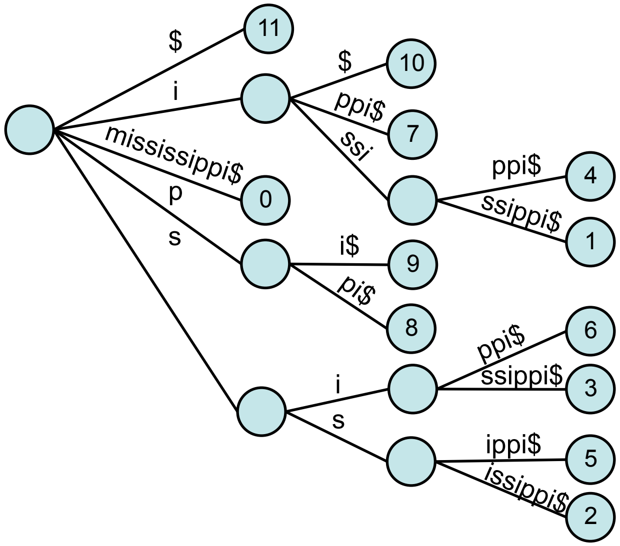
Lecture 17:
Suffix Arrays and
Burrows Wheeler Transforms

Not in Book

Homeworks #4 & #5
will be merged

Recall Suffix Trees

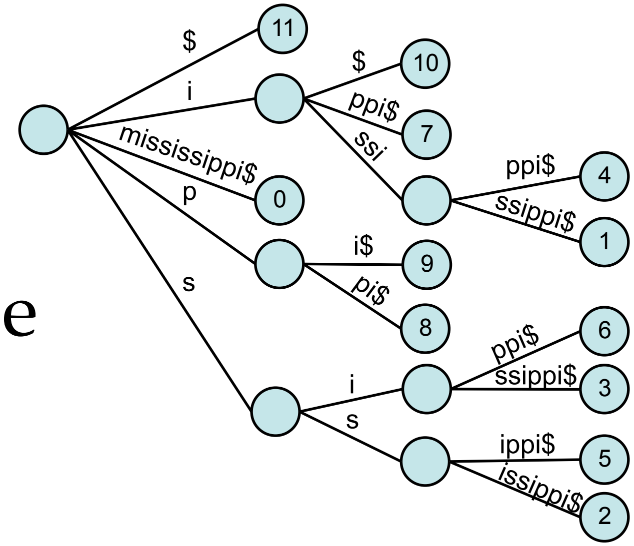
- A compressed keyword tree of suffixes from a given sequence
- Leaf nodes are labeled by the starting location of the suffix that terminates there
- Note that we now add an end-of-string character ‘$’



0. mississippi$
1. ississippi$
2. ssissippi$
3. sissippi$
4. issippi$
5. ssippi$
6. sippi$
7. ippi$
8. ppi$
9. pi$
10. i$
11. $

Suffix Tree Features

- How many leaves in a sequence of length m? O(m)
- How many nodes? (assume an alphabet of k characters) O(m)
- Given a suffix tree for a sequence. How long to determine if a pattern of length n occurs in the sequence? O(n)



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4. issippi$
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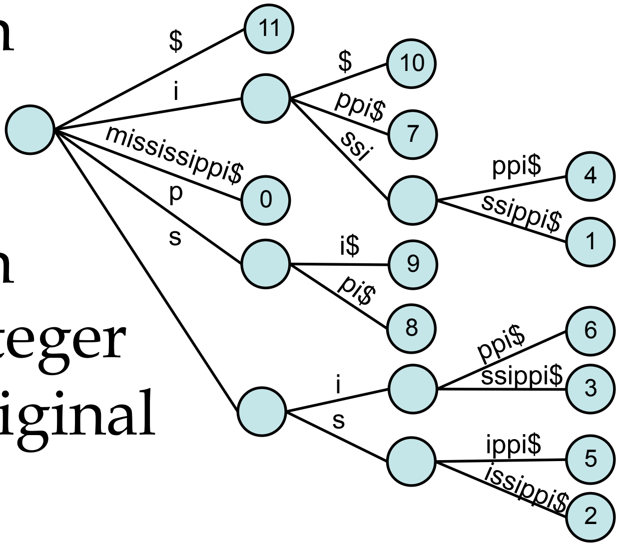
6. sippi$
7. ippi$
8. ppi$
9. pi$
10. i$
11. $

