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Biological Sequence Analysis

Suffix Arrays

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[For more details, refer to "Jewels of Stringology" by Maxime Crochemore and Wojciech Rytter]

1 Suffix arrays

The *suffix array* of a given *string* of length n (including a *sentinel* \$) is an integer array containing the *suffix IDs* of the lexicographically sorted suffixes of the *original string* (the *sentinel* \$ simplifies algorithms and is considered the smallest character). A *suffix ID* is the start index of this suffix inside the *original string*.

The purpose of the *suffix array* is the same as the *suffix tree*, but *suffix array* is less powerful (enables less operations than *suffix tree*) but more compact (needs less space than *suffix tree*).

Consider the suffixes of the string ACGACTACGATAAC\$ of length n = 15:

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
А	С	G	А	С	Т	Α	С	G	А	Τ	Α	А	С	\$

The right table shows the suffixes of the string ACGACTACGATAAC\$ sorted lexicographically:

Suffix ID	Suffix string
0	ACGACTACGATAAC\$
1	CGACTACGATAAC\$
2	GACTACGATAAC\$
3	ACTACGATAAC\$
4	CTACGATAAC\$
5	TACGATAAC\$
6	ACGATAAC\$
7	CGATAAC\$
8	GATAAC\$
9	ATAAC\$
10	TAAC\$
11	AAC\$
12	AC\$
13	C\$
14	\$

Suffix ID	Suffix string
14	\$
11	AAC\$
12	AC\$
0	ACGACTACGATAAC\$
6	ACGATAAC\$
3	ACTACGATAAC\$
9	ATAAC\$
13	C\$
1	CGACTACGATAAC\$
7	CGATAAC\$
4	CTACGATAAC\$
2	GACTACGATAAC\$
8	GATAAC\$
10	TAAC\$
5	TACGATAAC\$

Therefore, the *suffix array* of the string ACGACTACGATAAC\$ is:

Index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Suffix array	14	11	12	0	6	3	9	13	1	7	4	2	8	10	5

Using the *suffix array* and the *original string*, we can search for any *substring query* of length m inside the *original string* in $O(m \times (\log n + occ))$ time using *binary search*, where *occ* is the number of occurrences of the *substring query* inside the *original string*.

The above complexity is achieved because each of the $O(\log n)$ binary search iterations includes an O(m) string comparison of the substring query to an original string suffix. After the binary search is done, we perform string comparison of the substring query to all suffixes starting from the result location of the binary search until we encounter a suffix which is not prefixed by the substring query. The number of such suffixes is occ.

The third column of *suffix* strings in the following figure is not part of the *suffix array* and is shown for illustration only since it can be deduced easily from the *suffix array* and the *original string*.

Index	Suffix array	Corresponding suffix
0	14	\$
1	11	AAC\$
2	12	AC\$
3	0	ACGACTACGATAAC\$
4	6	ACGATAAC\$
5	3	ACTACGATAAC\$
6	9	ATAAC\$
7	13	C\$
8	1	CGACTACGATAAC\$
9	7	CGATAAC\$
10	4	CTACGATAAC\$
11	2	GACTACGATAAC\$
12	8	GATAAC\$
13	10	TAAC\$
14	5	TACGATAAC\$

Here we trace the *binary search* for the substring CGA using the above *suffix array* only. We start with an unexplored interval [0, 15] representing $[first_index, last_index + 1]$.

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Middle index is \lfloor (0+15)/2 \rfloor = 7. CGA > C$. Interval shrinks to [8,15]. Middle index is \lfloor (8+15)/2 \rfloor = 11. CGA < GACTACGATAAC$. Interval shrinks to [8,11]. Middle index is \lfloor (8+11)/2 \rfloor = 9. CGA < CGATAAC$. Interval shrinks to [8,9]. Middle index is \lfloor (8+9)/2 \rfloor = 8. CGA < CGACTACGATAAC$. Interval shrinks to [8,8].
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Then, we test if CGA is prefix of suffixes at indexes ≥ 8 in *suffix array*: CGA is prefix of CGACTACGATAAC\$ at index 8. Report occurrence at index 1 in *original string*. CGA is prefix of CGATAAC\$ at index 9. Report occurrence at index 7 in *original string*. CGA is not prefix of CTACGATAAC\$ at index 10. Stop.

The complexity can be improved to $O(m \log n + occ)$ by performing another binary search instead of comparing all suffixes starting from result index of the first binary search. The second binary search is similar to the first one, except that if query substring is prefix of compared suffix, it is considered greater than this suffix. In the above example, the second binary search will result the interval [10, 10] which is 1+ index of the last occurrence of query substring in suffix array.

