



Linear Time Suffix Array Construction

Algorithms for Sequence Analysis

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Summer 2021

Overview

Previous Lectures

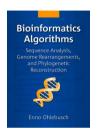
- Ukkonen's algorithm: linear time suffix tree construction
- Suffix links
- Kasai's algorithm: linear time LCP array construction

Today

■ Direct linear time suffix array construction using induced sorting



Recommended Literature



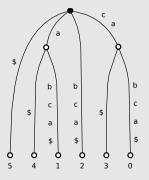
Further Reading

- Shrestha et al. A bioinformatician's guide to the forefront of suffix array construction algorithms. Brief. Bioinformatics 2014 Mar;15(2):138-54
- G. Nong, S. Zhang and W. H. Chan. Linear Suffix Array Construction by Almost Pure Induced-Sorting. Proceedings of 19th Data Compression Conference (IEEE DCC), 2009.



Suffix trees and suffix arrays

Suffix tree for the string T = cabca\$.

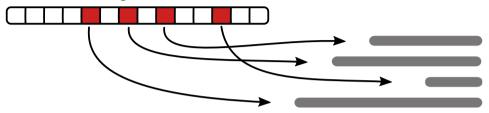


A suffix array of a string s\$ with |s\$| = n is defined as the permutation pos of $\{0,...,n-1\}$ that represents the lexicographic ordering of all suffixes of s\$. pos = [5,4,1,2,3,0].

Induced Sorting Idea

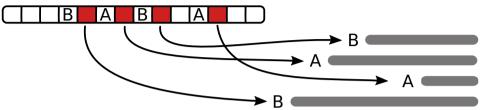


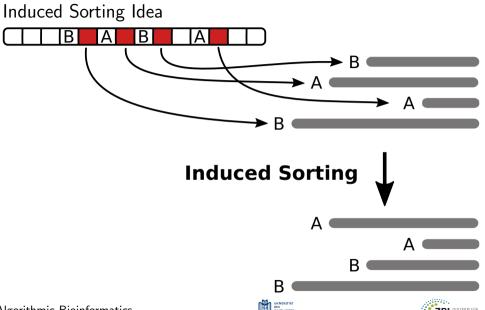
Induced Sorting Idea





Induced Sorting Idea





Definition of L-/S-positions

Definition (L-position, S-position)

Let s\$ be a string of length n with sentinel, such that s[n-1] = \$. Let $0 \le p < n-1$ be a position in the text. We say,

- p is an L-position (L means larger), if s[p...] > s[p+1...],
- p is an S-position (S means smaller), if s[p...] < s[p+1...],
- The position of the sentinel n-1 is defined as S-position.

(Note that no two suffixes can be identical.)



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- The position of the sentinel n-1 is defined as S-position.

(Note that no two suffixes can be identical.)

```
O......1.....2.

Position p 0123456789012345678901

Sequence s gccttaacattattacgccta$

type LSSLLSSLSLLSSLSSLLS
```



Computing the L-/S-positions in the type array

The type information can be computed in linear time with a scan through the text from right to left:

In a real implementation, we use a bit vector (0/1) to represent the types.



Definitions: LMS position / interval / substring

Definition (LMS-interval, LMS-substring)

- S-positions located to the right of an L-position are called LMS positions (for leftmost S position).
- A pair of positions [i, j] is called LMS interval of s, if either
 - i < j and both i and j are LMS-positions and there are no LMS-positions between i and j, or
 - i = j = n 1.
- Each LMS interval [i, j] is associated with its LMS substring s[i ... j].

Observations

- Position n-1 with the sentinel is always an LMS-position.
- Whether an S-position is an LMS-position can be determined in constant time, looking up its type and the type to the left in the typearray.



Example: type array, LMS substrings

position p 0123456789012345678901 sequence s gccttaacattattacgccta\$



Example: type array, LMS substrings

position p 0123456789012345678901 sequence s gccttaacattattacgccta\$ type LSSLLSSLSSLLSLLSSLSSLLS

Example: type array, LMS substrings

```
position p 0123456789012345678901
sequence s gccttaacattattacgccta$

type LSSLLSSLSLLSLLSSLSSLLS

LMS? * * * * * * *

LMS-substr cctta atta acgc $

aaca atta ccta$
```



Overview of Induced Sorting

Notation

- s is the input sequence,
- pos is the desired output suffix array of s.

