# Biosequence Algorithms, Spring 2005 Lecture 4: Set Matching and Aho-Corasick Algorithm 

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## Exact Set Matching Problem

In the exact set matching problem we locate occurrences of any pattern of a set $\mathcal{P}=\left\{P_{1}, \ldots, P_{k}\right\}$, in target $T[1 \ldots m]$ Let $n=\sum_{i=1}^{k}\left|P_{i}\right|$. Exact set matching can be solved in time

$$
O\left(\left|P_{1}\right|+m+\cdots+\left|P_{k}\right|+m\right)=O(n+k m)
$$

by applying any linear-time exact matching $k$ times
Aho-Corasick algorithm (AC) is a classic solution to exact set matching. It works in time $O(n+m+z)$, where $z$ is number of pattern occurrences in $T$
(Main reference here [Aho and Corasick, 1975])
$A C$ is based on a refinement of a keyword tree

## Keyword Trees

A keyword tree (or a trie) for a set of patterns $\mathcal{P}$ is a rooted tree $\mathcal{K}$ such that

1. each edge of $\mathcal{K}$ is labeled by a character
2. any two edges out of a node have different labels

Define the label of a node $v$ as the concatenation of edge labels on the path from the root to $v$, and denote it by $\mathcal{L}(v)$
3. for each $P \in \mathcal{P}$ there's a node $v$ with $\mathcal{L}(v)=P$, and
4. the label $\mathcal{L}(v)$ of any leaf $v$ equals some $P \in \mathcal{P}$

## Example of a Keyword Tree

A keyword tree for $\mathcal{P}=\{$ he, she, his, hers $\}$ :


A keyword tree is an efficient implementation of a dictionary of strings

## Keyword Tree: Construction

Construction for $\mathcal{P}=\left\{P_{1}, \ldots, P_{k}\right\}$ :
Begin with a root node only;
Insert each pattern $P_{i}$, one after the other, as follows:
Starting at the root, follow the path labeled by chars of $P_{i}$;
If the path ends before $P_{i}$, continue it by adding new edges and nodes for the remaining characters of $P_{i}$

- Store identifier $i$ of $P_{i}$ at the terminal node of the path

This takes clearly $O\left(\left|P_{1}\right|+\cdots+\left|P_{k}\right|\right)=O(n)$ time

## Keyword Tree: Lookup

Lookup of a string $P$ : Starting at root, follow the path labeled by characters of $P$ as long as possible;

- If the path leads to a node with an identifier, $P$ is a keyword in the dictionary
- If the path terminates before $P$, the string is not in the dictionary
Takes clearly $O(|P|)$ time - An efficient look-up method!
Naive application to pattern matching would lead to $\Theta(n m)$ time
Next we extend a keyword tree into an automaton, to support linear-time matching


## Aho-Corasick Automaton (1)

States: nodes of the keyword tree initial state: $0=$ the root
Actions are determined by three functions:

1. the goto function $g(q, a)$ gives the state entered from current state $q$ by matching target char $a$
if edge $(q, v)$ is labeled by $a$, then $g(q, a)=v$;
$g(0, a)=0$ for each $a$ that does not label an edge out of the root
$\rightsquigarrow$ the automaton stays at the initial state while scanning non-matching characters

- Otherwise $g(q, a)=\emptyset$


## Aho-Corasick Automaton (2)

2. the failure function $f(q)$ for $q \neq 0$ gives the state entered at a mismatch
$f(q)$ is the node labeled by the longest proper suffix
$w$ of $\mathcal{L}(q)$ s.t. $w$ is a prefix of some pattern
$\rightarrow$ a fail transition does not miss any potential occurrences
NB: $f(q)$ is always defined, since $\mathcal{L}(0)=\epsilon$ is a prefix of any pattern
3. the output function out $(q)$ gives the set of patterns recognized when entering state $q$

## Example of an AC Automaton



Dashed arrows are fail transitions

## AC Search of Target $T[1 \ldots m]$

```
q:= 0; // initial state (root)
for }i:=1\mathrm{ to }m\mathrm{ do
        while }g(q,T[i])=\emptyset d
        q:= f(q);// follow a fail
        q:=g(q,T[i]);// follow a goto
        if out (q) \not=\emptyset then print }i,\operatorname{out}(q)
endfor;
```


