Building Suffix Arrays
Recap from Last Time
Suffix Trees

- A **suffix tree** for a string $T$ is an Patricia trie of $T\$ where each leaf is labeled with the index where the corresponding suffix starts in $T\$. 

- (A Patricia trie is one where each node with one child and one parent is compacted into its parent.)
Suffix Arrays

- A **suffix array** for a string $T$ is an array of the suffixes of $T\$, stored in sorted order.

- By convention, $\$ precedes all other characters.
Representing Suffix Arrays

- Suffix arrays are typically represented implicitly by just storing the indices of the suffixes in sorted order rather than the suffixes themselves.
- Space required: $\Theta(m)$.
- More precisely, space for $T\$$, plus one extra word for each character.

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New Stuff!
Some History

- Historically, suffix trees were the main object of study in stringology (yes, that’s a word), with considerable effort focused on fast construction algorithms.

- Recently, suffix arrays have taken over from suffix trees, primarily because they use considerably less memory.

- **Fun fact:** Given either a suffix tree or a suffix array, it’s possible to construct the other in time $O(m)$. 
From Suffix Trees to Suffix Arrays
Algorithm: Run a DFS of the suffix tree, visiting children in sorted order, and output suffixes in the order you find them.
From Suffix Arrays to Suffix Trees
A Linear-Time Algorithm

- Construct the LCP array for the suffix array.
- Construct a Cartesian tree from that LCP array.
- Run a DFS over the Cartesian tree, adding in the suffixes in the order they appear whenever a node has a missing child.
- Fuse together any parent and child nodes with the same number in them.
- Assign labels to the edges based on the LCP values.
- Total time: $O(m)$.

*Question to ponder:* Why does this work?
Constructing Suffix Arrays
Building Suffix Arrays

• Once we have a suffix array for a string $T$, we can answer all sorts of questions about $T$ (or build a suffix tree for $T$ if we need it!)
• However, we need to be mindful of the preprocessing time – if it’s too great, then this data structure is a lot less useful.
• **Question:** How fast can we construct suffix arrays?
A Naïve Algorithm

- Here's a simple algorithm for building a suffix array for a string $T$:
  - Form an array of length $m+1$ consisting of the indices of all the suffixes in the string $T$.
  - Sort those indices using mergesort or heapsort, comparing indices by comparing the suffixes at those positions.
    - Makes $O(m \log m)$ comparisons, but each comparison takes $O(m)$ time.
  - Total time: $O(m^2 \log m)$.
  - *Can we do better?*
SA-IS

- In 2002, Ko and Aluru published an $O(m)$-time suffix array construction algorithm based on \textit{induced sorting}.

- In 2008, Nong, Zhang, and Chan found an improvement to Ko and Aluru’s algorithm, keeping the asymptotic runtime but improving the practical performance.

- That latter algorithm is called \textit{SA-IS} ("Suffix Array – Induced Sorting") and is the focus for the rest of today.
Some Observations about Suffix Arrays
Observation: We can partition the suffix array into **buckets**, where each bucket consists of all suffixes starting with the same first character.
We’ll call the suffix at position 4 an **S-type** suffix (\(S\) for *smaller*), since it lexicographically precedes the suffix at the position immediately after it.
We’ll call the suffix at position 18 an *L-type* suffix (*L* for *larger*), since it lexicographically comes after the suffix at the position immediately after it.
<table>
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<tr>
<th>$</th>
<th>A</th>
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<td>0</td>
<td>14</td>
<td>9</td>
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Table: |
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<td>C C G A T G T C A T G T C A G G A $</td>
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<td>C G A T G T C A T G T C A G G A $</td>
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Diagram: |
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<tbody>
<tr>
<td>S S</td>
</tr>
<tr>
<td>G T C C C C G A T G T C A T G T C A G G A $</td>
</tr>
</tbody>
</table>
By definition, the suffix starting at the sentinel is considered an S-type suffix.
**Theorem:** A suffix starting at position $k$ is an $S$-type suffix if

- $\text{Text}[k] < \text{Text}[k+1]$, or
- $\text{Text}[k] = \text{Text}[k+1]$ and the suffix at index $k+1$ is $S$-type, or
- $\text{Text}[k] = \$.  