Induced sorting

- Scan s to compute the type array
- Scan type to find all LMS positions in s
- Phase I Sort suffixes at LMS positions (complex; recursive)
- Phase II Sort all remaining suffixes of s (easy)
- Output pos



Code: Overview

```
def sais_main(T, alphabet_size):
      # T: text (bytes, numpy array, not str!), T[n-1]=0
      # alphabet_size, 1 <= T[i] < alphabet_size for all i < n-1</pre>
      pos = np.emptv(len(T), dtvpe=np.int64)
     # B[a]: total number of characters in T that are <= a
      B = count_cumulative_characters(T, alphabet_size)
      types = compute_types(T)
      lms_positions = find_lms_positions(types)
      # Phase 1 sorts lms_positions lexicographically in-place,
10
      # may recurse into sais_main() with a reduced text.
11
      phase1(T, B, types, lms_positions, pos)
12
      # Phase 2 sorts all suffixes from correctly sorted LMS.
13
      phase2(T, B, types, lms_positions, pos)
14
      return pos
15
```



Code: Initialization, buckets and types

```
def count_cumulative_characters(T, alphabet_size):
    # B[a]: total number of characters in T that are <= a
    B = np.zeros(alphabet_size, dtype=np.uint64)
    for a in T:
        B[a] += 1
    for a in range(1, alphabet_size):
        B[a] += B[a-1]
   return B
```

```
def compute_types(T):
    # Compute position types (SMALLER=0, LARGER=1) for T
   n = len(T)
   types = np.zeros(n, dtype=np.uint8) # types[n-1] = SMALLER
    for i in range (n-2, -1, -1):
        types[i] = LARGER if T[i] > T[i+1] else \
                   SMALLER if T[i] < T[i+1] else types[i+1]
    return types
```

Code: Initialization, LMS positions

```
def find_lms_positions(types):
      n = len(types)
      # count the number of LMS positions first
      m = 0
      for p in range(1, n):
          m += (types[p] == SMALLER and types[p-1] == LARGER)
      # allocate array of just the correct size m
      lms_positions = np.empty(m, dtype=np.int64)
      # now fill the array with the actual LMS positions
      m = 0
10
      for p in range(1, n):
11
          if types[p] == SMALLER and types[p-1] == LARGER:
12
              lms_positions[m] = p
13
              m += 1
14
      return lms_positions
15
```