## Example:

Search text "ushers" with the preceding automaton

## Complexity of AC Search

Theorem Searching target $T[1 \ldots m]$ with an AC automaton takes time $O(m+z)$, where $z$ is the number of pattern occurrences
Proof. For each target character, the automaton performs 0 or more fail transitions, followed by a goto.
Each goto either stays at the root, or increases the depth of $q$ by $1 \Rightarrow$ the depth of $q$ is increased $\leq m$ times
Each fail moves $q$ closer to the root
$\Rightarrow$ the total number of fail transitions is $\leq m$
The $z$ occurrences can be reported in $z \times O(1)=O(z)$ time (say, as pattern identifiers and start positions of occurrences)

## Constructing an AC Automaton

The AC automaton can be constructed in two phases Phase I:

1. Construct the keyword tree for $\mathcal{P}$

- for each $P \in \mathcal{P}$ added to the tree, set out $(v):=\{P\}$ for the node $v$ labeled by $P$

2. complete the goto function for the root by setting

$$
g(0, a):=0
$$

for each $a \in \Sigma$ that doesn't label an edge out of the root
If the alphabet $\Sigma$ is fixed, Phase I takes time $O(n)$

## Result of Phase I



## Phase II of the AC Construction

$Q:=$ emptyQueue();
for $a \in \Sigma$ do

$$
\text { if } \begin{aligned}
q(0, a) & =q \neq 0 \text { then } \\
f(q) & :=0 \text {; enqueue }(q, Q) ;
\end{aligned}
$$

while not isEmpty $(Q)$ do

$$
r:=\text { dequeue }(Q) \text {; }
$$

$$
\text { for } a \in \Sigma \text { do }
$$

$$
\text { if } g(r, a)=u \neq \emptyset \text { then }
$$

$$
\text { enqueue }(u, Q) ; v:=f(r) ;
$$

$$
\text { while } g(v, a)=\emptyset \text { do } v:=f(v) ; / /\left(^{*}\right)
$$

$$
f(u):=g(v, a) ;
$$

$$
\operatorname{out}(u):=\operatorname{out}(u) \cup \operatorname{out}(f(u)) ;
$$

What does this do?

## Explanation of Phase II

Functions fail and output are computed for the nodes of the trie in a breadth-first order
$\rightsquigarrow$ nodes closer to the root have already been processed
Consider nodes $r$ and $u=g(r, a)$, that is, $r$ is the parent of $u$ and $\mathcal{L}(u)=\mathcal{L}(r) a$
Now what should $f(u)$ be?
A: The deepest node labeled by a proper suffix of $\mathcal{L}(u)$.
The executions of line (*) find this, by locating the deepest node $v$ s.t. $\mathcal{L}(v)$ is a proper suffix of $\mathcal{L}(r)$ and $g(v, a)$ $(=f(u))$ is defined.
(Notice that $v$ and $g(v, a)$ may both be the root.)

## Completing the Output Functions

What about

$$
\operatorname{out}(u):=\operatorname{out}(u) \cup \operatorname{out}(f(u)) ; ?
$$

This is done because the patterns recognized at $f(u)$ (if any), and only those, are proper suffixes of $\mathcal{L}(u)$, and shall thus be recognized at state $u$ also.

## Complexity of the AC Construction

Phase II can be implemented to run in time $O(n)$, too:
The breadth-first traversal alone takes time proportional to the size of the tree, which is $O(n)$;

OK; ...
Is there also an $O(n)$ bound for the number of times that the $f$ transitions are followed (on line (*))?