Suffix Tree Features

- How much storage?
  - Just for the edge strings $O(n^2)$
  - Trick: Rather than storing an actual string at each edge, we can instead store 2 integer offsets into the original text



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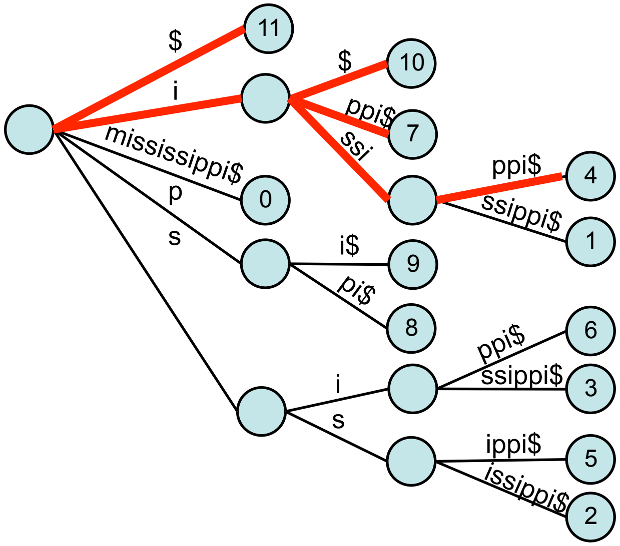
8. ppi$
9. pi$
10. i$
11. $

- In practice the storage overhead of Suffix Trees is too high, O(n) vertices with data and O(n) edges with associated data

Suffix Tree Properties

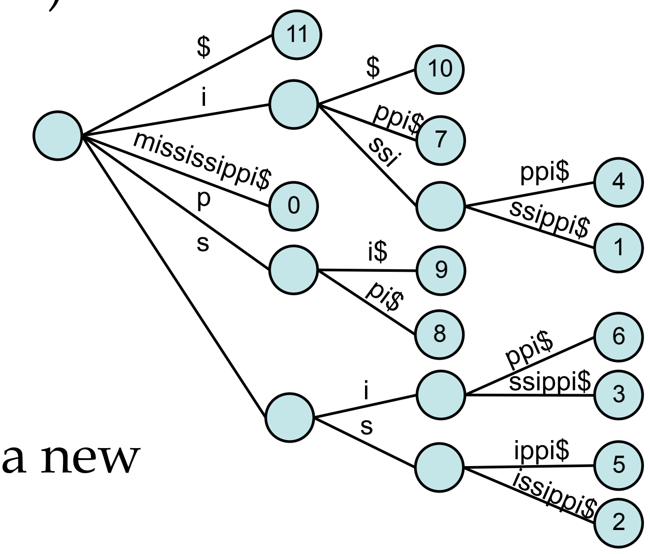
- There exists a depth-first traversal that corresponds to lexigraphical ordering (alphabetizing) all suffixes

11. $
10. i$
7. ippi$
4. issippi$
1. ississippi$
0. mississippi$
9. pi$
8. ppi$
6. sippi$
3. sissippi$
5. ssippi$
2. ssissippi$



Suffix Tree Construction

- One could exploit this property to construct a Suffix Tree
  - Make a list of all suffixes: O(m)
  - Sort them: O(m log m)
  - Traverse the list from beginning to end while threading each suffix into the tree created so far, when the suffix deviates from a known path in the tree, add a new node with a path to a leaf.



