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 $\verb|https://hdl.handle.net/2324/3033|$

出版情報: DOI Technical Report. 175, 2000-06. Department of Informatics, Kyushu University

バージョン: 権利関係:

DOI Technical Report

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June 2000



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Abstract

Given two sets of strings, consider the problem to find a subsequence that is common to one set but never appears in the other set. The problem is known to be NP-complete. We generalize the problem to an optimization problem, and give a practical algorithm to solve it exactly. Our algorithm uses pruning heuristic and subsequence automata, and can find the best subsequence. We show some preliminary experiments, that convinced us that the approach is quite promising.

1 Introduction

String is one of the most fundamental structure to express and reserve information. In these days, a lot of string data are available. String processing has vast application area, such as Genome Informatics and Internet related works. It is quite important to discover useful rules from large text data or sequential data [1, 6, 9, 22]. Finding a good rule to separate two given sets, often referred as *positive examples* and *negative examples*, is a critical task in Discovery Science as well as Machine Learning.

Shimozono et al. [20] developed a machine discovery system that produces a decision tree over regular patterns with alphabet indexing, from given positive set and negative set of strings. The core part of the system is to generate a decision tree which classifies positive examples and negative examples as correctly as possible. For that purpose, we have to find a pattern that maximizes the goodness according to the entropy information gain measure, recursively at each node of trees. In the current implementation, a pattern associated with each node is restricted to a substring pattern, due to the limit of computation time. One of our motivations of this study is to extend the BONSAI system to allow subsequence patterns as well as substring patterns at nodes, and accelerate the computation time.

However, there is a large gap between the complexity of finding the best *substring* pattern and *subsequence* pattern. Theoretically, the former problem can be solved in linear time, while the latter is NP-hard.

In this paper, we propose a practical algorithm to find the best subsequence pattern which separates a given set of strings from the other set of strings. Since the problem is NP-hard, essentially we are forced to examine exponentially many candidate patterns in the worst case. Basically, for each pattern w, we have to count the number of strings that contain w as a subsequence in each of two sets. We call the task of counting the numbers as answering subsequence query. The computational cost to find the best subsequence pattern mainly comes from the total amount of time to answer these subsequence queries, since it is relatively heavy task if the sets are large, and many queries will be needed. In order to reduce the time, we have to either (1) asking queries as few as possible, or (2) speeding up to answer queries. We attack the problem from both these two directions.

At first, we reduce the search space by appropriately pruning redundant branches that are guaranteed not to contain the best pattern. We use a heuristics inspired by Morishita and Sese [18], combined with some properties on the subsequence languages.

Next, we accelerate answering for subsequence queries. Since the sets of strings are fixed in finding the best subsequence pattern, it is reasonable to preprocess the sets so that answering subsequence query for any pattern will be fast. We take an approach based on a deterministic finite automaton that accepts all subsequences of a string. Actually, we use subsequence automata for sets of strings, developed in [11]. Subsequence automaton can answer quickly for subsequence query, at the cost of preprocessing time and space requirement to construct it.

Since these two approaches are different in their aims, we expect that a balanced integration of these two would result in the most efficient way to find the best subsequence patterns. In order to verify the performance of our algorithm, we are performing some experiments on these two approaches. We report some preliminary results of the experiments, that convinced us it is quite promising.

2 Preliminaries

Let Σ be a finite alphabet, and let Σ^* be the set of all strings over Σ . For a string w, we denote by |w| the length of w, and for a set S, we denote by |S| the cardinality of S. We say that a string v is a prefix (substring, suffix, resp.) of w if w = vy (w = xvy, w = xv, resp.) for some strings $x, y \in \Sigma^*$. We say that a string v is a subsequence of a string w if v can be obtained by removing zero or more characters from w, and say that w is a supersequence of v. We denote by $v \preceq_{\text{seq}} w$ that v is a substring of w, and by $v \preceq_{\text{seq}} w$ that v is a subsequence of w. For a string v, we define the substring

language $L^{\text{str}}(v)$ and subsequence language $L^{\text{seq}}(v)$ as follows:

$$L^{\text{str}}(v) = \{w \in \Sigma^* \mid v \leq_{\text{str}} w\}, \text{ and }$$

 $L^{\text{seq}}(v) = \{w \in \Sigma^* \mid v \leq_{\text{seq}} w\}, \text{ respectively.}$

The following lemma is obvious from the definitions.

