Handling Weighted Sequences Employing Inverted Files and Suffix Trees

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Abstract: In this paper, we address the problem of handling weighted sequences. This is by taking advantage of the inverted files machinery and targeting text processing applications, where the involved documents cannot be separated into words (such as texts representing biological sequences) or word separation is difficult and involves extra linguistic knowledge (texts in Asian languages). Besides providing a handling of weighted sequences using n-grams, we also provide a study of constructing space efficient n-gram inverted indexes. The proposed techniques combine classic straightforward n-gram indexing, with the recently proposed two-level n-gram inverted file technique. The final outcomes are new data structures for n-gram indexing, which perform better in terms of space consumption than the existing ones. Our experimental results are encouraging and depict that these techniques can surely handle n-gram indexes more space efficiently than already existing methods.

1 INTRODUCTION

In this paper we focus on handling weighted sequences (Makris and Theodoridis, 2011). The difference between weighted sequences and regular strings is that in the former, we permit in each position the appearance of more than one character, each with a certain probability (Makris and Theodoridis, 2011). Specifically, a weighted word \( w = w_1w_2\cdots w_n \) is a sequence of positions, where each position \( w_i \) consists of a set of couples; each couple has the form \((s, \pi_i(s))\), where \( \pi_i(s) \) is the probability of having the character \( s \) at position \( i \). Also, for every position \( w_i, 1 \leq i \leq n \), \( \sum \pi_i(s) = 1 \). Moreover, it is usually assumed that a possible subword is worth the effort to be examined if the probability of its existence is larger than \( 1/k \); with \( k \) being a user defined parameter. In order to handle weighted sequences the Weighted Suffix Tree data structure was implemented (Iliopoulos et al., 2006). We consider this specific data structure as a proper suffix tree generalization.

The novelty in our approach is that for the first time, we exploit inverted files and n-grams in the handling of weighted sequences, thus providing an interesting alternative to weighted suffix trees for a variety of applications that involve weighted sequences. Our approach is interesting since it offers interesting alternatives to approaches using suffix arrays and suffix trees with inverted files. This lacked in the bibliography in contrast to traditional pattern search applications such as in search engines where both alternatives were offered (see for example (Puglisi et al., 2006)). We do not delve into details of various pattern matching operations but merely focus on how to space efficiently transform weighted sequences into normal and then handle them using the well known technique of n-grams. Our target is not only at biological, but also at natural language applications. n-grams are sequences of consecutive text elements (either words or symbols); they are widely used in Information Retrieval (Ogawa and Iwasaki, 1995), (Lee and Ahn, 1996), (Navarro and Baeza-Yates, 1998), (Millar et al., 2000), (Navarro et al., 2000), (Navarro et al., 2001), (Gao et al., 2002), (Mayfield and McNamie, 2003), (Kim et al., 2007), (Yang et al., 2007), especially in applications employing text that cannot be separated into words.

The indexes produced with the n-gram inverted index technique, have a number of advantages. One of them is that they work on any kind of sequences, even if the sequence consists of words which have no practical meaning, such as DNA and protein sequences. Moreover, the n-gram technique is language neutral since it can be applied on different languages. Ano-
other major benefit is that this indexing method is error-tolerant, putting up with errors that occur during the construction of the index; this is as it uses for its construction, the 1-sliding technique.

Nevertheless, the \( n \)-gram inverted index has also some drawbacks; the size tends to be very large and the performance of queries tends to be inefficient. This is the reason why a wide amount of research on how to use this technique space efficiently has been performed (Kim et al., 2005), (du Mouza et al., 2009), (Tang et al., 2009).

In (Kim et al., 2005), an efficient method for constructing a two-level index is proposed. Specifically, this method reduces significantly the size of the index and improves the query performance when comparing to the straightforward \( n \)-gram inverted index technique; while preserving all the advantages of the \( n \)-gram inverted index. This technique extracts substrings of fixed length \( m \) from the original sequence and then applies the classic \( n \)-gram technique on each of those extracted substrings. As shown in (Kim et al., 2005), this technique can provide significant space improvements, but as it can be observed in our experimental results, when the original sequence is not enough repetitive, the performance of this two-level indexing technique deteriorates.

