Sampling the suffix array with minimizers

Szymon Grabowski and Marcin Raniszewski

Lodz University of Technology, Institute of Applied Computer Science, Al. Politechniki 11, 90–924 Lódź, Poland {sgrabow|mranisz}@kis.p.lodz.pl

Abstract. Sampling (evenly) the suffixes from the suffix array is an old idea trading the pattern search time for reduced index space. A few years ago Claude et al. showed an alphabet sampling scheme allowing for more efficient pattern searches compared to the sparse suffix array, for long enough patterns. A drawback of their approach is the requirement that sought patterns need to contain at least one character from the chosen subalphabet. In this work we propose an alternative suffix sampling approach with only a minimum pattern length as a requirement, which seems more convenient in practice. Experiments show that our algorithm achieves competitive time-space tradeoffs on most standard benchmark data.

1 Introduction

Full-text indexes built over a text of length $n$ can roughly be divided into two categories: those requiring at least $n \log_2 n$ bits and the more compact ones. Classical representatives of the first group are the suffix tree and the suffix array. Succinct solutions, often employing the Burrows–Wheeler transform and other ingenious mechanisms (compressed rank/select data structures, wavelet trees, etc.), are object of vivid interest in theoretical computer science [19], but their practical performance does not quite deliver; in particular, the locate query is significantly slower than using e.g. the suffix array [20,9,11].

A very simple, yet rather practical alternative to both compressed indexes and the standard suffix array is the sparse suffix array (SpaSA) [15]. This data structure stores only the suffixes at regular positions, namely those being a multiple of $q$ ($q > 1$ is a construction-time parameter). The main drawback of SpaSA is that instead of one (binary) search over the plain SA it has to perform $q$ searches, in $q - 1$ cases of which followed by verification of the omitted prefix against the text. If, for example, the pattern $P[1\ldots6]$ is tomcat and $q = 4$, we need to search for tomcat, omcat, mcat and cat, and 3 of these 4 searches will be followed by verification. Obviously, the pattern length must be at least $q$ and this approach generally works better for longer patterns.

The sampled suffix array (SamSA) by Claude et al. [4] is an ingenious alternative to SpaSA. They choose a subset of the alphabet and build a sorted array over only those suffixes which start with a symbol from the chosen subalphabet. The search starts with finding the first (leftmost) sampled symbol of the pattern, let us say at position $j$, and then the pattern suffix $P[j\ldots m]$ is sought
in the sampled suffix array with standard means. After that, each occurrence of the pattern suffix must be verified in the text with the previous $j-1$ symbols. A great advantage of SamSA over SpaSA is that it performs only one binary search. On the other hand, a problem is that the pattern must contain at least one symbol from the sampled subalphabet. It was shown however that a careful selection of the subalphabet allows for leaving out over 80% suffixes and still almost preserving the pattern search speed for the standard array, if the patterns are long (50–100).

An idea most similar to ours was presented more than a decade ago by Crescenzi et al. [6,7] and was called text sparsification via local maximia. Using local maxima, that is, symbols in text which are lexicographically not smaller than the symbol just before them and lexicographically greater than the next symbol, has been recognized even earlier as a useful technique in string matching and dynamic data structures, for problems like indexing dynamic texts [1], maintaining dynamic sequences under equality tests [17] or parallel construction of suffix trees [22]. Crescenzi et al., like us, build a suffix array on sampled suffixes, yet in their experiments (only on DNA) the index compression by factor about 3 requires patterns of length at least about 150 (otherwise at least a small number of matches are lost). Our solution does not suffer a similar limitation, that is, the minimum pattern lengths with practical parameter settings are much smaller.