Lemma 1 For any strings $v, w \in \Sigma^*$,

- 1. if v is a prefix of w, then $v \leq_{str} w$,
- 2. if v is a suffix of w, then $v \leq_{str} w$,
- 3. if $v \leq_{str} w$ then $v \leq_{seq} w$,
- 4. $v \leq_{str} w$ if and only if $L^{str}(v) \supseteq L^{str}(w)$,
- 5. $v \leq_{seq} w$ if and only if $L^{seq}(v) \supseteq L^{seq}(w)$.

3 Formulation of the Problem

Let good be a function from $\Sigma^* \times 2^{\Sigma^*} \times 2^{\Sigma^*}$ to the set of real numbers. We formulate the problem to be solved as follows.

Definition 1 (Finding the best pattern according to good) Input Two sets $S, T \subseteq \Sigma^*$ of strings.

Output A string $w \in \Sigma^*$ that maximizes the value good(w, S, T).

Intuitively, the value good(w, S, T) expresses the goodness to distinguish S from T using the rule specified by a string w. The definition of good varies for each application. For examples, the χ^2 values, entropy information gain, and gini index are frequently used (See [18]). Essentially, these statistical measures are defined by the numbers of strings that satisfy the rule specified by w. In this paper, we only consider the rules defined as substring languages and subsequence languages. We call these problems as finding best substring pattern, and finding best subsequence pattern, respectively. Let L be either L^{str} or L^{seq} . Then any of the above examples of the measures can be described in the following form.

$$good(w, S, T) = f(x_w, y_w, |S|, |T|), \text{ where}$$

$$x_w = |S \cap L(w)|,$$

$$y_w = |T \cap L(w)|.$$

For example, the entropy information gain, which is introduced by Quinlan [19] and also used in BONSAI system [20], can be defined in terms of the function f as follows:

$$f(x, y, x_{\text{max}}, y_{\text{max}}) = -\frac{x + y}{x_{\text{max}} + y_{\text{max}}} I(x, y) - \frac{x_{\text{max}} - x + y_{\text{max}} - y}{x_{\text{max}} + y_{\text{max}}} I(x_{\text{max}} - x, y_{\text{max}} - y),$$
where $I(s, t) = \begin{cases} 0 & \text{(if } s = 0 \text{ or } t = 0), \\ -\frac{s}{s + t} \log \frac{s}{s + t} - \frac{t}{s + t} \log \frac{t}{s + t} & \text{(otherwise)}. \end{cases}$

When the sets S and T are fixed, the values $x_{\text{max}} = |S|$ and $y_{\text{max}} = |T|$ become constants. Thus, we abbreviate the function $f(x, y, x_{\text{max}}, y_{\text{max}})$ to f(x, y) in the sequel.

Since the function good(w, S, T) expresses the goodness of a string w to distinguish two sets, it is natural to assume that the function f satisfies the *conicality*, defined as follows.

Definition 2 We say that a function f(x,y) is conic if

- for any $0 \le y \le y_{\text{max}}$, there exists an x_1 such that
 - $f(x,y) \ge f(x',y)$ for any $0 \le x < x' \le x_1$, and
 - $f(x,y) \le f(x',y)$ for any $x_1 \le x < x' \le x_{\text{max}}$.
- for any $0 \le x \le x_{\text{max}}$, there exists a y_1 such that
 - $f(x,y) \ge f(x,y')$ for any $0 \le y < y' \le y_1$, and
 - $f(x,y) \le f(x,y')$ for any $y_1 \le y < y' \le y_{max}$.

Actually, all of the above statistical measures are conic. We remark that any convex function is conic.

Lemma 2 Let f(x,y) be a conic function defined over $[0, x_{\text{max}}] \times [0, y_{\text{max}}]$. For any $0 \le x < x' \le x_{\text{max}}$ and $0 \le y < y' \le y_{\text{max}}$, we have

$$f(x,y) \le \max\{f(x',y'), f(x',0), f(0,y'), f(0,0)\}, \text{ and } f(x',y') \le \max\{f(x,y), f(x,y_{\max}), f(x_{\max},y), f(x_{\max},y_{\max})\}.$$

Proof 1 We show the first inequality only. The second can be proved in the same way. Since f is conic, we have $f(x,y) \leq \max\{f(x,0), f(x,y')\}$. Moreover, we have $f(x,0) \leq \max\{f(0,0), f(x',0)\}$ and $f(x,y') \leq \max\{f(0,y'), f(x',y')\}$. Thus the inequality holds.