A suffix starting at position $k$ is a $L$-type suffix if

- $\text{Text}[k] > \text{Text}[k+1]$, or
- $\text{Text}[k] = \text{Text}[k+1]$ and the suffix at position $k+1$ is $L$-type.

We can tag each suffix as $S$-type or $L$-type in time $O(m)$ by scanning $\text{Text}$ from right-to-left and applying the above rules.
Since the suffix of just $ is defined to be $S$-type, everything in this bucket is $S$-type.

$T$ is the lexicographically last character, so all suffixes starting with it are $L$-type.

Well *that’s* unexpected. What’s going on here?
**Theorem:** Let $i$ and $j$ be indices of two suffixes that start with the same character. Then if $i$ is $L$-type and $j$ is $S$-type, the suffix beginning at position $i$ lexicographically precedes the suffix beginning at position $j$. 
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\[ \text{...} \]
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Where We Stand

- We can efficiently classify each suffix as either $S$-type or $L$-type in time $O(m)$.
- We know a good amount about the relative positioning of the suffixes:
  - All suffixes are bucketed by their first character.
  - All $L$-type suffixes come before all $S$-type suffixes.
- If we can get everything relatively positioned within its group, we’re done!
SA-IS at a Glance

- There are three core insights that collectively give us the SA-IS algorithm.

  - First:
    
    *There is a proper subset of the suffixes that, if sorted, can be used to recover the order of all the remaining suffixes.*

  - Second:
    
    *Those suffixes can be broken apart into blocks of characters such that the order of the suffixes depends purely on the order of the blocks.*

  - Third:
    
    *With the proper preprocessing, those suffixes can be sorted via a recursive call on a smaller input string.*
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- **Third:**
  
  *With the proper preprocessing, those suffixes can be sorted via a recursive call on a smaller input string.*
These suffixes are called **LMS suffixes** (*Left Most S*-type).

A suffix is an LMS suffix if it’s *S*-type and the suffix before it is *L*-type.

This suffix isn’t an LMS suffix because it isn’t preceded by a suffix at all!

This suffix isn’t LMS because the suffix before it isn’t *L*-type.

The sentinel by itself is always considered an LMS suffix.

This suffix isn’t LMS because the suffix before it isn’t *L*-type.
**Key Theorem:** If we can get the LMS suffixes – and just the LMS suffixes – in sorted order, then we can, in time $O(m)$, get all the other suffixes in order as well.

The algorithm for doing this is called **induced sorting**. This is the “IS” in SA-IS.
All LMS suffixes and all L-type suffixes are here. We're missing some S-type suffixes; we'll fix that later.

This is a multiway merge! Each list is sorted, and we want to unify them all together.
These other suffixes starting with A are S-type, but suffix 19 is L-type. Therefore, suffix 19 wins on tiebreaks.
| S | L | S | S | S | S | S | L | S | S | S | S | S | L | L | L | L | L | L | L | S |
| G | T | C | C | C | G | A | T | G | T | C | A | T | G | T | C | A | G | G | A | $ |
This needs to go with the other G suffixes. Suffix 18 is L-type and the others are S-type, so suffix 18 wins on tiebreaks.
14 > 15 > 16 s A G G A S
9 > 10 > 11 s A T G T C A G G G ...
5 > 6 s A T G T C A T G ...
1 > 2 s C C C G A T G T ...
17 > 18 L G A S
12 > 13 s G T C A G G A S
7 > 8 s G T C A T G T C ...

20 19

S L S S S L S S L S L S L S L L S L S
G T C C C C G A T G T C A T G T C A G G A S
| 14 > 15 > 16 | S | AGGGA $ |
| 9 > 10 > 11 | S | ATGTCAAGG ... |
| 5 > 6 > 11 | S | ATGTCAATG ... |
| 1 > 2 > 11 | S | CCCCCGATGTG ... |
| 17 > 18 | L | GA $ |
| 12 > 13 | S | GTCAGGGAGA $ |
| 7 > 8 | S | GTCATGTC ... |

20 19
Suffix 15 needs to go with the other C suffixes. Again, it’s L-type and the others are S-type, so suffix 15 wins on tiebreaks.
We need to move this to the C suffixes.