Code: Overview again

```
def sais_main(T, alphabet_size):
      # T: text (bytes, numpy array, not str!), T[n-1]=0
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      return pos
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```



Phase II





Let's start with Phase II (Phase I uses elements of Phase II):

Definition (Bucket)

A maximal interval of the suffix array pos, in which the referenced suffixes start with the same character, is called a bucket.

There are as many buckets as characters in the used alphabet, plus the one for the sentinel character.



Lemma

Within each bucket of the suffix array, the L-positions appear before the S-positions.

Proof

Let p be an S-position, and let q be an L-position, let $s[p] = s[q] = b \in \Sigma$, so both p and q are in the b-bucket. Then the suffix p+1 is larger than suffix p, and suffix p+1 is smaller than suffix p. Because s[p] = s[q], the order of p vs. p+1 vs. p+1 vs. p+1 vs. p+1 vs. p+1 to ones before p+1 in the lexicographic order.

Illustration

Let a < b < c; suffix q is b^+a , whereas p is b^+c :



Lemma

Within each bucket of the suffix array, the L-positions appear before the S-positions.

Bucket	\$		а		С		t		
	L	S	L	S	L	S	L	S	

Idea

- Use the already sorted LMS-positions (a subset of the S-positions)
 to sort the L-positions correctly, and then
- use the sorted L-positions to sort all S-positions.

This is why the algorithm is called **induced sorting**:

The order of one type of suffixes completely induces the ordering of the others.



Preparing the Suffix Array

Step (1)

- Initialize pos with unknown at each position
- Mark the beginning and end of each bucket by pointers
- Write the sorted LMS-positions (phase I) at the end of their respective buckets.



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Sorting the L-positions (Induced Sorting)

Step (2)

- Iterate through pos from left to right with index r.
- If pos[r] is unknown, skip index r.
- Otherwise, look at pos[r] 1:
 - 1 If pos[r] 1 is an L-position, enter it at the first free position in its bucket.
 - 2 If pos[r] 1 is an S-position, skip index r.

Result

All L-positions are entered in the suffix array in correct order.



Example: Sorting the L-positions

0 1 2
position p 0123456789012345678901
sequence s gccttaacattattacgccta\$
type LSSLLSSLSSLLSSLSSLLS
LMS? * * * * * * *

rank r	0 1	2	3	4	5	6	7	8	9	10	11	12 13	14 15	16	17	18	19	20	21
bucket	\$ a	a	a	a	a	al	С	С	С	С	С	cl g	g t	t	t	t	t	t	tΙ
pos	21 .		5	14	11	81					17		. .						٠,۱
	^S vL					- 1						- 1	- 1						- 1
pos	21 20		5	14	11	81					17	1 .	. .						٠. ا
	^L					- 1						- 1	vL						- 1
pos	21 20		5	14	11	81					17	1 .	. 19						٠.
			^S			- 1						- 1	- 1	vL					- 1
pos	21 20		5	14	11	81					17	1 .	. 19	4					. 1
	1 1			^S		- 1						- 1	1		νL				- 1
pos	21 20		5	14	11	81					17	1 .	. 19	4	13				. 1
	1 1				^S	- 1						- 1	1			νL			- 1
pos	21 20		5	14	11	8	7				17	1 16	0 19	4	13	10	3	12	9

Sorting the S-positions (Induced Sorting)

Step (3)

- 1 Remove all the S-positions from pos, except \$.
- 2 Iterate through pos from right to left with index r.
- 3 If pos[r] is unknown, skip index r.
- 4 Otherwise, look at pos[r] 1:
 - If pos[r] 1 is an S-position, enter it at the rightmost free position in its bucket.
 - If pos[r] 1 is an L-position, skip index r.

Result

All S-positions are entered in the suffix array in correct order.



Example: Sorting the S-positions (Induced Sorting)