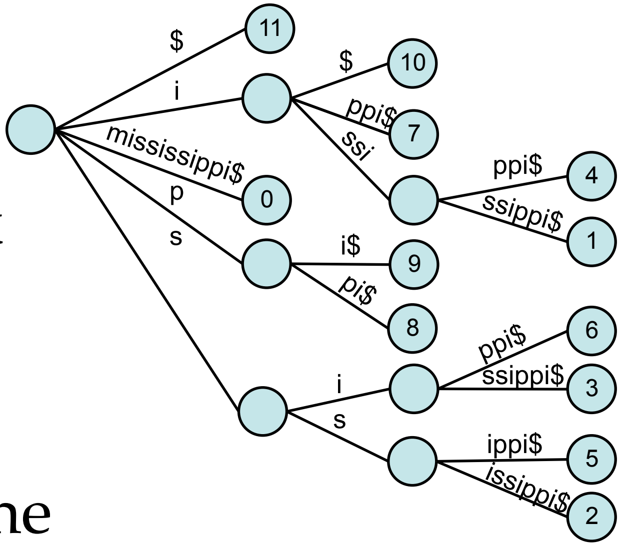
11. $
10. i$
7. ippi$
4. issippi$
1. ississippi$
0. mississippi$
9. pi$
8. ppi$
6. sippi$
3. sissippi$
5. ssippi$
2. ssissippi$

- ☹ Slower than the O(m) Ukkonen algorithm given last time

Saving space

- Sorting however did capture important aspects of the suffix trees structure
- A sorted list of tree-path traversals, our sorted list, can be considered a “compressed” version of a suffix tree.
- Save only the index to the beginning of each suffix

  11, 10, 7, 4, 1, 0, 9, 8, 6, 3, 5, 2



- Key: Argsort(text): returns the indices of the sorted elements of a text

Argsort

- One of the smallest Python functions yet:

```
def argsort(text):
    return sorted(range(len(text)), cmp=lambda i,j: -1 if text[i:] < text[j:] else 1)

print argsort("mississippi$")
```

```
$ python suffixarray.py
[11, 10, 7, 4, 1, 0, 9, 8, 6, 3, 5, 2]
```

- What types of queries can be made from this "compressed" form of a suffix tree
- We call this a "Suffix Array"

Suffix Array Queries

- Has similar capabilities to a Suffix Tree
- Does 'sip' occur in "mississippi"?
- How many times does 'is' occur?
- How many 'i''s?
- What is the longest repeated subsequence?
- Given a *suffix array* for a sequence. How long to determine if a pattern of length *n* occurs in the sequence? O(*n* log*m*)

11. $
10. i$
7. ippi$
4. issippi$
1. ississippi$
0. mississippi$
9. pi$
8. ppi$
6. sippi$
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5. ssippi$
2. ssissippi$

Searching Suffix Arrays

- Separate functions for finding the first and last occurrence of a pattern via binary search

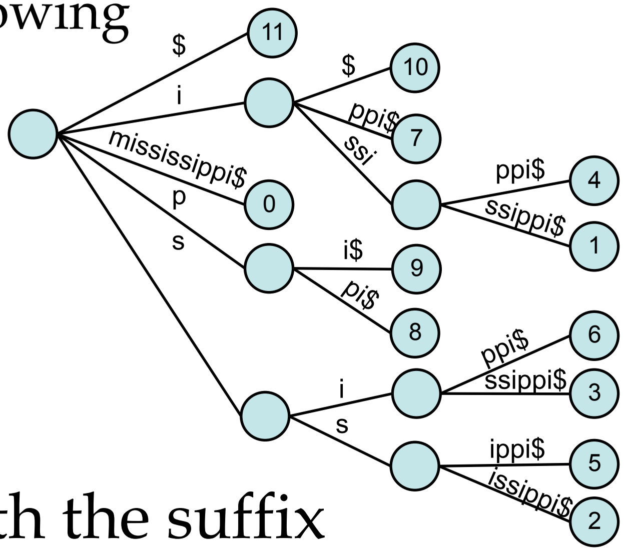
```
def findFirst(pattern, text, sfa):
    """ Finds the index of the first occurrence of pattern in the suffix array """
    hi = len(text)
    lo = 0
    while (lo < hi):
        mid = (lo+hi)//2
        if (pattern > text[sfa[mid]:]):
            lo = mid + 1
        else:
            hi = mid
    return lo

def findLast(pattern, text, sfa):
    """ Finds the index of the last occurrence of pattern in the suffix array """
    hi = len(text)
    lo = 0
    m = len(pattern)
    while (lo < hi):
        mid = (lo+hi)//2
        i = sfa[mid]
        if (pattern >= text[i:i+m]):
            lo = mid + 1
        else:
            hi = mid
    return lo-1
```

