# A Practical Algorithm to Find the Best Subsequence Patterns 

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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 experiments, that convinced us 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 BONSAI 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 give a practical solution to find the best subsequence pattern which separates a given set of strings from the other set of strings. We propose a practical implementation of exact search algorithm that practically
avoids exhaustive search. 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 results of the experiments, that convinced us it is quite promising.

## 2 Preliminaries

Let $\Sigma$ be a finite alphabet, and let $\Sigma^{*}$ be the set of all strings over $\Sigma$. 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 $w=v y\left(w=x v y, w=x v\right.$, 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 $v \preceq_{\text {str }} w$ 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 $L^{\operatorname{str}}(v)$ and subsequence language $L^{\text {seq }}(v)$ as follows:

$$
\begin{aligned}
& L^{\text {str }}(v)=\left\{w \in \Sigma^{*} \mid v \preceq_{\text {str }} w\right\}, \text { and } \\
& L^{\text {seq }}(v)=\left\{w \in \Sigma^{*} \mid v \preceq_{\text {seq }} w\right\}, \text { respectively. }
\end{aligned}
$$

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 $v \preceq_{s t r} w$,
2. if $v$ is a suffix of $w$, then $v \preceq_{s t r} w$,
3. if $v \preceq_{\text {str }} w$ then $v \preceq_{\text {seq }} w$,
4. $v \preceq_{s t r} w$ if and only if $L^{s t r}(v) \supseteq L^{s t r}(w)$,
5. $v \preceq_{\text {seq }} w$ if and only if $L^{s e q}(v) \supseteq L^{s e q}(w)$.

## 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 $\operatorname{value} \operatorname{good}(w, S, T)$.
Intuitively, the value $\operatorname{good}(w, S, T)$ 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 $\chi^{2}$ 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 the best substring pattern, and finding the best subsequence pattern, respectively. Let $L$ be either $L^{\text {str }}$ or $L^{\text {seq }}$. Then any of the above examples of the measures can be described in the following form.

$$
\begin{aligned}
\operatorname{good}(w, S, T) & =f\left(x_{w}, y_{w},|S|,|T|\right), \text { where } \\
x_{w} & =|S \cap L(w)|, \\
y_{w} & =|T \cap L(w)| .
\end{aligned}
$$

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:

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

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

Since the function $\operatorname{good}(w, S, T)$ 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 $0 \leq y \leq y_{\max }$, there exists an $x_{1}$ such that
- $f(x, y) \geq f\left(x^{\prime}, y\right)$ for any $0 \leq x<x^{\prime} \leq x_{1}$, and
- $f(x, y) \leq f\left(x^{\prime}, y\right)$ for any $x_{1} \leq x<x^{\prime} \leq x_{\max }$.
- for any $0 \leq x \leq x_{\text {max }}$, there exists a $y_{1}$ such that
- $f(x, y) \geq f\left(x, y^{\prime}\right)$ for any $0 \leq y<y^{\prime} \leq y_{1}$, and
- $f(x, y) \leq f\left(x, y^{\prime}\right)$ for any $y_{1} \leq y<y^{\prime} \leq y_{\max }$.

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 $\left[0, x_{\max }\right] \times\left[0, y_{\max }\right]$. For any $0 \leq x<x^{\prime} \leq x_{\max }$ and $0 \leq y<y^{\prime} \leq y_{\max }$, we have

$$
\begin{aligned}
f(x, y) & \leq \max \left\{f\left(x^{\prime}, y^{\prime}\right), f\left(x^{\prime}, 0\right), f\left(0, y^{\prime}\right), f(0,0)\right\}, \text { and } \\
f\left(x^{\prime}, y^{\prime}\right) & \leq \max \left\{f(x, y), f\left(x, y_{\max }\right), f\left(x_{\max }, y\right), f\left(x_{\max }, y_{\max }\right)\right\}
\end{aligned}
$$