```
position p
             0123456789012345678901
             gccttaacattattacgccta$
sequence s
             LSSLLSSLSSLLSLLSSLSSLLS
type
LMS?
                                8
                                   9 10 11 12 13 14 15 16 17 18 19 20 21 1
                          alccccclg
                          8 7 . . . 17 1 1 16 0 19 4 13 10
pos(2) |21|20 .
                 5 14 11
                                            .116
                                                  0|19
pos
                    . . 817
       121120
               . . . 11 81 7
                                             . 116
                                                  0|19
                                                        4 13 10
pos
       121120
                          81 7
                                            2|16
                                                  0|19
pos
                                                        4 13 10
                          817
                                 . . . 18
                                            2|16
                                                  0|19
                                                        4 13 10
pos
pos
       121120
               . . . 11
                          8I 7
                               . . 15 18
                                            2|16
                                                  0|19
                                                        4 13 10
                          81 7
                                   1 15 18
                                            2|16
                                                  0|19
       121120
                                                        4 13 10
pos
pos
       121120
                 . . 11
                          8I 7 17
                                   1 15 18
                                            2116
                                                  0119
                                                        4 13 10
       121120
                 . 14 11
                                   1 15 18
                                            2116
                                                  0119
                                                        4 13 10
pos
       121120
                 6 14 11
                          81 7 17
                                   1 15 18
                                            2|16
                                                  0|19
                                                        4 13 10
pos
       121120
                 6 14 11
                          8| 7 17
                                   1 15 18
                                            2116
                                                  0119
                                                        4 13 10
pos
                 6 14 11
                          81 7 17
                                   1 15 18
                                            2|16
                                                  0|19
                                                        4 13 10
pos
```



Summary and Analysis of Phase II

Phase II:

- 1 Enter sorted LMS suffixes into pos, set bucket pointers
- Sort L-suffixes based on sorted LMS-suffixes (induced sorting)
- 3 Sort S-suffixes based on sorted L-suffixes (induced sorting)



Summary and Analysis of Phase II

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Running Time Analysis

- Step (1) can be done in linear time.
- Step (2) and (3) each do a linear scan through the suffix array in linear time.
- ⇒ Phase II takes linear time.



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Correctness?



Correct Sorting of L-Positions

Lemma: Correctness of Step (2)

Assuming correctly ordered LMS-positions in each bucket, then after Step (2), all L-positions can be found at their **correct** positions.



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Proof idea

If p is a text position with rank r in pos and p-1 is a L-position, then p-1 has a rank r' with r'>r by definition of an L-position.



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- If p is a text position with rank r in pos and p-1 is a L-position, then p-1 has a rank r' with r'>r by definition of an L-position.
- This assures that each L-position p-1 will
 - **1** be induced by an LMS- or L-position *p*
 - 2 be induced by a position further to the left



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- This assures that each L-position p-1 will
 - **1** be induced by an LMS- or L-position *p*
 - 2 be induced by a position further to the left
- Complete proof by induction:
 Show that the first k LMS- and L-positions all appear in the correct order.



Lemma: Correctness of Step (3)

Assuming correctly ordered L-positions in each bucket, then after step (3), all positions can be found at their correct positions.



Lemma: Correctness of Step (3)

Assuming correctly ordered L-positions in each bucket, then after step (3), all positions can be found at their correct positions.

Proof idea

Let p be a text position with rank r in pos and p-1 is a S-position, then p-1 has a rank r' with r' < r (by definition of an S-position).



Lemma: Correctness of Step (3)

Assuming correctly ordered L-positions in each bucket, then after step (3), all positions can be found at their correct positions.

Proof idea

- Let p be a text position with rank r in pos and p-1 is a S-position, then p-1 has a rank r' with r' < r (by definition of an S-position).
- This assures that each S-position p-1 will be induced by a position p further to the right.



Lemma: Correctness of Step (3)

Assuming correctly ordered L-positions in each bucket, then after step (3), all positions can be found at their correct positions.

Proof idea

- Let p be a text position with rank r in pos and p-1 is a S-position, then p-1 has a rank r' with r' < r (by definition of an S-position).
- This assures that each S-position p-1 will be induced by a position p further to the right.
- Complete proof by induction (in k):
 Show that the last k positions all appear in the correct order.



Code: Phase II

```
def phase2(T, B0, types, lms, pos):
      # T: Text, B0: cumulative bucket sizes, types: type array
     # lms: sorted or unsorted LMS positions
      # pos: suffix array (output)
     # O. Initialize pos by inserting LMS positions,
      B = B0.copy() # working copy of C, to be modified
      initialize_pos_from_lms(T, B, lms, pos)
      # 1. Do a left-to-right induction scan for L-positions,
      B[:] = B0[:] # re-set B to a clean working copy of C
10
      induce_L_positions(T, B, types, pos)
11
      # 2. Do a right-to-left induction scan for S-positions.
12
     B[:] = B0[:] # re-set B to a clean working copy of C
13
      induce_S_positions(T, B, types, pos)
14
      # Result: pos has been modified as desribed.
15
```



Code: Phase II, Initialization

```
def initialize_pos_from_lms(T, B, lms, pos):
    pos[:] = -1  # set everything to "unknown"
    # Insert LMS positions at right end of their buckets,
    # right-to-left, so we know where to start in each bucket.
    for p in lms[::-1]:
        a = T[p]  # character determines the bucket
        B[a] -= 1
        pos[B[a]] = p
```



Code: Phase II, L-positions

```
def induce_L_positions(T, B, types, pos):
     # Left-to-right scan: Induce L-positions from LMS-positions
     n = len(T)
     for r in range(n):
          p = pos[r]
          if p <= 0: continue # unknown or 0 -> skip
          if types[p-1] == SMALLER: continue # skip S positions
          a = T[p-1] # determine bucket
         pos[B[a-1]] = p-1
         B[a-1] += 1
10
```



Code: Phase II, S-positions