Augmenting Suffix Arrays

- It is possible to augment a suffix array to facilitate converting it into a suffix tree
- Longest Common Prefix, (lcp)
  – Note than branches, and, hence, interior nodes if needed are introduced immediately following a shared prefix of two adjacent suffix array entries

$	lcp = 0
i$	lcp = 1
ippi$	lcp = 1
issipi$	lcp = 4
ississippi$	lcp = 0
mississippi$	lcp = 0



11. $
10. i$
7. ippi$
4. issippi$
1. ississippi$
0. mississippi$
9. pi$
8. ppi$
6. sippi$
3. sissippi$
5. ssippi$
2. ssissippi$

- If we store the lcp along with the suffix array it becomes a trivial matter to reconstruct and traverse the corresponding Suffix Array

Other Data Structures

- There is another trick for finding patterns in a text string, it comes from a rather odd remapping of the original text called a "Burrows-Wheeler Transform" or BWT.
- BWTs have a long history. They were invented back in the 1980s as a technique for improving lossless compression. BWTs have recently been rediscovered and used for DNA sequence alignments. Most notably by the Bowtie and BWA programs for sequence alignments.

String Rotation

- Before describing the BWT, we need to define the notion of Rotating a string. The idea is simple, a rotation of *i* moves the prefix_i, to the string's end making it a suffix.

Rotate("tarheel$", 3) → "heel$tar"

Rotate("tarheel$", 7) → "$tarheel"

Rotate("tarheel$", 1) → "arheel$t"

BWT Algorithm

```
BWT (string text)
    $table_i$ = Rotate(text, i) for i = 0..len(text)-1
    sort table alphabetically
    return (last column of the table)
```

```
tarheel$      $tarheel
arheel$t      arheel$t
rheel$ta      eel$tarh
heel$tar      el$tarhe
eel$tarh      heel$tar
el$tarhe      l$tarhee
l$tarhee      rheel$ta
$tarheel      tarheel$
```

BTW(“tarheels$”) = “ltherea$”

BWT in Python

- Once again, this is one of the simpler algorithms that we've seen

```
def BWT(s):
    # create a table, with rows of all possible rotations of s
    rotation = [s[i:] + s[:i] for i in xrange(len(s))]
    # sort rows alphabetically
    rotation.sort()
    # return (last column of the table)
    return "".join([r[-1] for r in rotation])
```

- Input string of length *m*, output a messed up string of length *m*

Inverse of BWT

- A property of a transform is that there is no information loss and they are invertible.

```
inverseBWT(string s)
    add s as the first column of a table strings
    repeat length(s)-1 times:
        sort rows of the table alphabetically
        add s as the first column of the table
    return (row that ends with the 'EOF' character)
```

l	l$	l$t	l$ta	l$tar	l$tarh	l$tarhe	l$tarhee
t	ta	tar	tarh	tarhe	tarhee	tarheel	tarheel$
h	he	hee	heel	heel$	heel$t	heel$ta	heel$tar
e	ee	eel	eel$	eel$t	eel$ta	eel$tar	eel$tarh
r	rh	rhe	rhee	rheel	rheel$	rheel$t	rheel$ta
e	el	el$	el$t	el$ta	el$tar	el$tarh	el$tarhe
a	ar	arh	arhe	arhee	arheel	arheel$	arheel$t
$	$t	$ta	$tar	$tarh	$tarhe	$tarhee	$tarheel

Inverse BTW in Python

- A slightly more complicated routine

```
def inverseBWT(s):
    # initialize table from s
    table = [c for c in s]
    # repeat length(s) - 1 times
    for j in xrange(len(s)-1):
        # sort rows of the table alphabetically
        table.sort()
        # insert s as the first column
        table = [s[i]+table[i] for i in xrange(len(s))]
    # return (row that ends with the 'EOS' character)
    return table[[r[-1] for r in table].index('$')]
```

How to use a BWT?

