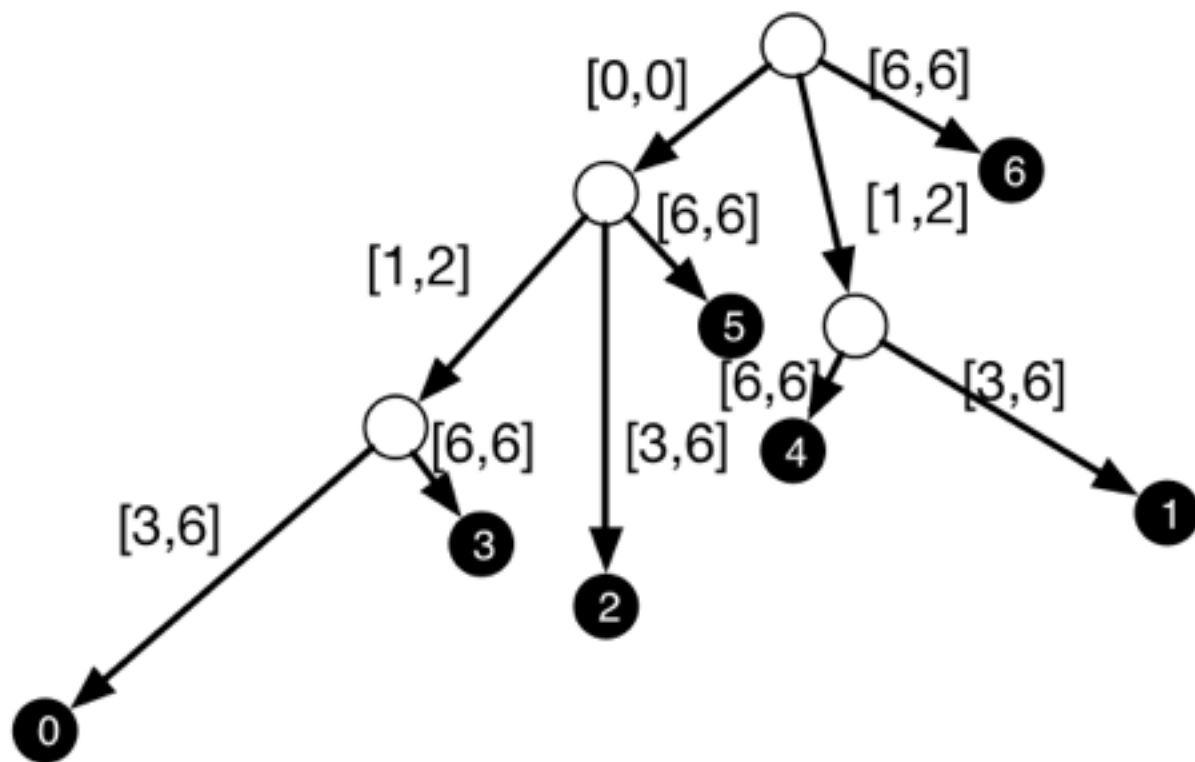
CMSC423 Fall 2014

Suffix Tree

T: abaaba$
   0123456

- Collapse non-branching nodes
  - #nodes O(|T|)

- Memory requirement is *not* O(|T|)
  - In the worst case, space required for edge labels is O(|T|)

Suffix Tree

T: abaaba$
   0123456

- Collapse non-branching nodes
  - #nodes O(|T|)

- Label edges with substring *[start,end]*
  - O(1) per edge

- Memory now O(|T|)

- Construction algorithm O(|T|) (see Gusfield)

Recap

Structure	Processing Time	Memory	Search
Suffix Trie	O(|T|)	O(|T|	O(|P|)
Suffix Tree	O(|T|)	O(|T|)*	O(|P|)
Suffix Array	O(|T|)	O(|T|) (but **much** smaller than Suffix Tree)	O(|P|log

*In best implementations about 20 bytes per character (as opposed to 4 bytes for suffix array)

Suffix Arrays

- Even though Suffix Trees are O(n) space, the constant hidden by the big-Oh notation is somewhat "big": ≈ 20 bytes / character in good implementations.

- If you have a 10Gb genome, 20 bytes / character = 200Gb to store your suffix tree. "Linear" but large.