2 Our algorithm

2.1 The idea

Our purpose is to combine the benefits of the sparse suffix array (searching any patterns of length at least the sampling parameter $q$) and the sampled suffix array (one binary search). To this end, we need the following property:

*For each substring $s$ of $T$, $|s| = q$, there exists its substring $s'$, $|s'| \leq q$, such that among the sampled suffixes there exists at least one which starts with $s'$. Moreover, $s'$ is obtained from $s$ deterministically, or in other words: for any two substrings of $T$, $s_1$ and $s_2$, if $s_1 = s_2$, then $s'_1 = s'_2$.*

This property is satisfied if a minimizer of $s$ is taken as $s'$. The idea of minimizers was proposed by Roberts et al. in 2004 [21] and seemingly first overlooked in the bioinformatics (or string matching) community, only to be revived in the last years (cf., e.g., [18,16,3,23]). The minimizer for a sequence $s$ of length $r$ is the lexicographically smallest of its all $(r-p+1)$ $p$-grams (or $p$-mers, in the term commonly used in computational biology); usually it is assumed that $p \ll r$. For a simple example, note that two DNA sequencing reads with a large overlap are likely to share the same minimizer, so they can be clustered together. That is, the smallest $p$-mer may be the identifier of the bucket into which the read is then dispatched.

Coming back to our algorithm: in the construction phase, we pass a sliding window of length $q$ over $T$ and calculate the lexicographically smallest substring
of length $p$ in each window (i.e., its minimizer). Ties are resolved in favor of the leftmost of the smallest substrings. The positions of minimizers are start positions of the sampled suffixes, which are then lexicographically sorted, like for a standard suffix array. The values of $q$ and $p$, $p \leq q$, are construction-time parameters.

In the actual construction, we build a standard suffix array and in extra pass over the sorted suffix indexes copy the sampled ones into a new array. This requires an extra bit array of size $n$ for storing the sampled suffixes and in total may take $O(n)$ time and $O(n)$ words of space. In theory, we can use one of two randomized algorithms by I et al. [14] which sort $n' = o(n)$ arbitrary suffixes of text of length $n$ either in $O(n')$ time using $O(n' \log n')$ words of space (Monte Carlo algorithm), or in $O(n \log n')$ time using $O(n')$ words of space (Las Vegas algorithm).

There is a small caveat: the minimizer at the new sampled position may be equal to the previous one, if only the window has been shifted beyond the position of its previous occurrence. The example illustrates. We set $q = 5$, $p = 1$ and the text is $T = \text{Once upon a time}$. In the first window (Once) the minimizer will be the blank space and it does not change until upon (including it), but the next window (upon) also has a blank space as its minimizer, yet it is a new string, in a different position. Both blank spaces are thus prefixes of the suffixes to sample.

The search is simple: in the prefix $P[1 \ldots q]$ of the pattern its minimizer is first found, at some position $1 \leq j \leq q - p + 1$, and then we binary search the pattern suffix $P[j \ldots m]$, verifying each tentative match with its truncated $(j - 1)$-symbol prefix in the text.

Note that any other pattern window $P[i \ldots i + q - 1]$, $2 \leq i \leq m - q + 1$, could be chosen to find its minimizer and continue the search over the sampled suffix array, but using no such window can result in a narrower range of suffixes to verify than the one obtained from the pattern prefix. This is because for any non-empty string $s$ with $occ_s$ occurrences in text $T$, we have $occ_x \geq occ_{xs}$, where $xs$ is the concatenation of a non-empty string $x$ and string $s$.

We call the described algorithm as the sampled suffix array with minimizers (SamSAMi).

### 2.2 Parameter selection

There are two free parameters in SamSAMi, the window length $q$ and the minimizer length $p$, $p \leq q$. Naturally, the case of $p = q$ is trivial (all suffixes sampled, i.e. the standard suffix array obtained). For a settled $p$ choosing a larger $q$ has a major benefit: the expected number of selected suffixes diminishes, which reduces the space for the structure. On the other hand, it has two disadvantages: $q$ is also the minimum pattern length, which excludes searches for shorter patterns, and for a given pattern length $m \geq q$ the average length of its sought suffix $P[j \ldots m]$ decreases, which implies more occurrence verifications.

For a settled $q$ the optimal choice of the minimizer length $p$ is not easy; too small value (e.g., 1) may result in frequent changes of the minimizer, especially...
for a small alphabet, but on the other hand its too large value has the same effect, since a minimizer can be unchanged over at most $p - q + 1$ successive windows. Yet, the pattern suffix to be sought has in the worst case exactly $p$ symbols, which may be a suggestion that $p$ should not be very small.