- A BWT is a "*last-first*" mapping meaning the ith occurrence of a character in the first column corresponds to the ith occurrence in the last.
- Also, recall the first column is sorted
- BWT("mississippi$") → "ipssm$pissii"
- Compute from BWT(s) a sorted dictionary of the number of occurrences of each letter

  N = { '$':1, 'i':4, 'm':1, 'p':2, 's':4 }
- Using N it is a simple matter to find indices of the first occurrence of a character on the "left" sorted side

  I = { '$':0, 'i':1, 'm':5, 'p':6, 's':8 }
- We also use N to compute the "right-hand" offsets or C-index

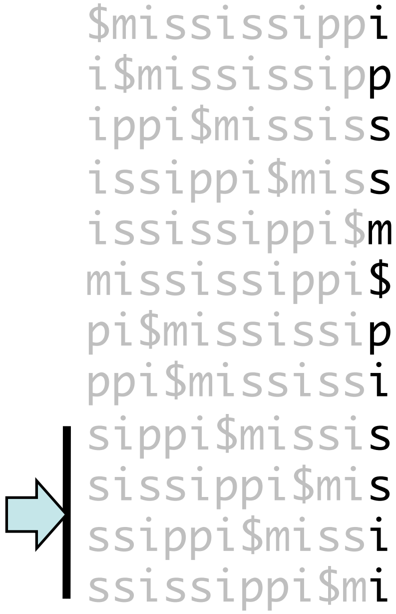
C-index

```
0 $mississippi 0
0 i$mississipp 0
1 ippi$mississ 0
2 issippi$miss 1
3 ississippi$m 0
0 mississippi$ 0
0 pi$mississip 1
1 ppi$mississi 1
0 sippi$missis 2
1 sissippi$mis 3
2 ssippi$missi 2
3 ssissippi$mi 3
```

Searching for a Pattern

- Find “iss” in “mississippi”
- Search for patterns take place in reverse order (last character to first)
- Use the I index to find the range of entries starting with the last character

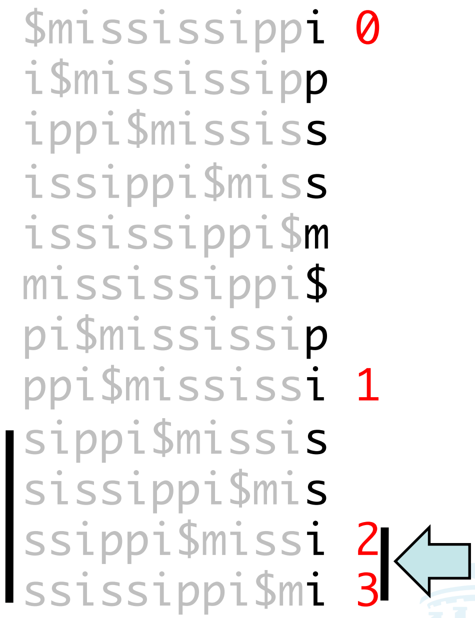
I = { ‘$’:0, ‘i’:1, ‘m’:5, ‘p’:6, ‘s’:8 }



```
$mississippi
i$mississipp
ippi$mississ
issippi$miss
ississippi$m
mississippi$
pi$mississip
ppi$mississi
sippi$missis
sissippi$mis
ssippi$missi
ssissippi$mi
```

Searching for a Pattern

- Find “sis” in “mississippi”
- Of these, how many BTW entries match the second-to-last character? If none string does not appear
- Use the C-index to find all offsets of occurrences of these second to last characters, which will be contiguous



```
$mississippi 0
i$mississipp
ippi$mississ
issippi$miss
ississippi$m
mississippi$
pi$mississip
ppi$mississi 1
sippi$missis
sissippi$mis
ssippi$missi 2
ssissippi$mi 3
```