- Suffix arrays are a more efficient way to store the suffixes that can do most of what suffix trees can do, but just a bit slower.

- Slight space vs. time tradeoff.

Example Suffix Array

- Idea: lexicographically sort all the suffixes.

- Store the starting indices of the suffixes in an array.

s = attcatg$

1	attcatg$
2	ttcatg$
3	tcatg$
4	catg$
5	atg$
6	tg$
7	g$
8	$

index of suffix   suffix of s

sort the suffixes alphabetically

→

the indices just "come along for the ride"

8	$
5	atg$
1	attcatg$
4	catg$
7	g$
3	tcatg$
6	tg$
2	ttcatg$

Example Suffix Array

- Idea: lexicographically sort all the suffixes.

- Store the starting indices of the suffixes in an array.

s = attcatg$

index of suffix	suffix of s
1	attcatg$
2	ttcatg$
3	tcatg$
4	catg$
5	atg$
6	tg$
7	g$
8	$

sort the suffixes alphabetically

→

the indices just "come along for the ride"

8
5
1
4
7
3
6
2

Search via Suffix Arrays

s = cattcat$

8	$
6	at$
2	attcat$
5	cat$
1	cattcat$
7	t$
4	tcat$
3	ttcat$

$\longleftarrow$ $\checkmark$ (at attcat$)

$\longleftarrow$ (at cattcat$)

- Does string "at" occur in s?
- Binary search to find "at".

- What about "tt"?

Counting via Suffix Arrays

s = cattcat$

|	
8	$
6	at$
2	attcat$
5	cat$
1	cattcat$
7	t$
4	tcat$
3	ttcat$

- How many times does "at" occur in the string?

- All the suffixes that start with "at" will be next to each other in the array.

- Find one suffix that starts with "at" (using binary search).

- Then count the neighboring sequences that start with at.

Constructing Suffix Arrays

- Easy $O(n^2 \log n)$ algorithm:

    sort the n suffixes, which takes $O(n \log n)$ comparisons, where each comparison takes $O(n)$.

- There are several direct $O(n)$ algorithms for constructing suffix arrays that use very little space.

- An simple $O(n)$ algorithm: build the suffix tree, and exploit the relationship between suffix trees and suffix arrays (next slide)

Relationship between Suffix Arrays and Suffix Trees

T: abaaba$
    0123456
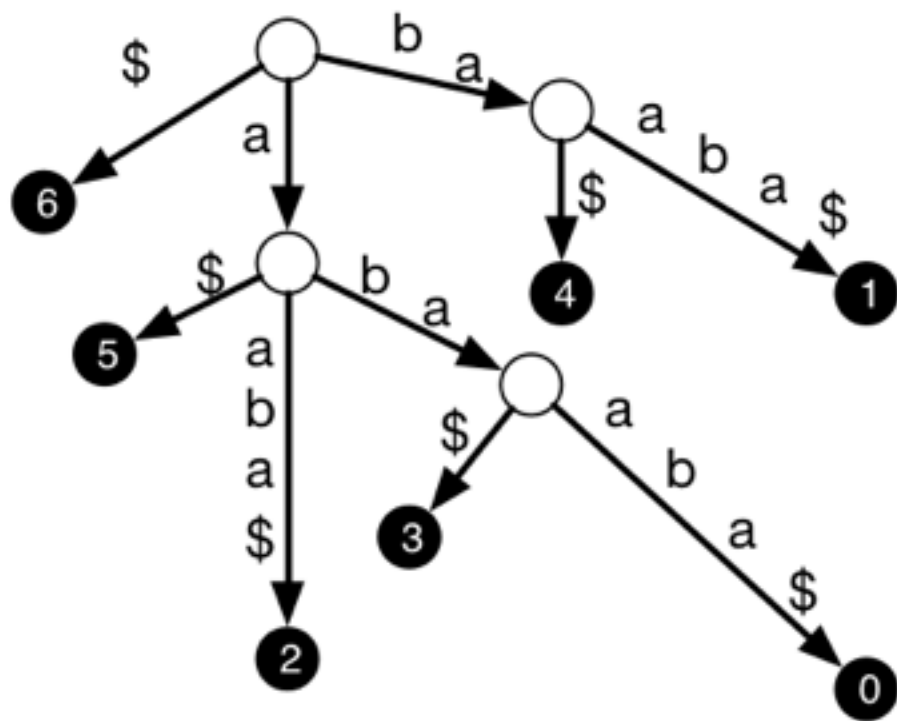
6	$
5	a$
2	aaba$
3	aba$
0	abaaba$
4	ba$
1	baaa$

