

Fast Optimal Algorithms for Computing All the Repeats in a String*

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Abstract. Given a string $\mathbf{x} = \mathbf{x}[1..n]$ on an alphabet of size α , and a threshold $p_{min} \geq 1$, we first describe a new algorithm PSY1 that, based on suffix array construction, computes all the complete *nonextendible* repeats in \mathbf{x} of length $p \geq p_{min}$. PSY1 executes in $\Theta(n)$ time independent of alphabet size and is an order of magnitude faster than the two other algorithms previously proposed for this problem. Second, we describe a new fast algorithm PSY2 for computing all complete *supernonextendible* repeats in \mathbf{x} that also executes in $\Theta(n)$ time independent of alphabet size, thus asymptotically faster than methods previously proposed. Both algorithms require $9n$ bytes of storage, including preprocessing (with a minor *caveat* for PSY1). We conclude with a brief discussion of applications to bioinformatics and data compression.

1 Introduction

A *repeating substring* \mathbf{u} in a string \mathbf{x} is a substring of \mathbf{x} that occurs more than once. A *repeat* in \mathbf{x} is a set of repeating substrings \mathbf{u} of \mathbf{x} ; it can be specified by the length $p \geq 1$ of \mathbf{u} (what we call its *period*) and the locations at which \mathbf{u} occurs. Thus in $\mathbf{x} = abaababa$, the tuple $(3; 1, 4, 6)$ describes the repeat of $\mathbf{u} = aba$ ($p = 3$) at positions 1, 4, 6.

Following [20] we say that a repeat $(p; i_1, i_2, \dots, i_k)$, $k \geq 2$, is *complete* iff it includes all occurrences of \mathbf{u} in \mathbf{x} ; *left-extendible* (LE) iff

$$\mathbf{x}[i_1 - 1] = \mathbf{x}[i_2 - 1] = \dots = \mathbf{x}[i_k - 1];$$

and *right-extendible* (RE) iff

$$\mathbf{x}[i_1 + p] = \mathbf{x}[i_2 + p] = \dots = \mathbf{x}[i_k + p].$$

A repeat is NLE iff it is not LE; NRE iff it is not RE; *nonextendible* (NE) iff it is both NLE and NRE. A repeat is *supernonextendible* (SNE) iff it is NE and its repeating substring \mathbf{u} is not a proper substring of any other repeating substring of \mathbf{x} .

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In [8, p. 147] an algorithm is described that, given the suffix tree $ST_{\mathbf{x}}$ of \mathbf{x} , computes all the NE (called “maximal”) *pairs of repeats* in \mathbf{x} in time $O(\alpha n + q)$, where q is the number of pairs output. [4] uses similar methods to compute all NE pairs $(p; i_1, i_2)$ such that $i_2 - i_1 \geq g_{min}$ (or $\leq g_{max}$) for user-defined *gaps* g_{min}, g_{max} . [1] shows how to use the suffix array $SA_{\mathbf{x}}$ of \mathbf{x} to compute the NE pairs in time $O(\alpha n + q)$. Since it may be that $\alpha \in O(n)$, all of these algorithms require $O(n^2)$ time in the worst case, though in applications usually $\alpha = 4$ (DNA alphabet). [7] uses the suffix arrays of both \mathbf{x} and its reversed string $\bar{\mathbf{x}} = \mathbf{x}[n]\mathbf{x}[n-1] \cdots \mathbf{x}[1]$ to compute all the complete NE repeats in \mathbf{x} in $\Theta(n)$ time. More recently, [17] describes suffix array-based $\Theta(n)$ -time algorithms to compute all *substring equivalence classes* — essentially the complete NE repeats — in \mathbf{x} .

In this paper we first describe an algorithm PSY1 that computes all the complete NE repeats in a given string \mathbf{x} whose length (period) $p \geq p_{min}$, where $p_{min} \geq 1$ is a user-specified minimum. PSY1 executes in $\Theta(n)$ time independent of alphabet size and requires $5n$ bytes of storage, plus a stack, but its preprocessing includes suffix array construction that raises the storage requirement to $9n$ bytes. PSY1 is an order of magnitude faster than the complete repeats algorithms described in [7,17].

We also describe a new fast algorithm PSY2 that computes all the complete SNE repeats in \mathbf{x} in time $\Theta(n + \alpha)$. This improves on the algorithm described in [8, p. 146] that does the same calculation (of “supermaximal” repeats) in time $O(n \log \alpha)$ using a suffix tree, as well as on the algorithm described in [1, p. 59] that uses a suffix array and requires $O(n + \alpha^2)$ time. For $\alpha \in O(n)$ these times become $O(n \log n)$ and $O(n^2)$, respectively, whereas PSY2 remains $\Theta(n)$.