Searching for a Pattern

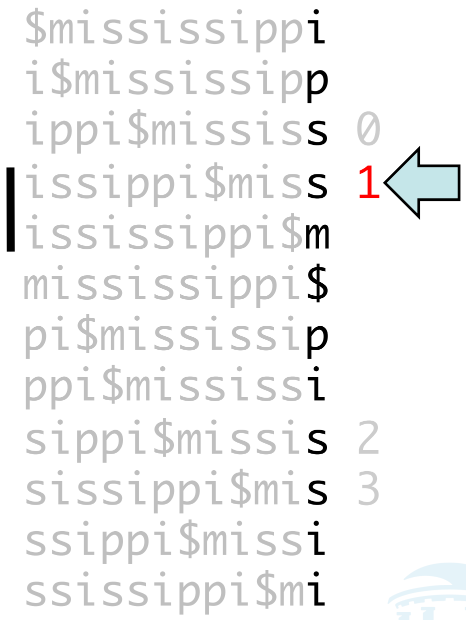
- Find “sis” in “mississippi”
- Combine offsets with I index entry to narrow search range
- Add the C-index offsets to the I-index of the second-to-last character to find new search range

I = { ‘$’:0, ‘i’:1, ‘m’:5, ‘p’:6, ‘s’:8 }

```
   $mississippi
0  i$mississipp
1  ippi$mississ
2  issippi$miss
3  ississippi$m
   mississippi$
   pi$mississip
   ppi$mississi
   sippi$missis
   sissippi$mis
   ssippi$missi
   ssissippi$mi
```

Searching for a Pattern

- Find "sis" in "mississippi"
- Find BTW entries that match the previous next-to-next-to-last character, 's'
- Use the C index to find the offsets of these second to last characters
- Now we know that the string appears in the text, but not where



```
$mississippi
i$mississipp
ippi$mississ 0
issippi$miss 1
ississippi$m
mississippi$
pi$mississip
ppi$mississi
sippi$missis 2
sissippi$mis 3
ssippi$missi
ssissippi$mi
```

Searching for a Pattern

- Find “sis” in “mississippi”
- We can find the pattern’s offset on the left side by combining the C index with the I index value for the first character
- Now, if we had a Suffix array we could use it to find the offset into the original text

```
  $mississippi
  i$mississipp
  ippi$mississ
  issippi$miss
  ississippi$m
  mississippi$
  pi$mississip
  ppi$mississi
0 sippi$missis
1 sissippi$mis
2 ssippi$missi
3 ssissippi$mi
```

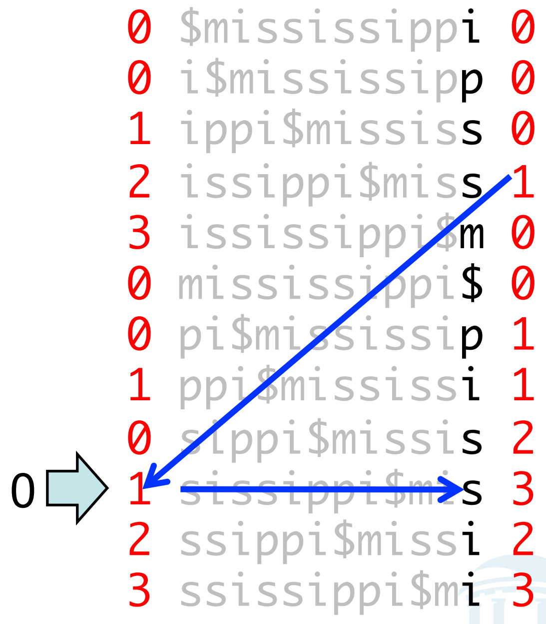
I = { ‘$’:0, ‘i’:1, ‘m’:5, ‘p’:6, ‘s’:8 }

8+1=9

sfa = [11, 10, 7, 4, 1, 0, 9, 8, 6, 3, 5, 2]

Searching for a Pattern

- Find "sis" in "mississippi"
- Actually, *there is an implicit suffix array* in our BWT
- We can use the last first-last property and the C index to thread back through the array to find the start position