Build suffix trees with edge labels sorted lexicographically
Order of leaves: 6,5,2,3,0,4,1

Recap

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Burrows-Wheeler Transform

Text transform that is useful for compression & search.

banana

banana$ $banana

anana$b   a$banan

nana$ba   sort   ana$ban

ana$ban   →   anana$b

na$bana   banana$

a$banan   nana$ba

$banana   na$bana

BWT(banana) =
annb$aa

Tends to put runs of the same character together.

Makes compression work well.

"bzip" is based on this.

Another Example

appellee$

appellee$
ppellee$a
pellee$ap
ellee$app   → sort →
llee$appe
lee$appel
ee$appell
e$appelle
$appellee

$appellee
appellee$
e$appelle
ee$appell
ellee$app
lee$appel
llee$appe
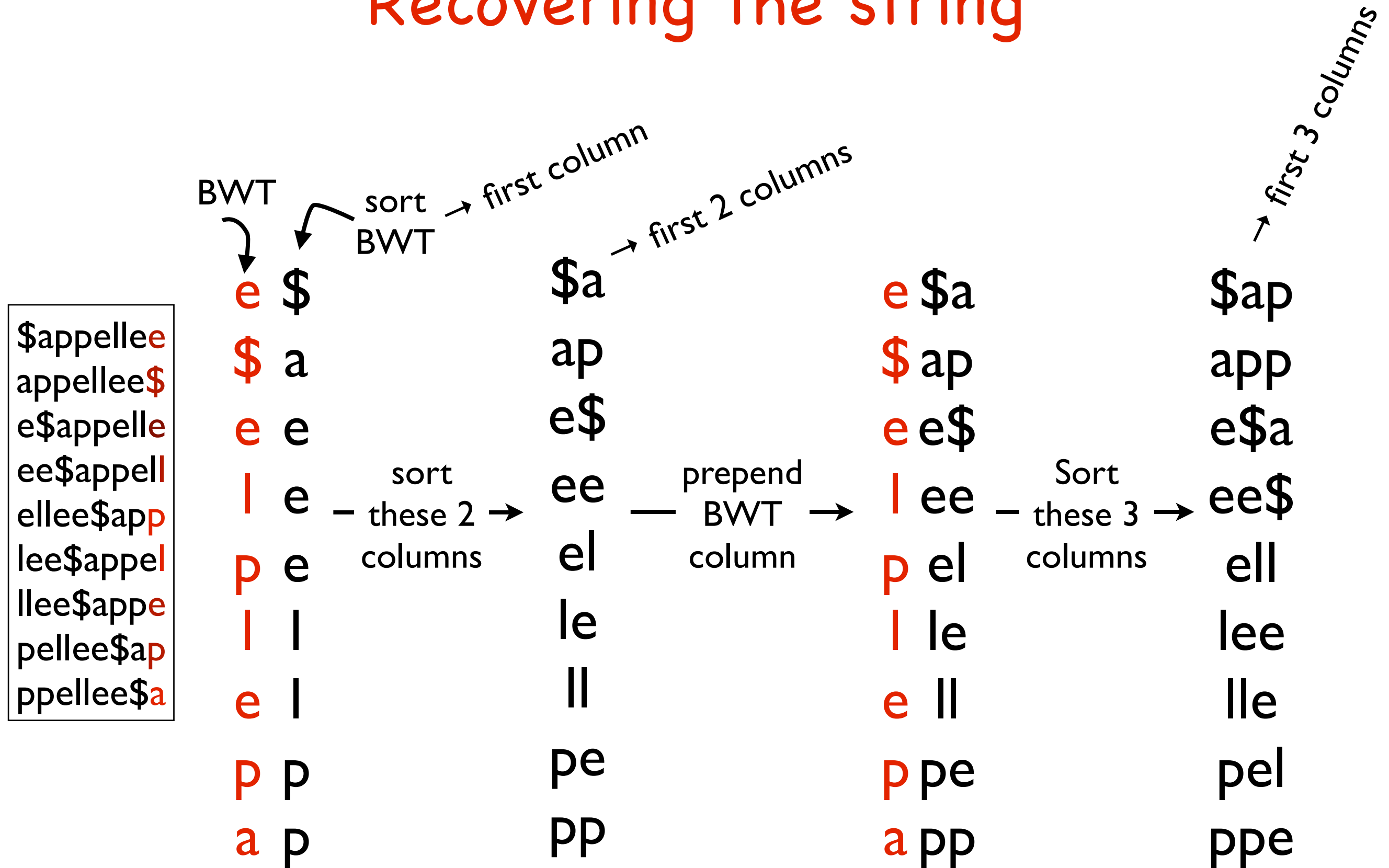pellee$ap
ppellee$a