3 SamSAMi-hash

In [12] we showed how to augment the standard suffix array with a hash table, to start the binary search from a much more narrow interval. The start and end position in the suffix array for each range of suffixes having a common prefix of length $k$ was inserted into the hash table, where the key for which the hash function was calculated was the prefix string. The same function was applied to the pattern’s prefix and after a HT lookup the binary search was continued with reduced number of steps. The mechanism requires $m \geq k$. To estimate the space needed by the extra table, the reader is advised to look at Table 1 presenting the number of distinct $q$-grams in five 200 MB datasets from the popular Pizza & Chili text corpus. For example for the text english the number of distinct 8-grams is 20,782,043, which is about 10% of the text length. This needed to be multiplied by 16 in our implementation (open addressing with linear probing and 50% load factor and two 4-byte integers per entry), which results in about $1.6n$ bytes overhead.

| $q$ | dna | english | proteins | sources | xml |
|-----|-----|---------|----------|---------|-----|
| 1   | 16  | 225     | 25       | 230     | 96  |
| 2   | 152 | 10,829  | 607      | 9,525   | 7,054 |
| 3   | 683 | 102,666 | 11,607   | 253,831 | 141,783 |
| 4   | 2,222 | 589,230 | 224,132 | 1,719,387 | 908,131 |
| 5   | 5,892 | 2,150,525 | 3,623,281 | 5,252,826 | 2,716,438 |
| 6   | 12,804 | 5,566,993 | 36,525,895 | 10,669,627 | 5,555,190 |
| 7   | 28,473 | 11,599,445 | 94,488,651 | 17,826,241 | 8,957,209 |
| 8   | 80,397 | 20,782,043 | 112,880,347 | 26,325,724 | 12,534,152 |

Table 1. The number of distinct $q$-grams (1 . . . 8) in the datasets. Each dataset is of length 209,715,200 bytes.

We can adapt this idea to SamSAMi. Again, the hashed keys will be $k$-long prefixes, yet now each of the sampled suffixes starts with some minimizer (or its prefix). We can thus expect a smaller overhead. Its exact value for a particular dataset depends on three parameters, $k$, $q$ and $p$. Note however that now the pattern length $m$ must be at least $\max(q - p + k, q)$.  

4 Compressing the text

All SA-like indexes refer to the text, so to reduce the overall space we can compress it. It is possible to apply a standard solution to it, like Huffman or Hu–Tucker coding (where the idea of the latter is to preserve lexicographical order of the code and thus enable direct string comparisons between the compressed pattern and the compressed text), but in SamSAMi it is more convenient to compress the text with aid of minimizers. More precisely, we partition \( T[1 \ldots n] \) into phrases: \( T[1 \ldots j_1], T[j_1 + 1 \ldots j_2], \ldots, T[j_{n'} - 1 + 1 \ldots n] \), \( n' \leq n \), \( j_1 \geq 0 \), where each \( T[j_i + 1] \) location is a start position of a new minimizer, considering all \( q \)-long text windows moved from the beginning to the end of the text, for the chosen parameters \( q \) and \( p \). Note that \( n'/n \) is the compression ratio (between 0 and 1) of the suffix array sampling. The resulting sequence of phrases \( T'[1 \ldots n'] \) is then compressed with a byte code [2]. The dictionary of phrases \( D \) has to be stored too. We note that \( q \) shouldn’t be too large in this variant, otherwise the phrases will tend to have a single occurrence and the dictionary representation will be dominating in space use.

In this variant we assume that \( m \geq 2q - p + 1 \). Searching for the pattern proceeds as follows. First the minimizer in \( P[1 \ldots q] \) is found, at some position \( 1 \leq j_1 \leq q - p + 1 \). Then the minimizer in \( P[j_1 + 1 \ldots j_1 + q] \) is found, at some position \( j_1 + 1 \leq j_2 \leq j_2 + q - p + 1 \). This means that the pattern comprises the phrase \( P[j_1 \ldots j_2 - 1] \). This phrase is encoded with its codeword in \( D \). If \( P[j_2 \ldots m] \) comprises \( k \) extra phrases, \( k \geq 1 \), then all of them are also translated to their codewords from \( D \). The resulting concatenation of codewords for \( k + 1 \) phrases, spanning \( P[j_1 \ldots j_{k+1} - 1] \) in the pattern, is the artificial pattern \( P' \) to be binary searched in the suffix array with \( n' \) sampled suffixes. Still, all the suffixes in the range starting with the encoding of \( P' \) have to be verified, both with the pattern prefix (of length \( j_1 - 1 \)) and pattern suffix (of length \( m - j_{k+1} + 1 \)). Each candidate occurrence is verified with decoding its preceding phrase in the text and then performing a comparison on the prefix, and decoding its following phrase in text with an analogous comparison.