Searching for a Pattern

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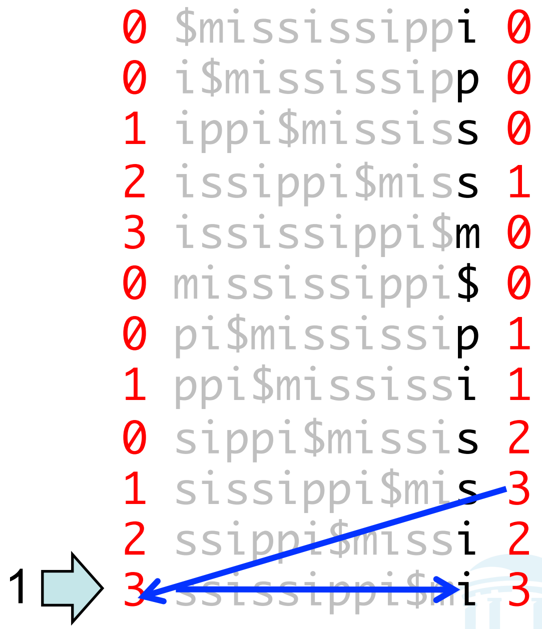

```
0 $mississippi 0
0 i$mississipp 0
1 ippi$mississ 0
2 issippi$miss 1
3 ississippi$m 0
0 mississippi$ 0
0 pi$mississip 1
1 ppi$mississi 1
0 sippi$missis 2
1 sissippi$mis 3
2 ssippi$missi 2
3 ssissippi$mi 3
```

Searching for a Pattern

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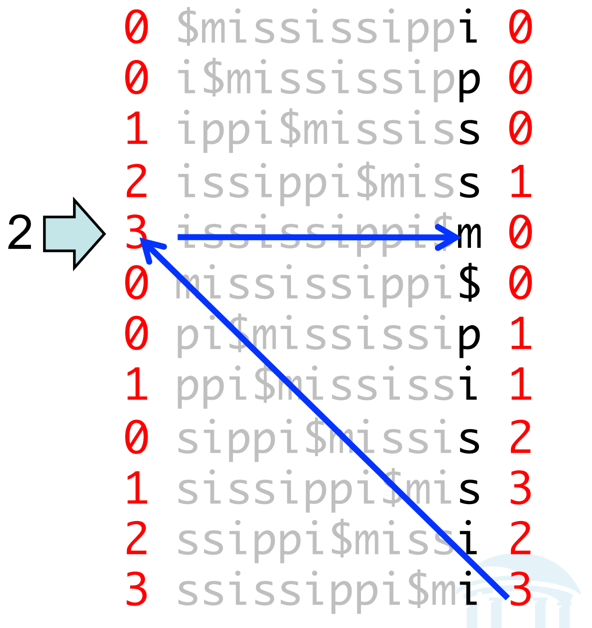
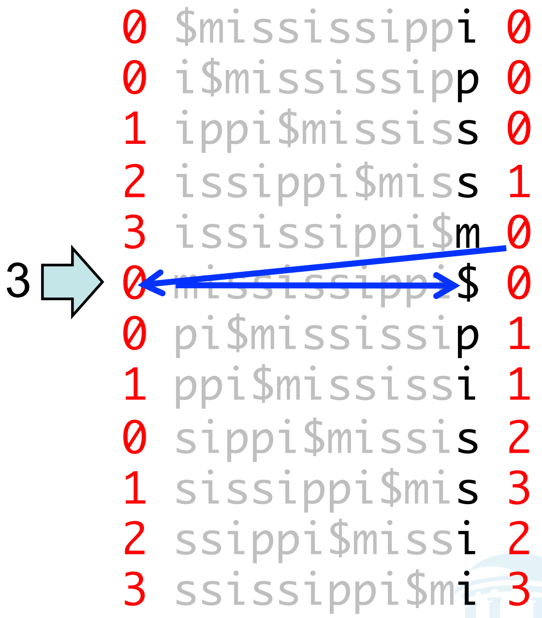


```
   0 $mississippi 0
   0 i$mississipp 0
   1 ippi$mississ 0
   2 issippi$miss 1
2  3 ississippi$m 0
   0 mississippi$ 0
   0 pi$mississip 1
   1 ppi$mississi 1
   0 sippi$missis 2
   1 sissippi$mis 3
   2 ssippi$missi 2
   3 ssissippi$mi 3
```

Searching for a Pattern

- Find "sis" in "mississippi"
- Actually, there is an implicit suffix array in our BWT
- We can use the last first-last property and the C index to thread back through the array to find the start position

- We're done. The text offset is 3.