BWT(appellee$) =
e$elplepa

Doesn't always improve
the compressibility...

Recovering the string

first 3 columns

BWT

sort BWT → first column

→ first 2 columns

$appellee	e $	$a	e $a	$ap
appellee$	$ a	ap	$ ap	app
e$appelle	e e	e$	e e$	e$a
ee$appell	l e	ee	l ee	ee$
ellee$app	p e	el	P el	ell
lee$appel	l l	le	l le	lee
llee$appe	e l	ll	e ll	lle
pellee$ap	P p	pe	P pe	pel
ppellee$a	a p	pp	a pp	ppe

sort these 2 columns →

prepend BWT column →

Sort these 3 columns →

Inverse BWT

```
def inverseBWT(s):
    B = [s_1,s_2,s_3,...,s_n]
    for i = 1..n:
        sort B
        prepend s_i to B[i]
    return row of B that ends with $
```

Another BWT Example

dogwood$ $dogwoo**d**
ogwood$d   d$dogwo**o**
gwood$do   dogwood**$**
wood$dog   *sort*→   gwood$d**o**   *last column*→
ood$dogw   od$dogw**o**
od$dogwo   ogwood$**d**   BWT(dogwood$) =
d$dogwoo   ood$dog**w**   **do$oodwg**
$dogwood   wood$do**g**

do$oodwg   Another BWT Example

	Prepend	Sort		Prepend	Sort		Prepend	Sort		Prepend	Sort
d	$	$d	d	$d	$do	d	$do	$dog	d	$dog	$dogw
o	d	d$	o	d$	d$d	o	d$d	d$do	o	d$do	d$dog
$	d	do	$	do	dog	$	dog	dogw	$	dogw	dogwo
o	g	gw	o	gw	gwo	o	gwo	gwoo	o	gwoo	gwood
o	o	od	o	od	od$	o	od$	od$d	o	od$d	od$do
d	o	og	d	og	ogw	d	ogw	ogwo	d	ogwo	ogwoo
w	o	oo	w	oo	ood	w	ood	ood$	w	ood$	ood$d
g	w	wo	g	wo	woo	g	woo	wood	g	wood	wood$

	Prepend	Sort		Prepend	Sort		Prepend	Sort
d	$dogw	$dogwo	d	$dogwo	$dogwoo	d	$dogwoo	$dogwood
o	d$dog	d$dogw	o	d$dogw	d$dogwo	o	d$dogwo	d$dogwoo
$	dogwo	dogwoo	$	dogwoo	dogwood	$	dogwood	dogwood$
o	gwood	gwood$	o	gwood$	gwood$d	o	gwood$d	gwood$do
o	od$do	od$dog	o	od$dog	od$dogw	o	od$dogw	od$dogwo
d	ogwoo	ogwood	d	ogwood	ogwood$	d	ogwood$	ogwood$d
w	ood$d	ood$do	w	ood$do	ood$dog	w	ood$dog	ood$dogw
g	wood$	wood$d	g	wood$d	wood$do	g	wood$do	wood$dog

Searching with BWT: LF Mapping

LF Mapping

Σ

BWT(unabashable)

	$	a	b	e	h	l	n	s	u
$unabashable	0	0	0	0	0	0	0	0	0
abashable$un	0	0	0	1	0	0	0	0	0
able$unabash	0	0	0	1	0	0	1	0	0
ashable$unab	0	0	0	1	1	0	1	0	0
bashable$una	0	0	1	1	1	0	1	0	0
ble$unabasha	0	1	1	1	1	0	1	0	0
e$unabashabl	0	2	1	1	1	0	1	0	0
hable$unabas	0	2	1	1	1	1	1	0	0
le$unabashab	0	2	1	1	1	1	1	1	0
nabashable$u	0	2	2	1	1	1	1	1	0
shable$unaba	0	2	2	1	1	1	1	1	1
unabashable$	0	3	2	1	1	1	1	1	1
	1	3	2	1	1	1	1	1	1

# of times letter appears before this position in the last column.

LF Property: The ith occurrence of a letter X in the last column corresponds to the ith occurrence of X in the first column.