In Section 2 we describe our algorithms. Section 3 summarizes the results of experiments that compare the algorithms with each other and with existing algorithms. Section 4 discusses these results, including the strategy of computing complete (NE and SNE) repeats in the context of applications to bioinformatics and data compression.

2 Description of the Algorithms

We suppose that a string $\mathbf{x} = \mathbf{x}[1..n]$ is given, defined on an ordered alphabet A of size α (where if there is no explicit bound on alphabet size, we suppose $\alpha \leq n$). We refer to the suffix $\mathbf{x}[i..n]$, $i \in 1..n$, simply as *suffix* i . Then the *suffix array* $SA_{\mathbf{x}}$ is an array $[1..n]$ in which $SA_{\mathbf{x}}[j] = i$ iff suffix i is the j^{th} in lexicographical order among all the suffixes of \mathbf{x} . Let $\text{lcp}_{\mathbf{x}}(i_1, i_2)$ denote the *longest common prefix* of suffixes i_1 and i_2 of \mathbf{x} . Then $LCP_{\mathbf{x}}$ is an array $[1..n+1]$ in which $LCP_{\mathbf{x}}[1] = LCP_{\mathbf{x}}[n+1] = -1$, while for $j \in 2..n$,

$$LCP_{\mathbf{x}}[j] = \left| \text{lcp}_{\mathbf{x}}(SA_{\mathbf{x}}[j-1], SA_{\mathbf{x}}[j]) \right|.$$

$SA_{\mathbf{x}}$ can be computed in $\Theta(n)$ worst-case time [9,12], though various supralinear methods [16,14] are certainly much faster, as well as more space-efficient, in practice [18], in some cases requiring space only for \mathbf{x} and $SA_{\mathbf{x}}$ itself. Given \mathbf{x} and $SA_{\mathbf{x}}$, $LCP_{\mathbf{x}}$ can also be computed in $\Theta(n)$ time [11,15]: the first algorithm described in [15] requires $9n$ bytes of storage and is almost as fast in practice as that of [11], which requires $13n$ bytes. (For space calculations, we make throughout the usual assumption that an integer occupies four bytes, a letter one.) When the context is clear, we write SA for $SA_{\mathbf{x}}$, LCP for $LCP_{\mathbf{x}}$.


```

— Preprocessing: compute SA, BWT & LCP
— in  $\Theta(n)$  time and  $9n$  bytes of space.
lcp  $\leftarrow$  LCP[1]; lb  $\leftarrow$  1; bwt1  $\leftarrow$  BWT[1]
push(LB; lcp, lb, bwt1)
for j  $\leftarrow$  1 to n do
  lb  $\leftarrow$  j; lcp  $\leftarrow$  LCP[j+1]
  — Compute LEletter of BWT[j] and BWT[j+1].
  bwt2  $\leftarrow$  BWT[j+1]; bwt  $\leftarrow$  LEletter(bwt1, bwt2); bwt1  $\leftarrow$  bwt2
  while top(LB).lcp > lcp do
    pop(LB; p, i, prevbwt)
    if prevbwt = $ and  $p \geq p_{min}$  then
      output(p; i, j)
    lb  $\leftarrow$  i
    top(LB).bwt  $\leftarrow$  LEletter(prevbwt, top(LB).bwt)
    bwt  $\leftarrow$  LEletter(prevbwt, bwt)
  if top(LB).lcp = lcp then
    top(LB).bwt  $\leftarrow$  LEletter(top(LB).bwt, bwt)
  else
    push(LB; lcp, lb, bwt)

function LEletter( $\ell_1, \ell_2$ )
if  $\ell_1 = \$$  or  $\ell_1 \neq \ell_2$  then return $
else return  $\ell_1$ 

```

Figure 1. Algorithm PSY1: compute all NE repeats of period $p \geq p_{min}$ as ranges in SA

It remains to determine whether or not the popped triple is NLE. For this the popped value *prevbwt* needs to be inspected to determine whether it is \$ — that is, whether the repeat is NLE, whether it should be output. To ensure that `top(LB).bwt` is maintained correctly, we use a simple property of ranges of repeats: two ranges are either disjoint (empty common prefix) or else one range contains the other (common prefix over the longer range). It follows that if `top(LB).bwt = $` for a contained range, then for every range that encloses it, we must also have `top(LB).bwt = $`. Moreover, if for some letter $\lambda \in A$, a contained range is LE with $bwt = \lambda$, then the enclosing range will be LE only if every other contained range also has $bwt = \lambda$. In PSY1 the correct *bwt* value for the enclosing range is maintained by invoking `LEletter` to update `top(LB).bwt` whenever $LCP[j+1] \leq \text{top(LB).lcp}$. For $LCP[j+1] < \text{top(LB).lcp}$, `LEletter` is used again to update the current *bwt* based on the *prevbwt* just popped.