In the rest of the paper, we assume that any function f associated with the objective function good is conic, and can be evaluated in constant time.

Now we consider the complexity of finding the best substring pattern and subsequence pattern, respectively. It is not hard to show that finding best substring pattern can be solved in polynomial time, since there are only $O(N^2)$ substrings from given sets of strings, where N is the total length of the strings, so that we can check all candidates in a trivial way. Moreover, we can solve it in linear time, by using generalized suffix trees [12].

Theorem 1 We can find the best substring pattern in linear time.

On the other hand, it is not easy to find the best subsequence pattern. First we introduce a very closely related problem.

Definition 3 (Consistency problem for subsequence patterns) Input: Two sets $S, T \subseteq \Sigma^*$ of strings.

Question: Is there a string w that is a subsequence for each string $s \in S$, but not a subsequence for any string $t \in T$?

The problem can be interpreted as a special case of the finding best subsequence pattern. The next theorem shows the problem is intractable.

Theorem 2 ([13, 16, 17]) The consistency problem for subsequence patterns is NP-complete.

Therefore, we are essentially forced to enumerate and evaluate exponential by many subsequence patterns in the worst case, in order to find the best subsequence pattern. In the next section, we show a practical solution based on pruning search trees. Our pruning strategy utilizes the property of subsequence languages and the conicality of the function.

4 Pruning Heuristics

In this section, we introduce two pruning heuristics, inspired by Morishita and Sese [18], to construct a practical algorithm to find the best subsequence pattern.

For a conic function f(x,y), we define

$$F(x,y) = \max\{f(x,y), f(x,0), f(0,y), f(0,0)\}, \text{ and } G(x,y) = \max\{f(x,y), f(x,y_{\text{max}}), f(x_{\text{max}},y), f(x_{\text{max}},y_{\text{max}})\}.$$

Theorem 3 For any strings $v, w \in \Sigma^*$ with $v \leq_{seq} w$,

$$f(x_w, y_w) \leq F(x_v, y_v), \tag{1}$$

$$f(x_v, y_v) \leq G(x_w, y_w). \tag{2}$$

Proof 2 By Lemma 1 (5), $v \leq_{seq} w$ implies that $L^{seq}(v) \supseteq L^{seq}(w)$. Thus $x_v = |S \cap L^{seq}(v)| \ge |S \cap L^{seq}(w)| = x_w$. In the same way, we can show $y_v \ge y_w$. By Lemma 2, we have $f(x_w, y_w) \le F(x_v, y_v)$. The second inequality can be verified similarly.

In Fig. 1, we show our algorithm to find the best subsequence pattern from given two sets of strings, according to the function f. Optionally, we can specify the maximum length of subsequences. We use the following data structures in the algorithm.

StringSet Maintain a set S of strings.

- void append(string w): append a string w into the set S.
- int $numOfSubseq(\mathbf{string}\ seq)$: return the cardinality of the set $\{w \in S \mid seq \leq_{seq} w\}$.
- int $numOfSuperseq(\mathbf{string}\ seq)$: return the cardinality of the set $\{w \in S \mid w \leq_{\text{seq}} seq\}$.

PriorityQueue Maintain strings with their priorities.

- **bool** *empty()* : return **true** if the queue is empty.
- void $push(string\ w,\ double\ priority)$: push a string w into the queue with priority priority.
- (string, double) pop(): pop and return a pair (string, priority), where priority is the highest in the queue.

The next theorem guarantees the completeness of the algorithm.

Theorem 4 Let S and T be sets of strings, and ℓ be a positive integer. The algorithm FindMaxSubsequence (S, T, ℓ) will return a string w that maximizes the value good(w, S, T) among the strings of length at most ℓ .

Proof 3 First of all, we consider the behavior of the algorithm whose lines marked by '*' are commented out. That is, we first assume that the lines 10, 13 and 20–23 are skipped. In this case, we show that the algorithm performs the exhaustive search in a breadth first manner. Since the value of upperBound is unchanged, **PriorityQueue** is actually equivalent to a simple queue. The lines 14–16 evaluate the value good(seq, S, T) of a string seq, and if it exceeds the current maximum value maxVal, we update maxVal and maxSeq in lines 17–19. Thus the algorithm will examine all strings of length at most ℓ , in increasing order of the length, and it can find the maximum.