BWT Search

BWTSearch(aba)   Start from the **end** of the pattern

LF Mapping

Step 1: Find the range of "a"s in the first column

Step 2: Look at the same range in the last column.

Step 3: "b" is the next pattern character. Set B = the LF mapping entry for b in the first row of the range.

Set E = the LF mapping entry for b in the last + 1 row of the range.

Step 4: Find the range for "b" in the first row, and use B and E to find the right subrange within the "b" range.

BWT(unabashable)

Σ

	$	a	b	e	h	l	n	s	u
$unabashable	0	0	0	0	0	0	0	0	0
abashable$un	0	0	0	1	0	0	0	0	0
able$unabash	0	0	0	1	0	0	1	0	0
ashable$unab	0	0	0	1	1	0	1	0	0
bashable$una	0	0	1	1	1	0	1	0	0
ble$unabasha	0	1	1	1	1	0	1	0	0
e$unabashabl	0	2	1	1	1	0	1	0	0
hable$unabas	0	2	1	1	1	1	1	0	0
le$unabashab	0	2	1	1	1	1	1	1	0
nabashable$u	0	2	2	1	1	1	1	1	0
shable$unaba	0	2	2	1	1	1	1	1	1
unabashable$	0	3	2	1	1	1	1	1	1
	1	3	2	1	1	1	1	1	1

BWT Searching Example 2

pattern = "bana"

(B,E) = 0, 2

(B,E) = 1, 2

(B,E) = 0, 1

BWT Searching Notes

- Don't have to store the LF mapping. A more complex algorithm (later slides) lets you compute it in $O(1)$ time in **compressed** data on the fly with some extra storage.

- To find the range in the first column corresponding to a character:
  - Pre-compute array $C[c]$ = # of occurrences in the string of characters lexicographically $< c$.
  - Then start of the "a" range, for example, is: $C["a"] + 1$.

- Running time: $O(|pattern|)$
  - Finding the range in the first column takes $O(1)$ time using the C array.
  - Updating the range takes $O(1)$ time using the LF mapping.

Relationship Between BWT and Suffix Arrays

`s = appellee$`
123456789

BWT matrix	The suffixes	Suffix array	Suffix position − 1
$appellee	$	9	s[9-1] = e
appellee$	appellee$	1	s[1-1] = $
e$appelle	e$	8	s[8-1] = e
ee$appell	ee$	7	s[7-1] = l
ellee$app	ellee$	4	s[4-1] = p
lee$appel	lee$	6	s[6-1] = l
llee$appe	llee$	5	s[5-1] = e
pellee$ap	pellee$	3	s[3-1] = p
ppellee$a	ppellee$	2	s[2-1] = a

These are still in sorted order because "$" comes before everything else

− subtract 1 →

BWT
matrix

The suffixes
are obtained
by deleting
everything
after the $

Suffix array
(start position
for the suffixes)