We know it precedes this S-type suffix.

How does it compare to this L-type suffix?
The suffix at index 15 is $C$, followed by the suffix at index 16.

The suffix at index 10 is $C$, followed by the suffix at index 11.

Conclusion: This suffix goes after the $L$-type suffixes starting with $C$ and before $S$-type suffixes starting with $C$. 

S L S S S L S L S L S L S L S S L L L L S S
G T C C C G A T G T C A T G T C A G G A $\$
We know it precedes these S-type suffixes.

How does it compare to this L-type suffix?
Suffix 5 is G followed by suffix 6. Suffix 18 is G followed by suffix 19.
Some Observations

• All the new suffixes we uncover are $L$-type.

• Whenever we uncover a new suffix:
  • that suffix comes *before* all $S$-type suffixes in the list with the same first character, and
  • that suffix comes *after* all $L$-type suffixes in the list with the same first character.

• Notice that *we never make any string comparisons* in the course of carrying out this multiway merge!

• If we can maintain these buckets efficiently, we could complete this merge in time $O(m)$. 
Okay, this next part is pretty cool. Props to Ko and Aluru for figuring it out.
We can compute the bucket boundaries in time $O(m)$ by just counting up how frequently each character appears in the string. If we store those boundaries in an array indexed by character, we can put each element in the right place in time $O(1)$.

Total time so far: $O(m)$. 

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
Watch how we implement the multiway merge.
for (each index i in SA) {
    if (SA[i] isn't empty and SA[i] > 0 and text[SA[i] - 1] is L-type) {
        put SA[i] - 1 at the next free slot at the front of text[SA[i] - 1];
    }
}
**Theorem:** If you have all the $L$-type suffixes in sorted order, you can use that to induce the order of the $S$-type suffixes by making a reverse pass over the array and following a similar algorithm.

Important detail: The ends of each bucket currently have some, but not all, of the $S$-type suffixes in them. These items may be out of place because we don't know how they relate to other $S$-type suffixes. Therefore, when doing this backwards pass, we'll allow ourselves to overwrite the old $S$-type suffixes as we go. Anything that wasn't overwritten was already in the right place.
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reset the indices of each bucket's next free slot at the end.
for (each index i in SA, in reverse order) {
    if (SA[i] isn't empty and SA[i] > 0 and
text[SA[i] - 1] is S-type) {
        put SA[i] - 1 at the next free slot
        at the end of text[SA[i] - 1];
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    }
}

S L S S S L S L S L L S L L S L L S L L S
G T C C C C G A T G T C A T G T C A T G G A $
To Recap

• Suppose that – somehow – we can sort the LMS suffixes.

• We can then make three linear scans to sort all the suffixes:
  
  • one **reverse** pass over the sorted LMS suffixes, placing them at the ends of their buckets;
  
  • one **forward** pass over the suffix array, placing L-type suffixes at the fronts of their buckets; and
  
  • one **reverse** pass over the suffix array, placing S-type suffix at the ends of their buckets (making sure to reset the end positions of each bucket first.)

• This runs in time $O(m)$ and has *excellent* locality of reference. It’s incredibly fast in practice.
Time-Out for Announcements!
Problem Sets

• Problem Set One was due today at 2:30PM.
  • Need some more time? You have two, 24-hour late days you can use throughout the quarter.
• Problem Set Two goes out today. It’s due next Tuesday at 2:30PM.
  • Play around with tries, suffix trees, suffix arrays, and their algorithms!
Back to CS166!
SA-IS at a Glance

• There are three core insights that collectively give us the SA-IS algorithm.

• First:

  There is a proper subset of the suffixes that, if sorted, can be used to recover the order of all the remaining suffixes.

• Second:

  Those suffixes can be broken apart into blocks of characters such that the order of the suffixes depends purely on the order of the blocks.

• Third:

  With the proper preprocessing, those suffixes can be sorted via a recursive call on a smaller input string.
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Third:

*With the proper preprocessing, those suffixes can be sorted via a recursive call on a smaller input string.*
Observation: The comparisons between these strings seem to be boiling down to comparisons between their blocks.