We now consider the lines 20, 21, and 23. Let v be the current value of the variable seq. At lines 14 and 15, x_v and y_v are computed. At line 20, upperBound = $F(x_v, y_v)$

```
string FindMaxSubsequence(StringSet S, T, int maxLength = \infty)
1
2
      string prefix, seq, maxSeq;
3
      double upperBound = \infty, maxVal = -\infty, val;
      int x, y;
4
5
      StringSet Forbidden = \emptyset;
      PriorityQueue queue; /* Best First Search*/
6
7
      queue.push("", \infty);
8
      while not queue.empty() do
9
          (prefix, upperBound) = queue.pop();
10 *
         if upperBound < maxVal then break;
11
         foreach c \in \Sigma do
                               /* string concatenation */
12
             seq = prefix + c;
13 *
             if Forbidden.numOfSuperseq(seq) == 0 then
                 x = S.numOfSubseq(seq);
14
15
                y = T.numOfSubseq(seq);
                 val = f(x, y);
16
17
                if val > maxVal then
18
                    maxVal = val;
19
                    maxSeq = seq;
20 *
                 upperBound = \max\{f(x, y), f(x, 0), f(0, y), f(0, 0)\};
21 *
                 if upperBound < maxVal then
22 *
                    Forbidden.append(seq);
23 *
                else
24
                    if |sea| < maxLength then
25
                       queue.push(seq, upperBound);
26
      return maxSeq;
```

Figure 1: Algorithm *FindMaxSubsequence*. In our pseudocode, indentation indicates block structure, and the **break** statement is to jump out of the closest enclosing loop.

is estimated and if upperBound is less than the current maximum value maxVal, the algorithm skips pushing v into the queue. It means that any string w of which v is a prefix will not evaluated. We can show that such a string w can never be the best subsequence as follows. Since v is a prefix of w, we know v is a subsequence of w, by Lemma 1 (1) and (3). By Theorem 3 (1), the value $f(x_w, y_w) \leq F(x_v, y_v)$, and since $F(x_v, y_v) < \max Val$, the string w can never be the maximum.

Assume the condition upperBound < maxVal holds at line 10. It implies that any string v in the queue can never be the best subsequence, since the queue is a priority queue so that $F(x_v, y_v) \le \text{upperBound}$, which means $f(x_v, y_v) \le F(x_v, y_v)$ by Theorem 3 (1). Therefore $f(x_v, y_v) < \text{maxVal}$ for any string v in the queue, and we can jump out of the loop immediately.

Finally, we take account of lines 13 and 22. Initially, the set Forbidden of strings

is empty. At line 22, a string v is appended to Forbidden only if upperBound = $F(x_v, y_v) < \max \text{Val.}$ At line 13, if the condition

Forbidden.numOfSuperseq(seq) == 0

does not hold, seq will not be evaluated. Moreover, any string of which seq is a prefix will not be evaluated either, since we does not push seq in the queue at line 25 in this case. Nevertheless, we can show that these cuts never affect the final output as follows. Assume that Forbidden.numOfSuperseq(seq) $\neq 0$ for a string seq. It implies that there exists a string $u \in$ Forbidden such that seq is a supersequence of u. In another word, u is a subsequence of seq. Since u is in Forbidden, we know that $F(x_u, y_u) < \max v$ at some moment. By Theorem 3 (2), the value $f(x_{seq}, y_{seq})$ can never exceeds maxVal. Thus the output of the algorithm is not changed by these cuts.

By the above theorem, we can safely prune the branches. We now consider the cost of performing these heuristics. The cost of the first heuristics at lines 20, 21, and 23 is negligible, since evaluating the upperBound at line 20 is negligible compared to evaluate x and y at lines 14 and 15. On the other hand, the second heuristics at lines 13 and 22 may be expensive, since the evaluation of Forbidden.numOfSuperseq(seq) may not be so easy when the set Forbidden becomes large.

Anyway, one of the most time-consuming part of the algorithm is the lines 14 and 15. Here, for a string seq, we have to count the number of strings in the sets S and T that are subsequences of seq. We remark that the set S and T are fixed within the algorithm FindMaxSubsequence. Thus we have a possibility to speed up counting, at the cost of some appropriate preprocessing. We will discuss it in the next section.

5 Using Subsequence Automata

In this section, we pay our attention to the following problem.

Definition 4 (Counting the matched strings) Input A finite set $S \subseteq \Sigma^*$ of strings.