```
def induce_S_positions(T, B, types, pos):
      # Right-to-left scan: Induce S-positions from L-positions
     n = len(T)
      for r in range(n-1, -1, -1):
          p = pos[r]
          if p == 0: continue # skip position 0 (no p-1)
          if types[p-1] == LARGER: continue # skip L positions
          a = T[p-1] # determine bucket
         B[a] -= 1
          pos[B[a]] = p-1
10
```



Phase I





Idea for Phase 1

Goal (hard)

Sort the LMS suffixes (i.e., suffixes starting at LMS positions)



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Goal (hard)

Sort the LMS suffixes (i.e., suffixes starting at LMS positions)

Plan

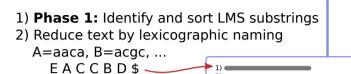
- Only sort the LMS substrings (up to next LMS position): shorter total length (O(n)) instead of $O(n^2)$.
- Expand alphabet and reduce text length (LMS substring → character), keeping lexicographic order of LMS substrings ("lexicographic naming").
- If all LMS substrings are distinct, we have also sorted the LMS suffixes, done!
- If there are equal LMS substrings, compute suffix array of reduced text (recursively with SAIS), use that to infer correct order of LMS suffixes.



Example: Alphabet Expansion and Text Reduction

```
0123456789012345678901
position p
             gccttaacattattacgccta$
text T
             LSSLLSSLSLLSLLSSLSSLLS
type
LMS?
LMS-substr
              cctta
                     atta
                           acgc
                  aaca
                        atta ccta$
p'
red. text R
r,
pos'[r']
                                      reduced suffix array
RT[pos'[r']] 21 5 14 11 8 17
                                      sorted LMS-positions
```

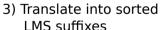
Overview with Recursion



Input

Suffix array of reduced text [6 1 4 3 2 5 0]





4) **Phase 2:** Use sorted LMS suffixes to induce order of non-LMS suffixes

Innut



Questions

- 1 How to sort the LMS substrings in linear time?
- 2 How to compare and name LMS substrings in linear time?
- 3 How to obtain order of LMS suffixes after recursive call?

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Sorting LMS Substrings

Surprisingly, it can be done by another run of Phase II:

- Enter unsorted LMS-positions into correct buckets of pos
- Induce order of L-positions based on unsorted LMS-positions
- Induce order of S-positions based on sorted S-positions

Result: Suffixes at LMS positions correctly sorted up to next LMS position:

```
... SSSSLLLLLLS ...
```

... * * ..



Text Reduction and Lexicographic Naming

- 1 Sort LMS substrings (phase 2) into pos (previous slide)
- Extract partially sorted LMS positions from pos
- 3 Compare LMS substrings in lexicographic order, \$ first, assign new "name" (number) if different from previous string.
- 4 In parallel, build new reduced text *R* from names at LMS positions, build map RT from *R*-positions to *T*-LMS-positions.
- 5 If all LMS substrings are unique, we already have sorted LMS suffixes. Otherwise recurse on R (next slide) to obtain pos'.
- **6** Total time without recursion: O(n).



Recursion

Situation: We have

- paritally sorted LMS suffixes lms,
- reduced text R,
- map RT from *R*-positions to *T*-LMS-positions.

Left to do:

- **1** Recursively compute pos' of R by calling SAIS(R).
- 2 Overwrite 1ms by correct order of T is RT[pos'[0]], RT[pos'[1]],



Code: Phase I, Overview

```
def phase1(T, B, types, lms_positions, pos):
      # T: text: B: cumulative charachter counts
      # lms_positions: LMS positions in ANY ORDER
      # pos: uninitialized, used to sort LMS positions
      alphabet_size = len(B)
      phase2(T, B, types, lms_positions, pos)
      # Compute reduced text from LMS substrings
      (R, reduced_alphabet_size, position_map) \
        = reduce_text(T, alphabet_size, types, pos, lms_positions)
      # If there are equal LMS substrings, recurse on reduced text
10
      if len(R) != reduced_alphabet_size:
11
          reduced_pos = sais_main(R, reduced_alphabet_size)
12
          # Re-map reduced_pos to original text positions;
13
          # these are the lms_positions in lexicographic order,
14
          for i, redp in enumerate(reduced_pos):
15
              lms_positions[i] = position_map[redp]
16
```



Code: Phase I, Text Reduction (Lexicographic Naming)