Why is that?
An **LMS block** is a substring of $T$ that either spans from one LMS suffix to the next or is the sentinel itself, where each character is annotated with its L/S type.

Each LMS suffix is made of one or more (overlapping) LMS blocks.
**Theorem:** Treat each character in an LMS block as a pair of the character itself and its L/S type. Then no LMS block is a prefix of another LMS block.

**Corollary:** If two different LMS blocks are compared factoring in L/S types, a mismatch will be found somewhere inside the blocks.

**Claim 1:** Every suffix starting at an LMS character is a local minimum among the suffixes near it in the original string.

**Claim 2:** With the exception of the sentinel, the types of the characters in an LMS block match the regex $S^*L^*S$. 
Theorem: Treat each character in an LMS block as a pair of the character itself and its L/S type. Then no LMS block is a prefix of another LMS block.

Corollary: If two different LMS blocks are compared factoring in L/S types, a mismatch will be found somewhere inside the blocks.

Claim 2: With the exception of the sentinel, the types of the characters in an LMS block match the regex S*L*S.

Proof: A comparison of two different LMS blocks will result in a mismatch no later than the first occurrence of LS.
If we knew the relative order of the LMS blocks, we could compare these suffixes very quickly by just comparing them one block at a time.

**Question:** How can we get those blocks into sorted order?
This next bit is totally brilliant. A huge shoutout to Nong, Zhang, and Chan for figuring this one out.
These strings are *not* in the right order. They just appear in the relative order in which they appear in the original string.

Watch what happens if we run the rest of the induced sort here.
These suffixes are sorted, at least up to the first LMS character that appears after the first letter! (Why?)
By finding all the LMS suffixes in the order in which they appear in the above array, we get all the LMS blocks into sorted order!

So, basically, we did a mergesort with a list that wasn’t sorted and got back a list that is. Kinda.
To Recap

- The relative order of the LMS suffixes depends purely on the relative order of the LMS blocks.
- The order of the LMS blocks can be found by running the induced sorting algorithm on a list of all the LMS suffixes in any order we’d like!
- We’re almost done!
SA-IS at a Glance

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• Third:

*With the proper preprocessing, those suffixes can be sorted via a recursive call on a smaller input string.*
The relative order of the LMS suffixes depends purely on the relative order of the LMS blocks.
We can compute these numbers in time $O(m)$. Just compare each block to the one after it to test for equality.
We need a suffix array for this reduced string!

Now we just need to get these sequences of numbers into sorted order.
Recursion to the Rescue

- The SA-IS algorithm handles this step recursively, with a very cleverly-chosen base case.

- **Base Case:** If all blocks are unique, the suffix array can be computed manually in time $O(m)$ by writing down the indices of $0, 1, 2, ..., k$.

- **Recursive Case:** Otherwise, recursively invoke SA-IS to get the suffix array!
The Whole Algorithm, End-to-End
Step One: Scan the array from right-to-left to label each suffix as S-type or L-type.
**Step Two:** Run an induced sorting step on the LMS suffixes in the order they appear. This will get the LMS *blocks* (not the LMS *suffixes*) into sorted order.

**Pass One:** Place the LMS suffixes at the ends of their buckets.
**Pass Two:** Place the $L$-type suffixes at the fronts of their buckets.

**Step Two:** Run an induced sorting step on the LMS suffixes in the order they appear. This will get the LMS blocks (not the LMS suffixes) into sorted order.
**Step Two**: Run an induced sorting step on the LMS suffixes in the order they appear. This will get the LMS blocks (not the LMS suffixes) into sorted order.

**Pass Three**: Place the S-type suffixes at the ends of their buckets.
Step Three: Number the LMS blocks and form the reduced string.
Step Four: Use the suffix array of the reduced string to sort the LMS suffixes.

**recursion!**
Step Four: Use the suffix array of the reduced string to sort the LMS suffixes.
### Step Four:

Use the suffix array of the reduced string to sort the LMS suffixes.
Step Five: Run an induced sorting step on the sorted LMS suffixes to produce the overall suffix array.

Pass One: Place the sorted LMS suffixes at the ends of their buckets.
Step Five: Run an induced sorting step on the sorted LMS suffixes to produce the overall suffix array.