Query $A string seq \in \Sigma^*$.

Answer The cardinality of the set $S \cap L^{seq}(seq)$.

Of course, the answer to the query should be very fast, since many queries will arise. Thus, we should preprocess the input in order to answer the query quickly. On the other hand, the preprocessing time is also a critical factor in our application. In this paper, we utilize automata that accept subsequences of strings. Baeza-Yates [5] introduced the directed acyclic subsequence graph (DASG) of a string t as the smallest deterministic partial finite automaton that recognizes all possible subsequences of t. By using DASG of t, we can determine whether a string s is a subsequence of a string t in O(|s|) time. He showed a right-to-left algorithm for building the DASG for a single string. On the other hand, Troníček and Melichar [21] showed a left-to-right algorithm for building the DASG for a single string.

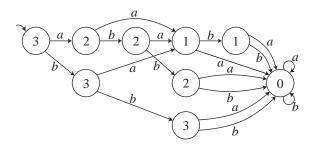


Figure 2: Subsequence automaton for $S = \{abab, abb, bb\}$, where $\Sigma = \{a, b\}$. Each number on a state denotes the number of matched strings. For example, by traverse the states according to a string ab, we reach the state whose number is 2. It corresponds to the cardinality $|L^{\text{seq}}(ab) \cap S| = 2$, since $ab \preceq_{\text{seq}} abab$, $ab \preceq_{\text{seq}} abb$ and $ab \npreceq_{\text{seq}} bb$.

We now turn our attention to the case of a set S of strings. A straightforward approach is to build DASGs for each string in S. Given a query string seq, we traverse all DASGs simultaneously, and return the total number of DASGs that accept seq. It clearly runs in O(k|seq|) time, where k is the number of strings in S. When the running time is more critical, we can build a product of k DASGs so that the running time becomes O(|seq|) time, at the cost of preprocessing time and space requirement. This is the DASG for a set of strings.

Baeza-Yates also presented a right-to-left algorithm for building the DASG for a set of strings [5]. Moreover, Troníček and Melichar [21], and Crochemore and Troníček [7] showed left-to-right algorithms for building the DASG for a set of strings.

In [11], we considered a subsequence automaton as a deterministic complete finite automaton that recognizes all possible subsequences of a set of strings, that is essentially the same as DASG. We showed an online construction of subsequence automaton for a set of strings. Our algorithm runs in $O(|\Sigma|(m+k)+N)$ time using $O(|\Sigma|m)$ space, where $|\Sigma|$ is the size of alphabet, N is the total length of strings, and m is the number of states of the resulting subsequence automaton. This is the fastest algorithm to construct a subsequence automaton for a set of strings, to the best of our knowledge. We can extend the automaton so that it answers the above Counting the matched strings problem in a natural way (See Fig. 2).

Although the construction time is linear to the size m of automaton to be built, unfortunately $m = O(n^k)$ in general, where we assume that the set S consists of k strings of length n. (The lower bound of m is only known for the case k = 2, as $m = \Omega(n^2)$ [7].) Thus, when the construction time is also a critical factor, as in our application, it may not be a good idea to construct subsequence automaton for the set S itself. Here, for a specified parameter mode > 0, we partition the set S into d = k/mode subsets S_1, S_2, \ldots, S_d of at most mode strings, and construct d subsequence automata for each S_i . When asking a query seq, we have only to traverse all automata similutaneously, and return the sum of the answers. In this way, we can

balance the preprocessing time with the total time to answer (possibly many) queries. In the next section, we experimentally evaluate the optimal value of the parameter mode in some situation.

6 Implementation and Experiments

In this section, we report some preliminary results on our experiment. We are implementing our algorithm in Fig. 1 using C++ language with Standard Template Library (STL). For the **PriorityQueue**, we use the standard priority_queue in STL. Concerning with the **StringSet**, we have implemented the function numOfSubseq(seq) in the following two ways depending on the value of mode. In case of mode = 0, we do not use subsequence automata. For each string w in the set, we check whether seq is a subsequence of w or not in a trivial way, and return the number of matched strings. Thus we do not need to preprocess the set. For the cases $mode \geq 1$, we construct k/mode subsequence automata in the preprocess, where k is the number of strings in the set. Unfortunately, the function numOfSuperseq(seq) is not implemented yet at the moment, and currently it returns 0 for any seq. In this sense, the effect of the second heuristics at lines 13 and 22 in Fig. 1 is not included in the following results.