In detail, we propose three new techniques for handling weighted sequences using \( n \)-grams indexing. We additionally propose a new framework for space compaction aiming to face the aforementioned space shortcomings of (Kim et al., 2005). In our space efficient framework, instead of resorting to the two-level indexing scheme, we judiciously select a set of substrings of the initial sequences for the \( n \)-grams of which, we employ the two-level indexing scheme; while for the rest of them, we employ the straightforward one-level indexing scheme. The substrings are selected based on the frequency of their appearance in the whole document set. Also, the length of substrings covering the initial sequence as well as the two distinct variants of the algorithmic scheme (variant for selecting these substrings employing a forest of suffix trees and a variant for the generalized suffix tree) are implemented and tested. It should be noted that these generalized suffix trees are the weighted suffix trees derived from the initial set of weighted sequences.

What is more, experiments on both synthetic and real data are performed in order to validate the performance of our constructions and the space reduction that they offer. Our work can be considered both an experimental research for the weighted sequences as well as a survey for validating the space efficiency of newly and previously proposed constructions in the area of \( n \)-gram indexing.

The rest of the paper is organized as follows. In section 2, the related work as well as the contribution is presented. In section 3, we present the techniques for handling weighted sequences. Subsequently, in section 4, we describe our space compaction heuristics. In following, section 5 presents a reference to our experimental results. Finally, section 6 concludes the paper and provides future steps and open problems.

2 RELATED WORK AND CONTRIBUTION

In (Christodoulakis et al., 2006), a set of efficient algorithms for string problems, involving weighted sequences arising in the computational biology area, were presented adapting traditional pattern matching techniques to the weighted scenario. What is more, in order to approximately match a pattern in a weighted sequence, a method was presented in (Amir et al., 2006) for the multiplicative model of probability estimation. In particular, two different definitions for the Hamming as well as for the edit distance, in weighted sequences, were given. Furthermore, we should refer to some more recent techniques (Zhang et al., 2010a), (Zhang et al., 2010b), (Alatabbi et al., 2012), that besides extending previous approaches, they also employ the Equivalence Class Tree for the problem at hand. From these papers, special mentioning deserves the work in (Zhang et al., 2010a), which generalizes the approach in (Iliopoulos et al., 2006), so as to handle effectively various approximate and exact pattern matching problems in weighted sequences.

In addition, there is a connection with the probabilistic suffix tree, which is basically a stochastic model that employs a suffix tree as its index structure. This connection aims to represent compactly the conditional distribution of probabilities for a set of sequences. Each node of the corresponding probabilistic suffix tree is associated with a probability vector that stores the probability distribution for the next symbol given the label of the node as the preceding segment (Marsan and Sagot, 2000), (Sun et al., 2004).

In our work, we will mainly employ the preprocessing techniques presented in (Iliopoulos et al., 2006), where an efficient data structure for computing string regularities in weighted sequences was presented; this data structure is called Weighted Suffix Tree. Our approach however can be also modified to incorporate the techniques presented in (Zhang et al., 2010a).

The main motivation for handling weighted sequences comes from Computational Molecular Bio-
However, there are possible applications in Cryptanalysis and musical texts (see for a discussion but in this time for the related area of Indeterminate Strings, which are strings having in positions, sets of symbols, (Holub and Smyth, 2003), (Holub et al., 2008)). In Cryptanalysis, undecoded symbols may be modeled as a set of letters with several probabilities, while in music, single notes may match chords or notes with several probabilities. In addition, our representation of n-grams and our space compaction heuristics are of general nature concerning the efficient handling of multilingual documents in web search engines and general in information retrieval applications.

Character n-grams are used especially in CJK (Chinese, Japanese and Korean) languages, which by nature cannot be easily separated into words. In these languages, 2-gram indexing seems to work well. For example in (Manning et al., 2008), it is mentioned that in these languages, the characters are more like syllables than letters and that most words are small in numbers of characters; also, the word boundaries are small and in these cases, it is better to use n-grams. Moreover, n-grams are helpful in Optical Character Recognition where the text is difficult to comprehend and it is not possible to introduce word breaks. Additionally, k-grams are useful in applications such as wildcard queries and spelling correction.

3 ALGORITHMS

We initially describe the n-gram based techniques for handling normal sequences, which are being presented in (Kim et al., 2005). Then we explain how these can be adapted so that we can handle weighted sequences. The algorithm proposed in (Kim et al., 2005) tries to improve the straightforward inverted file scheme that produces n-grams on the fly using a sliding window; afterwards the algorithm stores them in an inverted file by replacing it with a two-level scheme, which is shown to be more space efficient.

In particular, this novel two-level scheme is based on the following approach: (i) each of the initial sequences is processed and a set of substrings of length \(m\) is extracted so as to overlap with each other by \(n - 1\) symbols, (ii) an inverted index (called back-end index) for these substrings as well as the initial sequence set, considering the substrings as distinct words, are built, (iii) all the n-grams in each of the substrings are extracted, (iv) an inverted index (called front-index) is built, regarding the substrings as documents and the n-grams as words. This scheme, called by its authors n-gram/2L-v, can be applied to any text and in some cases, results to significant space reduction.