Pass Two: Place the $L$-type suffixes at the fronts of their blocks.
Step Five: Run an induced sorting step on the sorted LMS suffixes to produce the overall suffix array.

Pass Three: Place the S-type suffixes at the ends of their blocks.
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Pass Three: Place the S-type suffixes at the ends of their blocks.
| $ | A | A | A | A | A | A | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| $ | G | G | G | G | G | G | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| $ | G | G | G | G | G | G | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| $ | C | C | A | G | A | T | G | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| $ | A | A | $ | T | T | T | G | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| $ | G | T | C | C | C | C | A | T | G | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| $ | T | G | T | C | C | C | A | T | G | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| $ | G | T | C | C | C | C | A | T | G | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |

**Note:** The table represents a DNA sequence with the columns labeled 'G', 'T', 'C', 'A', and 'T'. The rows are numbered from 0 to 20.
SA-IS, End-to-End

SA-IS(T):
Scan T from right-to-left to mark each character as S-type or L-type.
Identify all the LMS suffixes of T.

Run induced sorting using the LMS suffixes in the order they appear in in T.

Scan the result, gathering LMS suffixes in the order they ended up in.
Number the LMS blocks, assigning duplicate blocks the same number.
Form the reduced string $T'$ from the block numbers.

If all blocks are unique, get a suffix array for $T'$ by directly inverting $T'$.
Otherwise, get a suffix array for $T'$ by calling SA-IS($T'$).

Use the suffix array for $T'$ to sort the LMS suffixes of T.
Do a second induced sorting pass of T using the LMS suffixes in sorted order.
The Overall Runtime

- The SA-IS algorithm does $O(m)$ work, then (optionally) makes a recursive call on the reduced string.
- The size of the reduced string is equal to the number of LMS characters.
- **Claim:** There are at most $m/2$ LMS characters.
  - Each LMS character appears when an $L$-type suffix is followed by an $S$-type suffix, and in the worst case the suffix types alternate between $L$-type and $S$-type.
- Recurrence relation is
  \[
  T(m) \leq T(m/2) + O(m),
  \]
  which solves to $O(m)$ total work.
Wow! What a nifty algorithm!
In Practice

- SA-IS is extremely fast in both theory and in practice.
  - Excellent locality of reference in the induced sorting and block numbering steps.
  - Recursive step usually has a great compression ratio.
- With a creative implementation, the memory overhead is minimal.
  - One implementation gets away with $4m$ machine words in total!
- The current fastest suffix array construction algorithm, DivSufSort, is essentially a highly optimized version of SA-IS using a slightly different approach to sorting LMS suffixes.
Why Study SA-IS?

- **Explore the theoretical structure of suffix arrays.**
  - The relative ordering of L-type and S-type suffixes, the idea of induced sorting, and the bit about LMS blocks are all really beautiful theoretical results.

- **See the idea of simulating one algorithm with another.**
  - Induced sorting is basically a multiway merge sort implemented really well, yet there’s little evidence of this in the final code!

- **Look at a really, really clever divide-and-conquer algorithm.**
  - Did you expect to see the suffix array reduced that way?

- **Probe the interface between theory and practice.**
  - This algorithm has an asymptotically optimal runtime, *and* it’s really fast in practice!
More to Explore

- **Constructing LCP using induced sorting.** (Fischer and Kurpicz, 2011)
  
  Kasai’s LCP algorithm was the first linear-time LCP algorithm. Turns out you can augment SA-IS to produce both the suffix array and the LCP array much, much faster than this.

- **Reducing SA-IS memory usage.** (Nong, 2013)
  
  A variation of SA-IS (by one of its original authors!) that cuts down on the memory usage and improves performance.

- **The Burrows-Wheeler transform.**
  
  Originally invented for data compression algorithms, now used extensively throughout computational genomics, and closely related to suffix arrays!
Next Time

- **Balanced Trees**
  - Fast, flexible data structures for sorted sequences.
- **B-Trees**
  - Built for databases, now popular in RAM!
- **2-3-4 Trees**
  - One of the simplest balanced trees around.
- **Red/Black Trees**
  - Where do they come from?