2 Suffix array construction

A *suffix array* can be constructed naively in $O(n^2 \log n)$ using an $O(n \log n)$ sorting algorithm such as *merge sort*. The additional n factor in complexity arises because the complexity of each *suffix* comparison performed by the algorithm is O(n), not O(1).

We can utilize the strong relation between *suffixes* of the same *original string* to improve the *suffix* array construction time to $O(n \log n)$ using the following *prefix doubling* algorithm.

Consider constructing *suffix array* of string ACGACTACGATAAC\$ using *prefix doubling*. The initial step is to sort all *suffixes* by their first character only, simply by assigning to each *suffix* the order of its first character in the alphabet. Remember that \$ is the smallest character.

	Index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Iteration	Sorted prefix len	А	С	G	А	С	Т	А	С	G	А	Т	А	А	С	\$
0	$2^0 = 1$	1	2	3	1	2	4	1	2	3	1	4	1	1	2	0

From the above table, we recognize that the smallest $suffix \$ gets the smallest integer 0. The immediately larger suffixes are those starting with A. They all got the next smallest integer 1, because they are equal if we look at their first character only which is A. The immediately larger suffixes are those starting with B. They all got the next smallest integer 2, because they are equal if we look at their first character only which is B.

The general rule is that, in iteration i, all *suffixes* are sorted according to their first 2^i characters only. That is, we assume that the length of each suffix is only 2^i . All *suffixes* starting with the same prefix of size 2^i are considered equal and assigned the same integer. Thus, the second iteration i = 1 assigns the same integer to all *suffixes* starting with the same $2^1 = 2$ characters:

	Index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Iteration	Sorted prefix len	А	С	G	А	С	Т	А	С	G	А	Т	А	А	С	\$
0	$2^0 = 1$	1	2	3	1	2	4	1	2	3	1	4	1	1	2	0
1	$2^1 = 2$	2	5	7	2	6	8	2	5	7	3	8	1	2	4	0

From the above table, we recognize that the smallest *suffix* \$ gets the smallest integer 0. The immediately larger *suffixes* are those starting with AA. It is exactly one *suffix* and it got the next smallest integer 1. The immediately larger *suffixes* are those starting with AC. They all got the next smallest integer 2, because they are equal if we look at their first two characters only which are AC.

Here we explain how to reduce time complexity. The next iteration i=2 of the algorithm is going to sort *suffixes* according to their first $2^i=2^2=4$ characters. Instead of comparing two *suffixes* by performing a string comparison of their first 4 characters, we will perform a more efficient *suffix* comparison using the results of the previous iteration i=1.

To compare two *suffixes* at iteration i, look at their assigned integers at iteration i-1. If the integers are not equal, their relative order remains the same. If the integers are equal, look at relative order of the two *suffixes* shifted by 2^i positions from the locations of the needed *suffixes*.

For example, to compare the first 4 characters of the two *suffixes* at indexes 4 (CTAC) and 7 (CGAT), look at their relative order according to their first 2 characters, appearing in last row in the above table to be 6 and 5, indicating that *suffix* 4 is larger than *suffix* 7. The relation remains the same.

	Index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Iteration	Sorted prefix len	A	С	G	A	С	Т	A	С	G	А	Т	А	A	С	\$
0	$2^0 = 1$	1	2	3	1	2	4	1	2	3	1	4	1	1	2	0
1	$2^1 = 2$	2	5	7	2	6	8	2	5	7	3	8	1	2	4	0

Another example for the other case, to compare the first 4 characters of the two *suffixes* at indexes 2 (GACT) and 8 (GATA). Their orders according to their first 2 characters, appearing in last row in the above table are 7 and 7, indicating that *suffix* 2 is equal to *suffix* 8 with respect to the first 2 characters (GA).

Since they are equal, we consider the two *suffixes* shifted by 2 from the original *suffixes* indexes, which are *suffixes* at indexes 2+2=4 (CT) and 8+2=10 (TA). Their orders according to their first 2 characters, appearing in last row in the above table are 6 and 8, indicating that *suffix* 4 is smaller than *suffix* 10 with respect to their first 2 characters (GA), which implies the same relation between the original two *suffixes* 2 (GACT) and 8 (GATA) with respect to their first 4 characters.