We note that the same text encoding can be used for online pattern search (cf. [10]).

5 Experimental results

So far, we have implemented only the basic SamSAMi index and compared it against SpaSA. All experiments were run on a laptop computer with an Intel i3 2.1 GHz CPU, equipped with 8 GB of DDR3 RAM and running Windows 7 Home Premium SP1 64-bit. All codes were written in C++ and compiled with Microsoft Visual Studio 2010.

We start with finding the fraction of sampled suffixes for multiple \((q, p)\) parameter pairs and the five 50 MB Pizza & Chili datasets. Table 2 presents the results.

Pattern searches were run for \( m \in \{10, 20, 50, 100\} \) and for each dataset and pattern length 500,000 randomly extracted patterns from the text were used.
|   |   | dna  |   |   |   |   |
|---|---|------|---|---|---|---|
| 4 | 1 | 46.1 | 39.7 | 40.5 | 46.1 | 45.8 |
| 4 | 2 | 55.2 | 51.0 | 51.0 | 55.8 | 54.1 |
| 5 | 1 | 40.9 | 32.3 | 34.0 | 38.8 | 39.3 |
| 5 | 2 | 44.9 | 39.9 | 40.8 | 46.2 | 45.9 |
| 6 | 1 | 37.6 | 27.7 | 29.4 | 34.5 | 32.5 |
| 6 | 2 | 38.0 | 32.3 | 34.1 | 38.8 | 39.3 |
| 8 | 1 | 33.7 | 22.1 | 23.2 | 28.3 | 22.0 |
| 8 | 2 | 29.5 | 23.8 | 25.5 | 30.5 | 26.6 |
| 10 | 1 | 31.8 | 19.3 | 19.4 | 25.0 | 17.1 |
| 10 | 2 | 24.5 | 18.5 | 20.5 | 25.9 | 18.5 |
| 10 | 3 | 25.8 | 20.8 | 22.7 | 27.9 | 21.9 |
| 12 | 1 | 30.7 | 17.9 | 16.8 | 22.5 | 13.7 |
| 12 | 2 | 21.2 | 15.4 | 17.1 | 22.8 | 15.1 |
| 12 | 3 | 21.4 | 16.8 | 18.6 | 24.2 | 17.0 |
| 16 | 1 | 29.7 | 16.4 | 13.7 | 19.3 | 11.0 |
| 16 | 2 | 17.1 | 12.0 | 12.9 | 18.6 | 11.3 |
| 16 | 3 | 16.1 | 12.6 | 13.7 | 19.4 | 11.9 |
| 24 | 2 | 13.3 | 8.4 | 8.7 | 13.6 | 7.1 |
| 24 | 3 | 11.1 | 8.7 | 9.0 | 13.9 | 7.4 |
| 32 | 2 | 11.7 | 6.5 | 6.6 | 10.6 | 5.1 |
| 32 | 3 | 8.7 | 6.7 | 6.7 | 10.6 | 5.4 |
| 40 | 2 | 10.8 | 5.3 | 5.3 | 8.5 | 4.2 |
| 40 | 3 | 7.3 | 5.4 | 5.3 | 8.4 | 4.3 |
| 64 | 2 | 9.8 | 2.9 | 3.4 | 4.7 | 3.1 |
| 64 | 3 | 5.4 | 3.0 | 3.3 | 4.4 | 2.6 |
| 64 | 4 | 4.4 | 3.1 | 3.4 | 4.3 | 2.7 |
| 80 | 2 | 9.6 | 1.9 | 2.7 | 3.5 | 2.9 |
| 80 | 3 | 4.8 | 1.8 | 2.7 | 3.1 | 2.2 |
| 80 | 4 | 3.7 | 1.9 | 2.7 | 3.0 | 2.2 |