The input data is a set of amino acid sequences taken from the PIR database, that are converted into strings over binary alphabet $\Sigma = \{0, 1\}$, according to the alphabet indexing discovered by BONSAI [20]. The average length of the strings is about 30, and |S| = 70 and |T| = 100.

In order to verify the effect of the first heuristics, we compared the searching time to find the best subsequence pattern of our algorithm (pruning search) with that of exhaustive search, where the lines 10, 14 and 20–23 are commented out. We set maxLength = 13, so that the exhaustive search will terminate.

Our experiment was carried out on an AlphaServer DS20 with an Alpha 21264 processor at 500MHz. Table 1 shows the preprocessing time, and search time for pruning search and for exhaustive search, where *mode* are changed from 0 to 10.

We can see that the preprocessing time increases with the *mode*, as we expected, since the total size of the automata increases. On the other hand, the search time decreases with the *mode* for both pruning and exhaustive searches, since each subsequence query will be answered quickly by using subsequence automata.

We now compare the search time of pruning with that of exhaustive. We can observe that the pruning dramatically reduced the search time, since the pruning reduce the number of subsequence queries.

In order to see the most preferable value of mode at which the total running time is minimized, refer to Fig. 3 that illustrates Table 1. The total running time, that is the sum of preprocessing and search time, is minimized at mode = 3 for exhaustive search, and at mode = 1 for pruning.

Table 1: Preprocessing time and search time (seconds).

| mode | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------------|------|------|------|------|------|------|------|------|------|-------|-------|
| preprocessing | - | 0.07 | 0.16 | 0.38 | 0.91 | 1.86 | 3.29 | 6.09 | 9.92 | 14.87 | 21.42 |
| exhaustive | 5.90 | 4.25 | 2.59 | 2.00 | 1.65 | 1.40 | 1.29 | 1.16 | 1.08 | 1.04 | 0.97 |
| pruning | 0.26 | 0.19 | 0.11 | 0.09 | 0.07 | 0.06 | 0.06 | 0.05 | 0.05 | 0.04 | 0.04 |

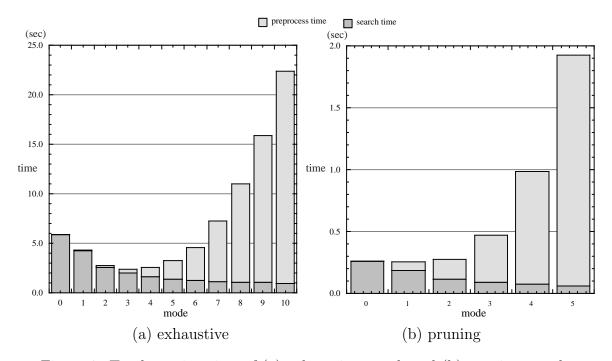


Figure 3: Total running time of (a) exhaustive search and (b) pruning search.

By these results, we can verify that the pruning heuristics and subsequence automata reduce the time to find the best subsequence pattern.

7 Concluding Remarks

We have discussed how to find a subsequence that maximally distinguishes given two sets of strings, according to a specified objective function. The only requirement to the objective function is the *conicality*, that is weaker than the *convexity*, and almost of all natural measures to distinguish two sets will satisfy the property.

In this paper, we focused on *finding the best* subsequence pattern. However, we can easily extend our algorithm to *enumerate all strings* whose values of the objective function exceed the given threshold, since essentially we examine all strings, with effective pruning heuristics. Enumeration may be more preferable in the context of *text data mining* [6, 9, 22].

Our preliminary experiments show that our approach is quite promising, where the

only one of our two heuristics are implemented. We will perform complete experiments and report the results in the final version of this paper.

In [8, 15] an *episode matching* is considered, where the total length of the matched strings is bounded by a given parameter. It will be very interesting to extend our approach to find the best *episode* to distinguish two sets of sequences. Moreover, it is also challenging to apply our approach to find the best *pattern* in the sense of *pattern languages* introduced by Angulin [2], where the related consistency problems are shown to be very hard [13, 14, 17]. Arimura et al. showed an another approach to find best *proximity pattern* [3, 4, 10]. It may be interesting to combine these approaches into one.

In future work, we are plan to install our algorithm into the core of the decision tree generator in the BONSAI system [20].

Acknowledgements

The authors would like to thank Prof. Albert Apostolico and Prof. Hiroki Arimura for fruitful discussion.

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