```
def reduce_text(T, alphabet_size, types, pos, lms_positions):
     n, m = len(pos), len(lms_positions)
      names = np.full(n, -1, dtype=np.int64) # the names
      last_lms = n-1; names[last_lms] = 0 # sentinel at n-1
      reduced_alphabet_size = 1; j = 0
      # go through the suffixes lexicographically, w/o sentinel
      for r in range(1, n):
          p = pos[r] # if not LMS, skip it:
          if p==0 or types[p]!=SMALLER or types[p-1]!=LARGER:
              continue
10
         lms_positions[j]=p; j+=1 # write sorted LMS positions
11
          if lms_substrings_unequal(T, types, last_lms, p):
12
              reduced_alphabet_size += 1
13
          names[p] = reduced_alphabet_size - 1
14
          last_lms = p
15
```



Code: Phase I, Comparison of LMS Substrings

```
def lms_substrings_unequal(T, types, p1, p2):
      """Return True iff LMS substrings at p1, p2 in T differ"""
      is_lms_p1 = is_lms_p2 = False
      while True:
          if T[p1] != T[p2]: return True # unequal
          if types[p1] != types[p2]: return True # unequal
          if is_lms_p1 and is_lms_p2: return False # equal
          p1 +=1; p2 += 1 \# look at next positions
          # check if both or only one LMS substring ends now
          is_lms_p1 = types[p1] == SMALLER and types[p1-1] == LARGER
10
         is_lms_p2 = types[p2] == SMALLER and types[p2-1] == LARGER
11
          if is_lms_p1 and is_lms_p2: continue # final test
12
          if is_lms_p1 or is_lms_p2: return True # unequal
13
```



Running Time Analysis

Observations about the recursion

- The alphabet size can grow, but is bounded by *n* (e.g. a, c, g, t expands to A–E).
- After each reduction step for a sequence of length n (including the sentinel), the new sequence has at most length $\lfloor n/2 \rfloor$ (again including the sentinel).



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Find a bound on the running time T(n) for these three parts:

- **1** Phase I without recursion: $\leq c_1 n$
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Claim

 $T(n) = \mathcal{O}(n)$, i.e., SAIS takes linear time in n = |T|.



Running Time Analysis (Proof)

Proof of Claim $T(n) = \mathcal{O}(n)$

- **1** Phase I without recursion: $\leq c_1 n$
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- **3** Phase II: $\leq c_2 n$

Let
$$C:=c_1+c_2$$
. Then $T(1)=\mathcal{O}(1)$, and thus

$$T(n) \le c_1 n + T(n/2) + c_2 n$$

= $C n + T(n/2)$
= $C n + C n/2 + T(n/4)$
 $\le C n(1 + 1/2 + 1/4 + ...) + T(1)$
= $2C n + O(1) = O(n)$.

q.e.d.

Summary

Linear suffix array construction by induced sorting (SAIS)

- Sorted LMS-suffixes can be used to induce sorting of L-suffixes.
- 2 Sorted L-suffixes can be used to induce sorting of S-suffixes.
- Sort LMS-suffixes by sorting LMS-substrings first (how? induced sorting on unsorted LMS-positions)
- Reduce text by lexicographic naming of LMS-substrings
- 5 If equal LMS-substrings exist, recurse on reduced text
- 6 LMS-order of original text is obtained from suffix array of reduced text



Possible exam questions

- Explain the principle of induced sorting.
- Why are L-positions on the left and S-positions on the right of each bucket?
- What is the goal of the text reduction step?
- Conduct the first iteration of induced sorting for a small example string.
- Explain why the induced sorting algorithm has linear running time.