**Table 2.** The percentage of suffixes that are sampled using the idea of minimizers with the parameters $q$ and $p$. 
Fig. 1. Pattern search time (count query). All times are averages over 500K random patterns of length 10. The patterns were extracted from the respective texts. Times are given in microseconds. The index space is a multiple of the text size, including the text.
Fig. 2. Pattern search time (count query). All times are averages over 500K random patterns of length 20. The patterns were extracted from the respective texts. Times are given in microseconds. The index space is a multiple of the text size, including the text.
Fig. 3. Pattern search time (count query). All times are averages over 500K random patterns of length 50. The patterns were extracted from the respective texts. Times are given in microseconds. The index space is a multiple of the text size, including the text.
Fig. 4. Pattern search time (count query). All times are averages over 500K random patterns of length 100. The patterns were extracted from the respective texts. Times are given in microseconds. The index space is a multiple of the text size, including the text.
Figs 1–4 present average search times with respect to varying parameters. For SpaSA we changed its parameter $k$ from 1 (which corresponds to the plain suffix array) to 8. For SamSAMi we varied $q$ from \{4, 5, 6, 8, 10, 12, 16, 24, 32, 40, 64, 80\} setting the most appropriate $p$ (up to 3 or 4) to obtain the smallest index, according to the statistics from Table 2. Obviously, $q$ was limited for $m < 100$; up to 6 for $m = 10$, up to 16 for $m = 20$, and up to 40 for $m = 50$.

We note that SamSAMi is rather competitive against the sparse suffix array, with two exceptions: short patterns ($m = 10$) and the XML dataset (for $m = 10$ and $m = 20$). We have not yet directly compared our algorithm against the sampled SA by Claude et al., however the results suggest that SamSAMi is more robust when aggressive suffix sampling is applied. (For a honest comparison one should also notice that our implementation uses 32-bit suffix indexes while the Claude et al. scheme was tested with $\lceil \log_2 n \rceil$ bits per index; which is 26 bits for the used datasets.)

6 Conclusions and future work

We presented a simple suffix sampling scheme making it possible to search for patterns effectively. The resulting data structure, called a sampled suffix array with minimizers (SamSAMi), achieves interesting time-space tradeoffs; for example, on English50 dataset the search for patterns of length 50 is still by about 10% faster than with a plain suffix array when only 5.3% of the suffixes are retained.

Apart from extra experiments, several aspects of our ideas require further research. We mentioned a theoretical solution for building our sampled suffix array in small space can be applied, but it is an interesting question if we can make use of our parsing properties to obtain $O(n)$ time and $O(n')$ space in the worst case. Such complexities are possible for the suffix array on $n'$ words, as shown by Ferragina and Fischer [8], and their idea can easily be used for the sampled SA by Claude et al. [4] as noted in the cited work.

How to find minimizers efficiently, both in a static sequence (i.e., a pattern prefix) and a sliding window, is also of some interest. Naïve implementations result in $O(pq)$ and $O(npq)$ times, respectively, but with a heap the latter can be reduced to $O(np \log q)$. One solution to get rid of the factor $q$ can be to use the Rabin-Karp rolling hash [5] Sect. 32.2 over the substrings of length $p$ and find the minimum hash value rather than the lexicographically lowest substring. Also, a heap may be replaced with a trie storing the $p$-grams. Assuming constant-time parent-child navigation over the trie (i.e., also a small enough alphabet), we update the trie for one shift of the window in $O(p)$ time (as one $p$-gram is removed, one $p$-gram is added, and the minimizer is the leftmost string in the trie), which results in $O(np)$ overall time.

A practical question concerns speeding up the pattern search when many verifications are needed (cf. the XML dataset). We are currently checking some possibilities.
Acknowledgement

We thank Kimmo Fredriksson for helpful comments. The work was supported by the Polish Ministry of Science and Higher Education under the project DEC-2013/09/B/ST6/03117 (both authors).