	Index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Iter	Sorted prefix len	А	С	G	А	С	Т	А	С	G	А	Т	А	А	С	\$
0	$2^0 = 1$	1	2	3	1	2	4	1	2	3	1	4	1	1	2	0
1	$2^1 = 2$	2	5	7	2	6	8	2	5	7	3	8	1	2	4	0
2	$2^2 = 4$	3	7	10	4	9	13	3	8	11	5	12	1	2	6	0

Here we explain how to obtain all *suffix* orders from of iteration 2 from iteration 1. There is exactly one *suffix* with order 0 which is *suffix* 14, its order remains the same. Also, only *suffix* 11 has order 1 and remains the same.

There are 4 *suffixes* with order 2 which are 0, 3, 6, 12. We look at shifted-by-2 *suffixes* 2, 5, 8, 14 their orders are 7, 8, 7, 0 to conclude that the smallest *suffix* is 12 so we assign to it order of 2 (because last assigned order was 1). Then, next smallest *suffixes* are 0 and 6 with the same order of 3, meaning that they are still equal with respect to their first 4 characters, then *suffix* 3 takes order of 4 (because last assigned order was 3).

Only *suffix* 9 has order 3 in iteration 1. It is assigned order 5 in iteration 2 (because last assigned order was 4). Only *suffix* 13 has order 4. It is assigned order 6. There are 2 *suffixes* with order 5 which are 1, 7. We look at shifted-by-2 *suffixes* 3, 9 their orders are 2, 3 to conclude that the smaller *suffix* is 1 so we assign to it order of 7, then *suffix* 7 takes order of 8. Only *suffix* 4 has order 6. It is assigned order 9.

There are 2 *suffixes* with order 7 which are 2, 8. We look at shifted-by-2 *suffixes* 4, 10 their orders are 6, 8 to conclude that the smaller *suffix* is 2 so we assign to it order of 10, then *suffix* 8 takes order of 11. There are 2 *suffixes* with order 8 which are 5, 10. We look at shifted-by-2 *suffixes* 7, 12 their orders are 5, 1 to conclude that the smaller *suffix* is 10 so we assign to it order of 12, then *suffix* 5 takes order of 13.

Note that actually there should not be any two equal *suffixes*, so the algorithm terminates only if there are no two *suffixes* with the same order.

To move to the next iteration 3, the only two suffixes with same order are 0, 6. We look at shifted-by-4 *suffixes* 4, 10 their orders in iteration 2 are 9, 12 to conclude that the smaller *suffix* is 0 so we assign to it a smaller order than suffix 6 as follows:

	Index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Iter	Sorted prefix len	А	С	G	А	С	Т	А	С	G	А	Т	А	А	С	\$
0	$2^0 = 1$	1	2	3	1	2	4	1	2	3	1	4	1	1	2	0
1	$2^1 = 2$	2	5	7	2	6	8	2	5	7	3	8	1	2	4	0
2	$2^2 = 4$	3	7	10	4	9	13	3	8	11	5	12	1	2	6	0
3	$2^3 = 8$	3	8	11	5	10	14	4	9	12	6	13	1	2	7	0

The algorithm terminates because all suffixes have different orders as they should. Since we terminated at iteration 3 we conclude that no two *suffixes* share the same prefix of $2^3 = 8$ characters.

The resulting array is not the *suffix array*, but it is the *inverse* of the *suffix array*. The resulting array tells the order given a *suffix ID* (example: suffix 12 has the order 2). The *suffix array* tells the *suffix ID* given an order (example: the suffix of order 2 is 12). The *suffix array* can be easily obtained from its *inverse* by O(n) sequential scan:

Index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Suffix array	14	11	12	0	6	3	9	13	1	7	4	2	8	10	5

In the worst case, no two *suffixes* share the same prefix of n characters because all *suffixes* are different. Therefore, the number of iterations is $O(\log n)$ can be concluded from the second column because maximum sorted prefix length is n and it is multiplied by 2 at each iteration.

At each iteration suffixes are sorted using $O(n \log n)$ sorting algorithm, then the required array in the figures above is obtained in O(n) sequential scan over the sorted array. Each suffix comparison needs only O(1) operations since we compare 2 orders, and when equal we compare 2 shifted orders. It can be viewed as comparing pairs of integers. Therefore, the total time complexity is $O(n \log^2 n)$. Since the sorting procedure compares two pairs of integers whose range is n, we can use two-pass O(n) radix sorting at each iteration to reduce the total complexity to $O(n \log n)$. There is also an O(n) suffix array construction algorithm called induced sorting.