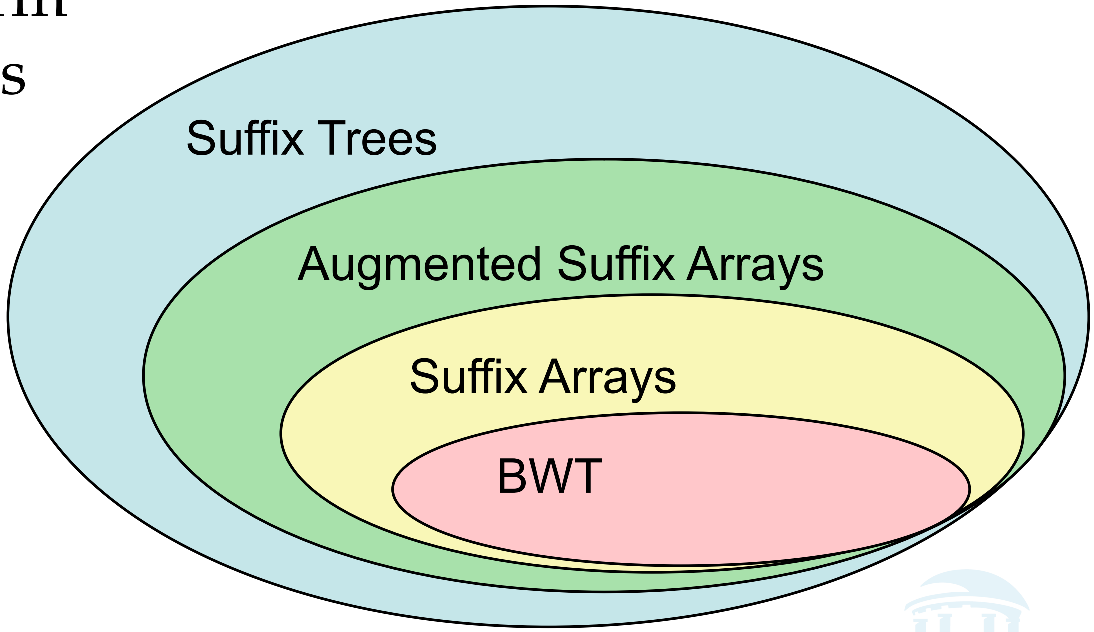
```
  0 $mississippi 0
  0 i$mississipp 0
  1 ippi$mississ 0
  2 issippi$miss 1
  3 ississippi$m 0
3 0 mississippi$ 0
  0 pi$mississip 1
  1 ppi$mississi 1
  0 sippi$missis 2
  1 sissippi$mis 3
  2 ssippi$missi 2
  3 ssissippi$mi 3
```

BWT Search Details

- The C-index can be easily compressed
  - Indices tend to appear in runs (a string of 0s, followed by a string of 1s, etc.)
  - Rather than store each index individually, store a 2-tuple, (index, # of times it is repeated)
- Speeding up the backtracking
  - Store a separate seeded array of BWT string positions of known text-string offsets
  - Obvious choices: C-index run boundaries and a few extra select positions
    - Starts of chromosomes
    - Uniformly every m/k positions

Summary

- Query Power (Big is good)
  - BWTs support the fewest query types of these data structs
  - Suffix Trees perform a variety of queries in O(m)



Summary

- Memory Footprint (Small is good)
  - BWTs compress very well on real data
  - Difficult to store the full suffix tree for an entire genome