Proof. We show the first inequality only. The second can be proved in the same way. Since $f$ is conic, we have $f(x, y) \leq \max \left\{f(x, 0), f\left(x, y^{\prime}\right)\right\}$. Moreover, we have $f(x, 0) \leq \max \left\{f(0,0), f\left(x^{\prime}, 0\right)\right\}$ and $f\left(x, y^{\prime}\right) \leq \max \left\{f\left(0, y^{\prime}\right), f\left(x^{\prime}, y^{\prime}\right)\right\}$. 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 the best substring pattern can be solved in polynomial time, since there are only $O\left(N^{2}\right)$ 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 the best subsequence pattern. The next theorem shows the problem is intractable.
Theorem $2([\mathbf{1 3}, \mathbf{1 6}, \mathbf{1 7}])$. The consistency problem for subsequence patterns is NP-complete.

Therefore, we are essentially forced to enumerate and evaluate exponentially 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

$$
\begin{aligned}
& F(x, y)=\max \{f(x, y), f(x, 0), f(0, y), f(0,0)\}, \text { and } \\
& G(x, y)=\max \left\{f(x, y), f\left(x, y_{\max }\right), f\left(x_{\max }, y\right), f\left(x_{\max }, y_{\max }\right)\right\} .
\end{aligned}
$$

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

$$
\begin{align*}
f\left(x_{w}, y_{w}\right) & \leq F\left(x_{v}, y_{v}\right)  \tag{1}\\
f\left(x_{v}, y_{v}\right) & \leq G\left(x_{w}, y_{w}\right) \tag{2}
\end{align*}
$$

Proof. By Lemma 1 (5), $v \preceq_{\text {seq }} w$ implies that $L^{\text {seq }}(v) \supseteq L^{\text {seq }}(w)$. Thus $x_{v}=$ $\left|S \cap L^{\text {seq }}(v)\right| \geq\left|S \cap L^{\text {seq }}(w)\right|=x_{w}$. In the same way, we can show $y_{v} \geq y_{w}$. By Lemma 2, we have $f\left(x_{w}, y_{w}\right) \leq F\left(x_{v}, y_{v}\right)$. 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(string seq) : return the cardinality of the set $\{w \in S \mid$ seq $\left.\preceq_{\text {seq }} w\right\}$.
- int numOfSuperseq(string seq) : return the cardinality of the set $\{w \in S \mid$ $\left.w \preceq_{\text {seq }} s e q\right\}$.

PriorityQueue Maintain strings with their priorities.

- bool empty() : return true if the queue is empty.
$-\operatorname{void}$ push(string $w$, double priority) : push a string $w$ into the queue with priority priority.
- (string, double) $\operatorname{pop}()$ : 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 $\ell$ be a positive integer. The algorithm FindMaxSubsequence ( $S, T, \ell$ ) will return a string $w$ that maximizes the value $\operatorname{good}(w, S, T)$ among the strings of length at most $\ell$.

Proof. 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

```
string FindMaxSubsequence(StringSet \(S, T\), int maxLength \(=\infty\) )
    string prefix, seq, maxSeq;
    double upperBound \(=\infty\), \(\operatorname{maxVal}=-\infty\), val;
    int \(x, y\);
    StringSet Forbidden \(=\emptyset\);
    PriorityQueue queue; /* Best First Search*/
    queue.push("", \(\infty\) );
    while not queue.empty() do
        \((\) prefix, upperBound \()=\) queue.pop ()\(;\)
        if upperBound \(<\) maxVal then break;
        foreach \(c \in \Sigma\) do
            seq \(=\) prefix \(+\mathrm{c} ; \quad /^{*}\) string concatenation */
            if Forbidden.numOfSuperseq \((\) seq \()=0\) then
                \(x=\) S.numOfSubseq(seq);
                \(y=T\).numOfSubseq(seq);
                \(v a l=f(x, y)\);
                if \(\mathrm{val}>\operatorname{maxVal}\) then
                    \(\operatorname{maxVal}=v a l ;\)
                    \(\operatorname{maxSeq}=s e q\);
                upperBound \(=\max \{f(x, y), f(x, 0), f(0, y), f(0,0)\}\);
                if upperBound \(<\max\) Val then
                    Forbidden.append(seq);
                else
                    if \(\mid\) seq \(\mid<\) maxLength then
                    queue.push(seq, upperBound);
    return maxSeq;
```