A: Yes! See next

## AC Construction: Number of fail

transitions

Consider the nodes $u_{1}, \ldots, u_{l}$ on a path created by entering a pattern $a_{1} \ldots a_{l}$ to the tree, and the depth of their $f$ nodes, denoted by $d f\left(u_{1}\right), \ldots, d f\left(u_{l}\right)$ (all $\geq 0$ )
Now $d f\left(u_{i+1}\right) \leq d f\left(u_{i}\right)+1 \Rightarrow$ the $d f$ values increase at most $l$ times along the path. When locating $f\left(u_{i+1}\right)$, each execution of line ( ${ }^{*}$ ) takes $v$ closer to the root, and thus makes value of $d f\left(u_{i+1}\right)$ smaller than $d f\left(u_{i}\right)+1$ by one at least
$\rightsquigarrow$ line $\left(^{*}\right.$ ) is executed in total $\leq l$ times (for a pattern of length $l$ )
$\rightsquigarrow$ line (*) is executed in total, for all patterns, $\leq n$ times

## AC Construction: Unions of output functions

Is it costly to perform

$$
\operatorname{out}(u):=\operatorname{out}(u) \cup \operatorname{out}(f(u)) ; ?
$$

No: Before the assignment, out $(u)=\emptyset$ or out $(u)=\{\mathcal{L}(u)\}$. Any patterns in out $(f(u))$ are shorter than $\mathcal{L}(u)$
$\Rightarrow$ the sets are disjoint
$\rightarrow$ Output sets can be implemented as linked lists, and united in constant time

## Biological Applications

## 1. Matching against a library of known patterns

A Sequence-tagged-site (STS) is, roughly, a DNA string of 200-300 bases whose left and right ends occur only once in the entire genome
ESTs (expressed sequence tags) are STSs that participate in gene expression, and thus belong to genes
Hundreds of thousands of STSs and tens of thousands of ESTs (by mid-90's) are stored in databases, and used to compare against new DNA sequences
$\rightsquigarrow$ Ability to search for occurrences of patterns in time that is independent of their number is very useful

## 2. Matching with Wild Cards

Let $\phi$ be a wild card that matches any single character
For example, ab $\phi \phi \mathrm{c} \phi$ occurs at positions 2 and 7 of 1234567890123
xabvccababcax
A transcription factor is a protein that binds to specific locations of DNA and regulates its transcription to RNA
Many transcription factors are separated into families characterized by substrings with wild cards
Example: Transcription factor Zinc Finger has signature
СффС $\varnothing \phi \phi \phi \phi \phi \phi \phi \phi \phi \phi \phi \phi Н \phi \phi H$
( $C=$ cysteine, $H=$ histidine; amino acids)

## Matching with Wild Cards (2)

If the number of wild cards is bounded by a constant, patterns with wild-cards can be matched in linear time, by counting occurrences of non-wild-card substrings of $P$ :
Let $\mathcal{P}=\left\{P_{1}, \ldots, P_{k}\right\}$ be the substrings of $P$ separated by wild-cards, and let $l_{1}, \ldots, l_{k}$ be their end positions in $P$

Preprocess: Build an AC automaton for $\mathcal{P}$; Initiate occurrence counts: for $i:=1$ to $|T|$ do $C[i]:=0$;
Search target $T$ with the AC automaton
When pattern $P_{j}$ is found to end at position $i \geq l_{j}$ of $T$, increment $C\left[i-l_{j}+1\right]$ by one;

Any $i$ with $C[i]=k$ is the start position of an occurrence

## Example

Let $P=\phi A T C \phi \phi T C \phi A T C$
Then $\mathcal{P}=\{A T C, T C, A T C\}$ with $l_{1}=4, l_{2}=8$ and $l_{3}=12$


Search on

$$
\begin{aligned}
& i: 12345678901234 . . . \\
& T: \text { ACGATCTCTCGATC... }
\end{aligned}
$$

$\rightsquigarrow C[1]=C[7]=C[11]=1$ and $C[3]=3$ ( $\sim$ occurrence)

## Complexity of AC Wild-Card

Matching

Let $|P|=n$ and $|T|=m$
Preprocessing: $O(n+m)\left(\leftarrow \sum_{i=1}^{k}\left|P_{i}\right| \leq n\right)$
Search: $O(m+z)$, where $z$ is the number of occurrences
Each occurrence increments a cell of $C$ by one, and each cell $C[1], \ldots, C[m]$ is incremented at most $k$ times $\Rightarrow z \leq k m(=O(m)$ if $k$ is bounded by a constant)

We have derived the following result:
Theorem 3.5.1 If the number of wild-cards in pattern $P$ is bounded by a constant, exact matching with wild-cards can be performed in time $O(|P|+|T|)$