If the text can be partitioned into words (natural language text), another scheme termed n-gram/2L-v is provided. So, the subsequences are defined as consecutive sequences of the text words, by exploiting the intuitive remark that words exhibit repetitiveness in natural language text. Their experiments show that when applied to natural text n-gram/2L-v, sample space savings, compared to the initial technique, are produced.

We attempt to adapt their techniques by presenting three algorithms for handling weighted sequences, which are based in the exploitation of the technique presented in (Kim et al., 2005); then we can adjust them to the problem at hand.

3.1 1st Technique - Subsequences Identification

In the first technique, we form separate sequences as we split each weighted sequence into weighted substrings; each one of length \(m\). Each one of these weighted substrings is used to produce normal substrings by employing the normal substrings generation phase of (Iliopoulos et al., 2006) (p.267, algorithm 2). In this phase, the generation of a substring stops when its cumulative possibility has reached the \(1/k\) threshold. The cumulative possibility is calculated by multiplying the relative probabilities of appearance of each character in every position. Each produced substring is of maximum size \(m\) and for every substring, we produce all the possible n-grams. After this procedure, we store all the produced n-grams in the n-gram/2L-v scheme.

Concerning the generation phase, all the positions in the weighted sequences are thoroughly scanned and at each branching position, a list of possible substrings, starting from this position, is created. Then moving from left to right, the current subwords are extended by adding the same single character whenever a non-branching position is encountered; in contrast there is also a creation of new subwords at branching positions where potentially many choices are supplied.

3.2 2nd Technique - On the fly n-grams Identification

This technique is much simpler as we don’t need to deploy all the generic sequences. Unlike the previous technique, we just need to produce all the possible n-grams and in following for each report, its corresponding weighted sequences as well as their offsets.
As a matter of fact, we don’t have to form separate sequences, as in the previous approach, but instead only split each generalized sequence into segments, each of size m, and for each segment, just produce the requested n-grams.

Hence, this particular scheme is by nature one-level and we propose its use due its simplicity. However, as it will be highlighted in the experiments, there are cases when the technique outperforms the previous one in terms of space complexity.

4 SPACE EFFICIENT INVERTED FILE IMPLEMENTATIONS FOR NORMAL SEQUENCES

Our crucial remark is that, in order for the n-gram/2L technique to provide space savings, the substrings, where the initial sequences are separated, should appear a large number of times and should cover a broad extent of the initial sequences, otherwise in case this does not apply (e.g. if there is a large number of unique substrings), then the space occupancy turns out to increase instead of shrinking.

Hence, it would be preferable to use a hybrid scheme instead of a two-level one; there we should extract from the initial sequences, substrings that appear repetitively enough and cover a large extent of the initial sequences. In following, for the specific substrings, we will employ a two-level scheme; while for the remaining parts of the sequences, we will use the straightforward one-level representation. During this separation, we elongate each selected substring by n-1, as in (Kim et al., 2005).

So, as to achieve our goal and build a hybrid one and two-level inverted index, we introduce three techniques:

4.1 One Simple Technique

A variant of the algorithm described in (Kim et al., 2005), called Hybrid indexing Algorithm version 0 - hybrid(0), is implemented. In this implementation, we decided to store the substrings of length m and of a number of occurrences in the back-end inverted file of the two-level scheme; provided that this number is greater than a trigger. The user is asked to provide the value of the trigger; the trigger is set equal to 1, for the results presented in the corresponding section.

The substrings, occurring less or equal to the provided trigger, are just decomposed in their n-grams and then saved in a one-level index. The substrings stored in the two-level scheme, are also decomposed in their n-grams, which we forward to the front-end index of the two-level scheme.

4.2 Two Techniques based on Suffix Trees

In these techniques, we locate substrings that (in contrast to hybrid(0)) can be of varying size, highly repetitive and cover a large extent of the initial sequences. So as to locate them, we employ suffix trees (McCreight, 1976) that have been previously used in similar problems (Gusfield, 1997) of locating frequent substrings. In particular, we provide two different variants in the implementation of our space efficient heuristic schema. Those two distinct versions share a common initial phase, while differing in their subsequent workings.