Fig. 1. Algorithm FindMaxSubsequence. In our pseudocode, indentation indicates block structure, and the break statement is to jump out of the closest enclosing loop.
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 $\operatorname{good}(s e q, S, T)$ of a string $s e q$, 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 $\ell$, 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 string currently represented by the variable seq. At lines 14 and $15, x_{v}$ and $y_{v}$ are computed. At line 20 , upperBound $=F\left(x_{v}, y_{v}\right)$ 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 $f\left(x_{w}, y_{w}\right) \leq F\left(x_{v}, y_{v}\right)$, and since $F\left(x_{v}, y_{v}\right)<\operatorname{maxVal}$, the string $w$ can never be the maximum.

Assume the condition upperBound $<\operatorname{maxVal}$ 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 $F\left(x_{v}, y_{v}\right) \leq$ upperBound, which means $f\left(x_{v}, y_{v}\right) \leq$ $F\left(x_{v}, y_{v}\right)$ by Theorem 3 (1). Therefore $f\left(x_{v}, y_{v}\right)<\operatorname{maxVal}$ 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 $=F\left(x_{v}, y_{v}\right)<\operatorname{maxVal}$. 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 $F\left(x_{u}, y_{u}\right)<$ maxVal at some moment. By Theorem 3 (2), the value $f\left(x_{\text {seq }}, y_{\text {seq }}\right)$ 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 $S \cap L^{s e q}(s e q)$.
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.

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 $O(k|s e q|)$ 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 $O(|s e q|)$ 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 $m=O\left(n^{k}\right)$ 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 $m=\Omega\left(n^{2}\right)[7]$.) 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.


Fig. 2. Subsequence automaton for $S=\{a b a b, a b b, b b\}$, 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 $a b$, we reach the state whose number is 2 . It corresponds to the cardinality $\left|L^{\text {seq }}(a b) \cap S\right|=2$, since $a b \preceq_{\text {seq }} a b a b, a b \preceq_{\text {seq }} a b b$ and $a b \preceq_{\text {seq }} b b$.

## 6 Implementation and Experiments

In this section, we report some results on our experiments. 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. On the other hand, the function numOfSuperseq( seq) is implemented in a trivial way without using any special data structure.

We examined the following two data as input.
Transmembrane 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 $30 . S_{1}$ consists of 70 transmembrane domains, and $T_{1}$ consists of 100 non-transmembrane domains.
DNA DNA sequences of yeast genome over $\Sigma=\{\mathrm{A}, \mathrm{T}, \mathrm{G}, \mathrm{C}\}$. The lengths of the strings are all 30 . We selected two sets $S_{2}$ and $T_{2}$ based on the functional categories. $\left|S_{2}\right|=31$ and $\left|T_{2}\right|=35$.

We note that $\left\langle S_{1}, T_{1}\right\rangle$ is an easy instance, while $\left\langle S_{2}, T_{2}\right\rangle$ is a hard instance, in the sense that the best score for $\left\langle S_{1}, T_{1}\right\rangle$ is high, while that for $\left\langle S_{2}, T_{2}\right\rangle$ is low. As we will report, the facts affect the practical behaviors of our algorithm.

In order to verify the effect of the first heuristics and the second heuristics, we compared the searching time to find the best subsequence pattern of our algorithm.


Fig. 3. Number of strings actually evaluated and running time, where maxLength varies.
pruning1 We use the first heuristics only, by commented out the lines 13 and 22.
pruning2 We use both the first and second heuristics.
exhaustive We do not use any heuristics, by commented out the lines 10, 13 and 20-23.