Suffix position - 1 =
the position of the
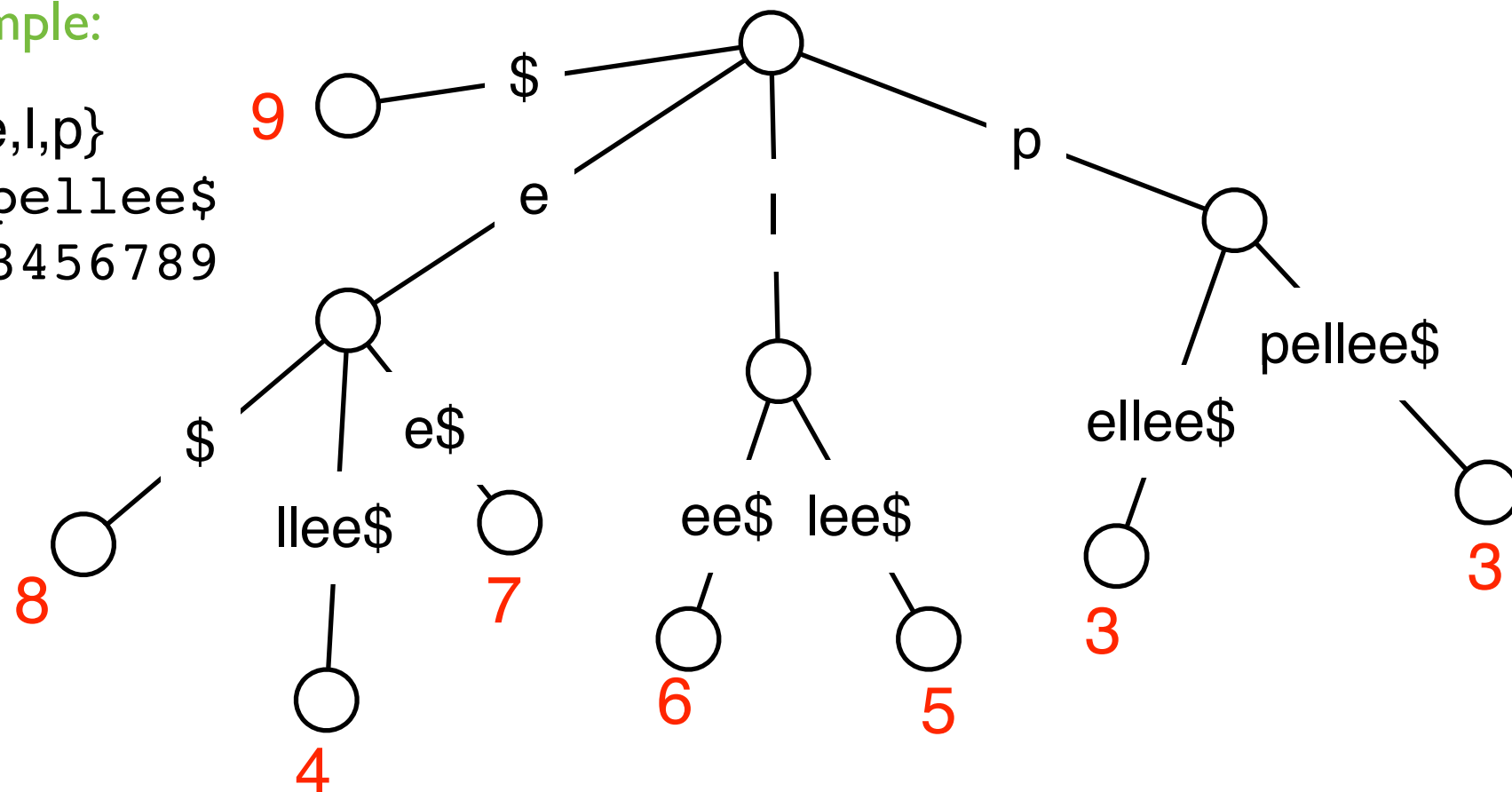last character of
the BWT matrix

($ is a special case)

Relationship Between BWT and Suffix Trees

- Remember: Suffix Array = suffix numbers obtained by traversing the leaf nodes of the (ordered) Suffix Tree from left to right.

- Suffix Tree ⇒ Suffix Array ⇒ BWT.

Ordered suffix tree for previous example:

$\Sigma = \{\$,e,l,p\}$
s = appellee\$
    123456789

Computing BWT in O(n) time

- Easy $O(n^2 \log n)$-time algorithm to compute the BWT (create and sort the BWT matrix explicitly).

- Several direct $O(n)$-time algorithms for BWT.
  These are space efficient.

- Also can use suffix arrays or trees:

  Compute the suffix array, use correspondence between suffix array and BWT to output the BWT.

  $O(n)$-time and $O(n)$-space, but the constants are large.

Recap

Structure	Processing Time	Memory	Search
Suffix Trie	O(|T|)	O(|T|	O(|P|)
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Suffix Array	O(|T|)	O(|T|) (but **much** smaller than Suffix Tree)	O(|P|log
BWT	O(|T|)	O(|T|)**	O(|P|)

*In best implementations about 20 bytes per character (as opposed to 4 bytes for suffix array)
**Compressed! For human genome ~2GB