More analytically, we insert all the sequences in a generalized suffix tree as described in (Gusfield, 1997) and in following we use this tree for counting the repetitions of each substring of the stored documents. Note that if the sequences have been produced by using mappings from weighted sequences, then the produced suffix tree is similar to the weighted suffix tree of the initial sequences. This operation is performed during the building of the generalized suffix tree; after that, each node of the tree keeps the information concerning the repetitions of the substrings stored in it.

Subsequently, in each repetition, our algorithm chooses a substring and a subset of each occurrence. These two objects are in following included in the two-level index. The selection procedure is described as follows:

1. The substring needs to have a length equal or greater than s; s is the least acceptable length of a substring and constitutes a user defined parameter at the start of the algorithm’s execution.
2. The substring has to be highly repetitive. This means that it should have more than a specific number of occurrences (trigger) in the set of indexed documents; this trigger is also a user defined parameter.
3. The appearances of the selected substring, which are to be included in the two-level index, should not overlap in more than half the length of the subsequence; i.e. if the substring has a length of 10 characters, consecutive appearances of this substring should not overlap on more than 5 characters. By setting this criterion, we keep only the discrete appearances of the selected substring.

After the end of the procedure, we have selected a collection of substrings. We then sort this collection
based on the total length of the original sequences that
the distinct occurrences cover (according to criterion
3). Furthermore, we select as best the occurrences
of specific subsequence that cover the majority of the
length of the initial sequences. We extract all these
substrings from the initial sequences, thus including
them in the two-level index. As a result, we have split
the initial sequences into a set of partitions that are
not included in the two-level index. Next, we elongate
them by $n - 1$, so as not to miss any $n$-gram; where $n$
is the $n$-gram length. Finally, we keep all these elon-
gated substrings in a list. As a result, we have per-
fomed the preprocessing step that allows us to follow
one out of two methods described below (see the pro-
cedure in Fig. 1):

(i) **Hybrid Indexing Algorithm version 1 - hybrid(1)**. We construct for each elongated substring,
a separate suffix tree and process best utilizing the
same method as above. Then, our algorithm continues
executing the process for each suffix tree constructed
as cited above. This process is repeated as many times
as the user chooses at the beginning of the algorithm
execution.

(ii) **Hybrid Indexing Algorithm version 2 - hybrid(2)**. We include all elongated substrings men-
tioned in a unified generalized suffix tree. In follow-
ing, our algorithm executes the process for the gen-
eralized suffix tree constructed. This process is re-
peated as many times as requested. Generally, the
more recursions we made, the better results we had;
however, because of the limited system resources, we
opted for 50 recursions in our experiments.

5 EXPERIMENTS

5.1 Experimental Setting

In our experiments, we used random weighted se-
quencies to test our $n$-gram mapping techniques as
well as one file (of size 1 GB) containing Protein data
and DNA data to test our space compaction heuris-
tics. We also performed experiments with 10MB and
100MB with similar results. Due to lack of space,
only figures and comments from the 1GB data are pre-
sented in the main body of the article. Our experi men-
tal data were downloaded from the NCBI databases
(ftp://ftp.ncbi.nih.gov/genomes/). Furthermore, we
use initials to designate both $m$ (length of substrings)
as well as the parameters $s$ (size in bytes) in our space
compaction heuristics.

The computer system, where the experiments
were performed, was an Intel Core i5-2410M 2.3
GHz CPU with a 3GB (1x1GB and 1x2GB in 2xDual
Channel) RAM. The techniques we implemented and
applied on the experimental data mentioned above,
were:

1. Weighted Sequences Identification:
   (i) Subsequences Identification,
   (ii) On the fly $n$-grams Identification and
   (iii) Offline Identification.

2. Space compaction heuristics:
   (i) One-Level Inverted File (using the classic
       straightforward technique),
   (ii) Two-Level Inverted File (using the technique
       in (Kim et al., 2005)),
   (iii) Hybrid Inverted File using the Simple Tech-
       nique - hybrid(0),
   (iv) Hybrid Inverted File with separate suffix trees
       - hybrid(1) and
   (v) Hybrid Inverted File with a unified generalized
       suffix tree - hybrid(2).

For our space compaction heuristics, we run all
techniques proposed in this paper (hybrid(0), hy-
brid(1) and hybrid(2)) in order to identify the most
space efficient solution available. So as to depict the
space compaction effectiveness of our approach, we
tried our approach on real data of significant size and
performed several experiments. As the experiments
show, our approach outstandingly reduces the space
complexity and stands by itself as a considerable im-
provement.

5.2 Weighted Sequences Results

As is depicted in Fig. 2, the offline approach is the
worst in the attained space complexity, as expected.
The reason is because all possible combinations of sequences are produced; not only those that are needed by the two-level scheme. On the other hand, the offline approach is more flexible since it can incorporate different values of variables $n$ and $s$.