Our experiments were carried out both on a workstation AlphaServer DS20 with an Alpha 21264 processor at 500 MHz running Tru64 UNIX operating system (WS), and on a personal computer with Pentium III processor at 733 MHz running Linux (PC).

First we verified the effect of the first heuristics and the second heuristics. Fig. 3 shows the numbers of strings actually evaluated and the running time at PC, when maxLength varies and mode was fixed to 0 . The both graphs (a)

Table 1. Preprocessing time and search time (seconds) at PC. The data is Transmembrane.

| mode | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| preprocessing | - | 0.023 | 0.054 | 0.120 | 0.273 | 0.470 | 0.796 | 1.378 | 2.108 | 3.083 | 4.543 |
| exhaustive | 1.502 | 1.560 | 0.906 | 0.710 | 0.599 | 0.535 | 0.494 | 0.460 | 0.425 | 0.414 | 0.379 |
| pruning1 | 0.067 | 0.077 | 0.046 | 0.037 | 0.031 | 0.025 | 0.023 | 0.022 | 0.020 | 0.019 | 0.018 |
| pruning2 | 0.060 | 0.069 | 0.047 | 0.040 | 0.035 | 0.033 | 0.031 | 0.030 | 0.029 | 0.029 | 0.028 |

and (c) show that the pruning2 gives the most effective pruning with respect to the number of evaluated strings, as we expected. For example, pruning2 reduces the search space approximately half compared to pruning1, when maxLength is 14 in (c). However, the running time behaves differently as we expected. The graph (b) shows that the running time reflects the number of evaluated strings, while the graph (c) shows that pruning2 was much slower than pruning1. This is because the overhead of maintaining the set Forbidden and the response time of the query to Forbidden, since we implemented it in a trivial way. By comparing (a) and (b) with (c) and (d) respectively, we see that the instance $\left\langle S_{1}, T_{1}\right\rangle$ of Transmembrane is easy to solve compared to $\left\langle S_{2}, T_{2}\right\rangle$ of DNA, because some short subsequences with high score were found in an early stage so that the search space is reduced drastically.

We now verify the effect of introducing subsequence automata. Table 1 shows the preprocess time, and search time for each search method, where mode is 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 monotonically with the mode for any search method except the case mode $=0$, since each subsequence query will be answered quickly by using subsequence automata. The search time in the case mode $=1$ is slightly slower than that in the case mode $=0$. It implies that traversing an automaton is not so faster than naive matching of subsequence when answering subsequence queries. We suppose that the phenomena arise mainly from the effect of CPU caches.

In order to see the most preferable value of mode at which the total running time is minimized, refer to Fig. 4 (a), (b), and (c) 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 (a). On the other hand, unfortunately, for both pruning1 in (b) and pruning2 in (c), the total running time is minimized at mode $=0$. It means that in this case, subsequence automata could not reduce the running time. Especially, at the workstation (d), search without using subsequence automata ( mode $=0$ ) is much faster than any other mode. We guess that it is also caused by the CPU caches.

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


Fig. 4. Total running time of (a) exhaustive search and (b)(c)(d) pruning search. The experiments (a), (b) and (c) are performed at PC, while (d) at WS.

## 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 $[6,9,22]$.

In our current implementation, the function numOfSuperseq is realized in a trivial way, that slows down the pruning2 in some situation. If we can construct a supersequence automata efficiently, the second heuristic will be more effective.

We remark that the function $G$ in Theorem 3 (2) is not actually used in our algorithm, since our algorithm starts from the empty string and tries to extend it. Another approach is also possible, that starts from a given string and tries to shrink it. In this case, the function $G$ will be applicable.

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 strings. 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 the best proximity pattern [ $3,4,10$ ]. It may be interesting to combine these approaches into one.

We plan to install our algorithm into the core of the decision tree generator in the BONSAI system [20].

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