References

1. S. Alstrup, G. S. Brodal, and T. Rauhe. Pattern matching in dynamic texts. In Proceedings of the 11th Annual Symposium on Discrete Algorithms (SODA), pages 819–828. Society for Industrial and Applied Mathematics, 2000.
2. N. Brisaboa, A. Fariña, G. Navarro, and J. Paramá. Lightweight natural language text compression. Information Retrieval, 10:1–33, 2007.
3. R. Chikhi, A. Limasset, S. Jackman, J. Simpson, and P. Medvedev. On the representation of de Bruijn graphs. arXiv preprint arXiv:1401.5383, 2014.
4. F. Claude, G. Navarro, H. Peltola, L. Salmela, and J. Tarhio. String matching with alphabet sampling. Journal of Discrete Algorithms (JDA), 11:37–50, 2012.
5. T. H. Cormen, C. E. Leiserson, R. L. Rivest, and C. Stein. Introduction to Algorithms (3. ed.). MIT Press, 2009.
6. P. Crescenzi, A. D. Lungo, R. Grossi, E. Lodi, L. Pagli, and G. Rossi. Text sparsification via local maxima. In Proceedings of the 20th Conference on the Foundations of Software Technology and Theoretical Computer Science (FSTTCS), volume 1974 of LNCS, pages 290–301. Springer, 2000.
7. P. Crescenzi, A. D. Lungo, R. Grossi, E. Lodi, L. Pagli, and G. Rossi. Text sparsification via local maxima. Theoretical Computer Science, 1–3(304):341–364, 2003.
8. P. Ferragina and J. Fischer. Suffix arrays on words. In CPM, volume 4580 of LNCS, pages 328–339. Springer–Verlag, 2007.
9. P. Ferragina, R. Gonzalez, G. Navarro, and R. Venturini. Compressed text indexes: From theory to practice. ACM Journal of Experimental Algorithmics (JEA), 13:article 12, 2009. 30 pages.
10. K. Fredriksson and S. Grabowski. A general compression algorithm that supports fast searching. Information Processing Letters, 100(6):226–232, 2006.
11. S. Gog and M. Petri. Optimized succinct data structures for massive data. Software–Practice and Experience, 2013. DOI: 10.1002/spe.2198.
12. S. Grabowski and M. Rakiszewski. Two simple full-text indexes based on the suffix array. CoRR, abs/1405.5919, 2014.
13. T. C. Hu and A. C. Tucker. Optimal computer search trees and variable-length alphabetical codes. SIAM Journal on Applied Mathematics, 21(4):514–532, 1971.
14. T. I. J. Kärkkäinen, and D. Kempa. Faster sparse suffix sorting. In STACS, volume 25 of LIPIcs, pages 386–396. Schloss Dagstuhl - Leibniz-Zentrum fuer Informatik, 2014.
15. J. Kärkkäinen and E. Ukkonen. Sparse suffix trees. In COCOON, volume 1090 of LNCS, pages 219–230, 1996.
16. Y. Li, P. Kamousi, F. Han, S. Yang, X. Yan, and S. Suri. Memory efficient minimum substring partitioning. In Proceedings of the 39th International Conference on Very Large Data Bases, pages 169–180. VLDB Endowment, 2013.
17. K. Mehlhorn, R. Sundar, and C. Uhrig. Maintaining dynamic sequences under equality tests in polylogarithmic time. Algorithmica, 17(2):183–198, 1997.
18. N. S. Movahedi, E. Forouzmand, and H. Chitsaz. De novo co-assembly of bacterial genomes from multiple single cells. In BIBM, pages 1–5, 2012.
19. G. Navarro and V. Mäkinen. Compressed full-text indexes. ACM Comput. Surv., 39(1):article 2, 2007.
20. S. J. Puglisi, W. F. Smyth, and A. Turpin. Inverted files versus suffix arrays for locating patterns in primary memory. In SPIRE, volume 4209 of LNCS, pages 122–133, 2006.
21. M. Roberts, W. Hayes, B. R. Hunt, S. M. Mount, and J. A. Yorke. Reducing storage requirements for biological sequence comparison. Bioinformatics, 20(18):3363–3369, 2004.
22. S. C. Sahinalp and U. Vishkin. Symmetry breaking for suffix tree construction. In Proceedings of the 26th Annual ACM Symposium on Theory of Computing (STOC), pages 300–309. ACM, 1994.
23. D. E. Wood and S. L. Salzberg. Kraken: ultrafast metagenomic sequence classification using exact alignments. Genome Biology, 15(3):R46, 2014.