Figure 2: Weighted Sequences 10MB for varying size of $s$ (a) $n=2$, (b) $n=3$ and (c) $n=4$.

With regards to the other two techniques, the on the fly approach is the most robust and stable in performance due to its fixed algorithmic behavior when handling every possible input. The identification of the subsequences, although better for small values of $s$, behaves worse for larger values. This can be attributed to the shortage of repetitions; being a vital ingredient of the success of this method’s heuristic, when the value of $s$ is increasing.

5.3 Protein Data Results

In the performed experiments, we never needed to make more than 50 recursions, as by this number we got the best possible results from the index method. Moreover, we ran experiments of substrings that have length from 4 to 10, in order to demonstrate the improvements that the two-level technique produces to the inverted file size.

Our hybrid(2) technique seems to be not as efficient as hybrid(1) is. Although, it theoretically considers the high repetitive sequence more efficiently than the hybrid(1) technique, it does not seem to have satisfactory results. A probable explanation could be that using separate suffix trees, this method permits more choices in the sequences that will be selected for separate indexing than the Generalized suffix tree; the latter demands the selection of the same substring across different substrings. Furthermore, the technique is sensitive to the number of performed recursions and needs a vast number of them to work effectively.

Figure 3: Protein Data 1GB for varying size of $s$ (a) $n=2$, (b) $n=3$ and (c) $n=4$.

Another finding is that hybrid(0) technique is quite similar to the two-level technique for substrings with length 4 and 5 and after that, it is not as efficient as our hybrid(1) technique. This behavior can be explained from the fact that this technique always takes advantage of the positive characteristics of the two-level techniques as long as it is better than one-level; otherwise it resorts to the one-level.

Generally, in Protein data, our methods achieve better results due to the fact that they take advantage of the repetitiveness of the initial sequence even when the number of the repetitions is quite low. This is something that does not hold for the two-level scheme, where the performance is clearly degraded.

5.4 DNA Data Results

In the results shown below, the maximum number of recursions made, was fixed to 50 for each experiment.
In case of DNA data, we experimented for substrings that have length from 4 to 13. We examined more substring sizes so as to clarify the inefficiency of the two-level technique when the repetitiveness becomes lower. It is obvious that the two-level technique increases the inverted file size produced, when the substring length becomes larger than 11.

Analyzing the results presented in figure with DNA data results, we can patently see that our hybrid(1) technique is not as efficient as the two-level index. The reason for this inefficiency is that two-level index takes advantage of the substrings of length from 6 to 11, which seems to be highly repetitive in the DNA sequences examined. As soon as the size of the substring becomes lower than 6 or larger than 11, our method becomes obviously better. This occurs because the DNA data file used, is not so highly repetitive for subsequences of length <6 or >11.

In cases when two-level technique performs better than hybrid(1), we use hybrid(0) to store our data. Hybrid(0) performs very similarly to two-level technique. The differences between the files produced by those two techniques are considered to be negligible. The reason why this phenomenon appears is due to the highly repetitive nature of DNA data (the limited alphabet) on limited size sequences.

As for our hybrid(2) method, we can clearly see that this method seems to be inefficient, and works worse than hybrid(1); this was something that was also noted in Protein data and can be explained in a similar way as previously mentioned. Perhaps a better tuning of the involved algorithmic parameters and a combination with hybrid(1) would result in a more efficient scheme; but this is left as future work.

By choosing hybrid(0) or hybrid(1) techniques to save the DNA data in inverted indexes, we are led to very compact inverted file sizes. These sizes generally outperform or at least approximate the two-level index efficacy.

In conclusion, our experiments clearly prove that our techniques can significantly reduce space complexity by handling n-gram indexes and can also stand as considerable improvements.

6 GENERAL CONCLUSIONS AND FUTURE WORK

In this article we presented a set of algorithmic techniques for efficiently handling weighted sequences by using inverted files. Also, these methods deal effectively with weighted sequences using the n-gram machinery. Three techniques, which act as alternatives to other techniques that mainly use suffix trees, were presented. We furthermore completed our discussion by presenting a general framework that can be employed so as to reduce the space complexity of the two-level inverted files for n-grams.

In the future, we intend to experiment with various inverted file intersection algorithms (Culpepper and Moffat, 2010), in order to test the time efficiency of our scheme when handling such queries. We could perhaps incorporate some extra data structures as those in (Kaporis et al., 2003) as a well thought out plan. Last but not least, we also plan to apply our technique to natural language texts.

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