In view of this discussion, we claim the correctness of PSY1. Execution time is $\Theta(n)$, since the number of executions of the **while** loop is at most the number of triples pushed onto LB, thus $O(n)$. Space required is $5n$ bytes plus maximum stack size at 9 bytes per entry (four bytes each for *lb* and *lcp*, plus a byte for *bwt*). The largest number of entries in LB is exactly the maximum depth of the suffix tree — in fact n for $x = a^n$ — but expected depth on an alphabet of size $\alpha > 1$ is $2 \log_\alpha n$ [10]. Thus even for $\alpha = 2$, expected space for LB is $18 \log_\alpha n$ bytes — if $n = 2^{20}$, 360 bytes. On strings arising in practice, LB requires negligible space (Section 4).

PSY2

The SNE (“supermaximal”) repeats algorithm described in [1] does not deal explicitly with the problem of determining whether or not a complete super NRE (SNRE) repeat is also SNLE. This determination requires that the left extensions (BWT values) of

```

— Preprocessing: compute SA, LAST & LCP.
j ← 0; p ← -1; q ← 0
while j < n do
  high ← 0
  repeat
    j ← j+1; p ← q; q ← LCP[j+1]
    if q > p then high ← q; i ← j
  until p > q
  if high > 0 and SNLE(i, j, LAST) then
    output(p; i, j)

function SNLE(start, end, LAST)
k ← end - start + 1
if k > α then return FALSE
else
  for h ← start+1 to end do
    if h - LAST[h] > start then return FALSE
  return TRUE

```

Figure 2. Algorithm PSY2 with a simplified SNLE function using LAST

the k positions in the repeat be pairwise distinct. The approach apparently proposed by the authors requires at most $\binom{k}{2}$ letter comparisons, where k can be order n , thus leading to $O(n^2)$ time in the worst case. A perhaps more efficient approach would be to use a bit map $B[1..\alpha]$ to determine if any letter in the alphabet has occurred more than once as a left extension over the range of the repeat. However, this would require initializing the α positions in B for each of $O(n)$ candidate repeats, and since possibly $\alpha \in O(n)$, the time required could again be $O(n^2)$. Our proposed algorithm PSY2 (Figure 2) incorporates two improvements, one to decrease execution time in practice, the other to reduce asymptotic complexity to $O(n+\alpha)$.

We observe first that the cardinality k of an SNE repeat cannot exceed the alphabet size α . Thus as shown in function SNLE of Figure 2, a single test suffices to eliminate candidate SNRE repeats of cardinality greater than α , thus substantially reducing processing time in many cases. We now describe a more sophisticated approach that reduces worst-case complexity to $\Theta(n+\alpha)$ with a negligible effect on actual processing time.

Instead of $\text{BWT}\mathbf{x}$, we compute an array $\text{LAST} = \text{LAST}[1..n]$ in which for every $j \in 1..n$, $\text{LAST}[j]$ is the offset between the BWT letter corresponding to the current position j in SA and the position j_{prev} of the rightmost previous occurrence in SA of the same BWT letter — if j_{prev} does not exist or if $j - j_{prev} \geq \alpha$, then $\text{LAST}[j] \leftarrow \alpha - 1$. However, if j_{prev} exists and satisfies $j - j_{prev} < \alpha$, we set $\text{LAST}[j] \leftarrow j - j_{prev} - 1$, so that $\text{LAST}[j]$ takes values in the range $0..\alpha - 2$. See Figure 3. Then when function SNLE processes a possibly supernonextendible repeat consisting of $end - start + 1$ substrings of \mathbf{x} , for every position $h \in start + 1..end$, the value of $\text{BWT}[h]$ will be unique within the range if and only if $h - \text{LAST}[h] > start$. See Figure 2.

In general it is possible that the offsets stored in LAST could be integers of size $O(n)$. But offsets of magnitude greater than $\alpha - 1$ need not be stored, since if the interval $start..end$ actually is an SNE repeat, it can contain no more than α positions. Thus LAST requires the same amount of storage as BWT, which stores letters that are also restricted to be at most $\alpha - 1$ in magnitude. The method can be implemented for any finite α , but with the usual convention that each letter in the

```

— Initialize an array storing rightmost positions of each letter.
for  $\ell \leftarrow 1$  to  $\alpha$  do
   $lastpos[\ell] \leftarrow 0$ 
— Compute LAST in a single left-to-right scan of SA.
 $\alpha' \leftarrow \alpha - 1$ 
for  $j \leftarrow 1$  to  $n$  do
   $i \leftarrow SA[j] - 1$ 
  if  $i \leftarrow 0$  then
     $LAST[j] \leftarrow \alpha'$ 
  else
     $letter \leftarrow x[i]; jprev \leftarrow lastpos[letter]$ 
    if  $jprev = 0$  or  $j - jprev \geq \alpha$  then
       $LAST[j] \leftarrow \alpha'$ 
    else
       $LAST[j] \leftarrow j - jprev - 1$ 
     $lastpos[letter] \leftarrow j$ 

```

Figure 3. Preprocessing for Algorithm PSY2 — computing LAST

alphabet is confined to a single byte ($\alpha \leq 256$), the array LAST becomes an array of bytes, just like BWT. (In fact, in order to take advantage of the CPU cache, our implementation of this algorithm actually computes BWT first, then makes a pass over BWT to convert it into LAST — an approach that turns out to be 2–3 times faster than a straightforward implementation of the preprocessing algorithm.)

3 Experimental Results

Experiments were conducted on a diverse selection of files (see Table 1) chosen from <http://www.cas.mcmaster.ca/~bill/strings/>. Tests were conducted using a 2.6 GHz Opteron 885 processor with 2 GB main memory available, under Red Hat Linux 4.1.2–14. The compiler was gcc with the -O3 option. The run times used were the minima over four runs, not including input/output.

File Type	Name	No. Bytes	Description
highly periodic	fib035	9,227,465	Fibonacci
	fib036	14,930,352	Fibonacci
	fss9	2,851,443	run-rich [6]
	fss10	12,078,908	run-rich [6]
random	rand2	8,388,608	$\alpha = 2$
	rand21	8,388,608	$\alpha = 21$
DNA	ecoli	4,638,690	<i>escherichia coli</i> genome
	chr22	34,553,758	human chromosome 22
	chr19	63,811,651	human chromosome 19
Genbank protein database	prot-a	16,777,216	sample
	prot-b	33,554,432	sample
English	bible	4,047,392	King James bible
	howto	39,422,105	Linux howto files
	mozilla	51,220,480	Mozilla source code

Table 1. Files used for testing.

Test results are shown in Table 2, where the vertical line separates preprocessing from processing. For SA construction the KS algorithm was used [9] — the fastest

such algorithm is perhaps MP2 [14] that, based on experiments documented in [14,18], would perform 5–10 times faster on average, using about $5.2n$ bytes of storage. For LCP construction the algorithm of Kasai *et al.* [11] was used, the fastest one known — according to experiments documented in [15], the first Manzini variant runs almost as fast. Table 2 compares PSY1 with the algorithm of [17]. The algorithm of [7] was not tested because it computes SA twice, and so could not be competitive. Not shown in the table are tests against three variants of PSY1, two of them using heuristics designed to speed up processing, another using a different approach that also achieves $\Theta(n)$ worst case time: on each of the test files listed in Table 1, PSY1 is at least as fast as any of the three. Note that for each program tested, the number of microseconds per letter is generally stable within each file type and not highly variable overall. Averages are not weighted by file size. Tests shown for PSY1 used $p_{min} = 1$; as expected, for larger p_{min} run time was unchanged.

File	SA	LCP	BWT	LAST	PSY1	[17]	PSY2
fib35	0.898	0.169	0.025	0.031	0.012	0.448	0.009
fib36	0.886	0.170	0.027	0.033	0.012	0.475	0.007
fss9	0.826	0.154	0.026	0.031	0.014	0.330	0.007
fss10	0.958	0.177	0.025	0.032	0.013	0.469	0.008
periodic AVG	0.892	0.168	0.026	0.032	0.013	0.430	0.008
rand2	0.947	0.188	0.026	0.031	0.017	0.215	0.012
rand21	1.135	0.199	0.025	0.031	0.012	0.122	0.012
random AVG	1.041	0.193	0.025	0.031	0.015	0.169	0.012
ecoli	1.413	0.175	0.025	0.031	0.015	0.155	0.011
chr22	1.635	0.285	0.035	0.040	0.016	0.278	0.012
chr19	1.873	0.333	0.044	0.053	0.016	0.242	0.012
DNA AVG	1.754	0.309	0.035	0.041	0.016	0.225	0.012
prot-a	1.778	0.222	0.027	0.032	0.013	0.211	0.012
prot-b	1.971	0.277	0.034	0.039	0.013	0.247	0.012
protein AVG	1.874	0.249	0.030	0.036	0.013	0.229	0.012
bible	1.417	0.151	0.024	0.030	0.015	0.168	0.012
howto	1.912	0.214	0.035	0.039	0.016	0.219	0.012
mozilla	1.815	0.187	0.032	0.036	0.013	0.139	0.011
English AVG	1.417	0.151	0.024	0.035	0.014	0.175	0.012
AVERAGE	1.390	0.207	0.029	0.035	0.014	0.266	0.011

Table 2. Microseconds per letter used by each run.

4 Discussion

We make the following observations:

- * Both new algorithms are very fast, especially on strings that arise in practice: even if SA were to execute 10 times faster, still each algorithm would require less than 5% of total SA/LCP time.
- * Computing LAST for PSY2 requires about 20% more time than computing BWT for PSY1. Both requirements are small compared to SA/LCP computation time.
- * For PSY1 we have computed maximum stack size for each of the test files: for `prot-a` (the worst case) the maximum storage for LB was less than 0.1% of the $5n$ bytes required for LCP and BWT.

- * The algorithm of [17] appears to execute 10–15 times slower than PSY1 on real-world files, while requiring $12n$ bytes of storage (SA, inverse of SA, and LCP). (The timing facilities for this algorithm were included in the code kindly provided by the authors.)
- * Assuming the use of a fast space-efficient SA construction algorithm, LCP construction turns out to be the main obstacle to further improvement, due to both its time and its space requirements.

The output of PSY1 and PSY2 can be used in various ways and for various purposes. For offline data compression the output can be used for phrase selection [2,13,21]. It is also useful for duplicate text/document detection [3]. If the user requires positions in \mathbf{x} to be output, this can trivially be achieved, since SA is available, by postprocessing that replaces $i..j$ by $\text{SA}[i], \text{SA}[i+1], \dots, \text{SA}[j]$. In applications to protein sequences, such as the detection of low-complexity regions, the use of either PSY1 or PSY2 will provide significant algorithmic speed-up over currently-proposed methods [19] that are effective but slow. In the context of genome analysis the postprocessing of interest may be to compute NE pairs as in [8,4,1]. Assuming an integer alphabet $1..\alpha$, this can be accomplished as follows for each range $i..j$. Introduce a new array $\text{BWT}' = \text{BWT}'[1..n]$, where for $\text{SA}[h] < n$, $\text{BWT}'[h] = \mathbf{x}[\text{SA}[h]+1]$, otherwise $\text{BWT}'[h] = \$$.

- (1) Perform a radix sort on the pairs

$$(\text{BWT}[i], \text{BWT}'[i]), (\text{BWT}[i+1], \text{BWT}'[i+1]), \dots, (\text{BWT}[j], \text{BWT}'[j])$$

into bins that are accessed from an array $\text{B} = \text{B}[1..\alpha, 1..\alpha]$. As a byproduct of the sort, positions in a Boolean array $\text{E} = \text{E}[1..\alpha]$ are set: $\text{E}[b] = \text{TRUE}$ if and only if row b of B is empty.

- (2) For every nonempty row b_1 of B , and for every $b_2 \in 1..\alpha$, perform the following simple processing:

```

for  $h_1 \leftarrow b_1+1$  to  $\alpha$  do
  if not  $\text{E}[h_1]$  then
    for  $h_2 \leftarrow (1 \text{ to } b_2-1)$  and  $(b_2+1 \text{ to } \alpha)$  do
      output all pairs  $\text{B}(b_1, b_2)$  with  $\text{B}(h_1, h_2)$ 

```

This approach requires checking at most $\alpha^2(\alpha-1)^2/2$ positions in B for each range processed; in the DNA case with $\alpha = 4$, this amounts to at most 72 (that is, $\alpha^3+2\alpha$) positions, but will for most ranges be much less. Otherwise the time required is proportional to the number of pairs output. Due to cache effects, we believe this will be an efficient algorithm for computing NE pairs: it depends only on $i, j, \text{BWT}, \text{BWT}'$.

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