Biosequence Algorithms, Spring 2005

Lecture 4: Set Matching and Aho-Corasick Algorithm

Pekka Kilpeläinen

University of Kuopio

Department of Computer Science

Exact Set Matching Problem

In the **exact set matching problem** we locate occurrences of any pattern of a set $\mathcal{P} = \{P_1, \ldots, P_k\}$, in target $T[1 \ldots m]$

Let $n = \sum_{i=1}^{k} |P_i|$. Exact set matching can be solved in time

$$O(|P_1| + m + \cdots + |P_k| + m) = O(n + km)$$

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])

AC 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

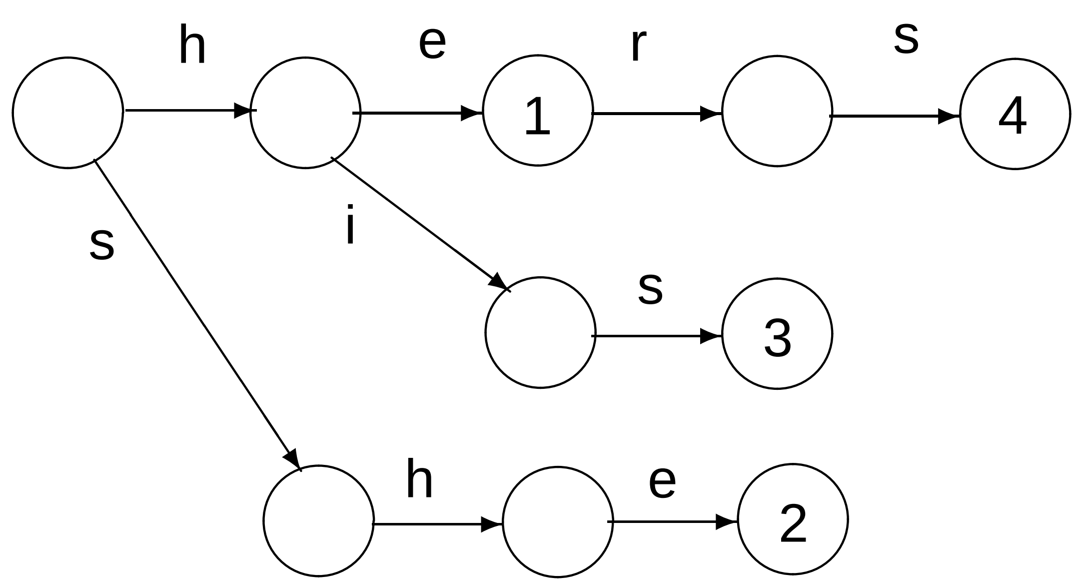
1. each edge of $\mathcal{K}$ is labeled by a character
2. any two edges out of a node have different labels

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 $\mathcal{P} = \{\text{he}, \text{she}, \text{his}, \text{hers}\}$:



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

Keyword Tree: Construction

Construction for $\mathcal{P} = \{P_1, \ldots, P_k\}$:

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 $O(|P_1| + \cdots + |P_k|) = O(n)$ 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 $\Theta(nm)$ 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

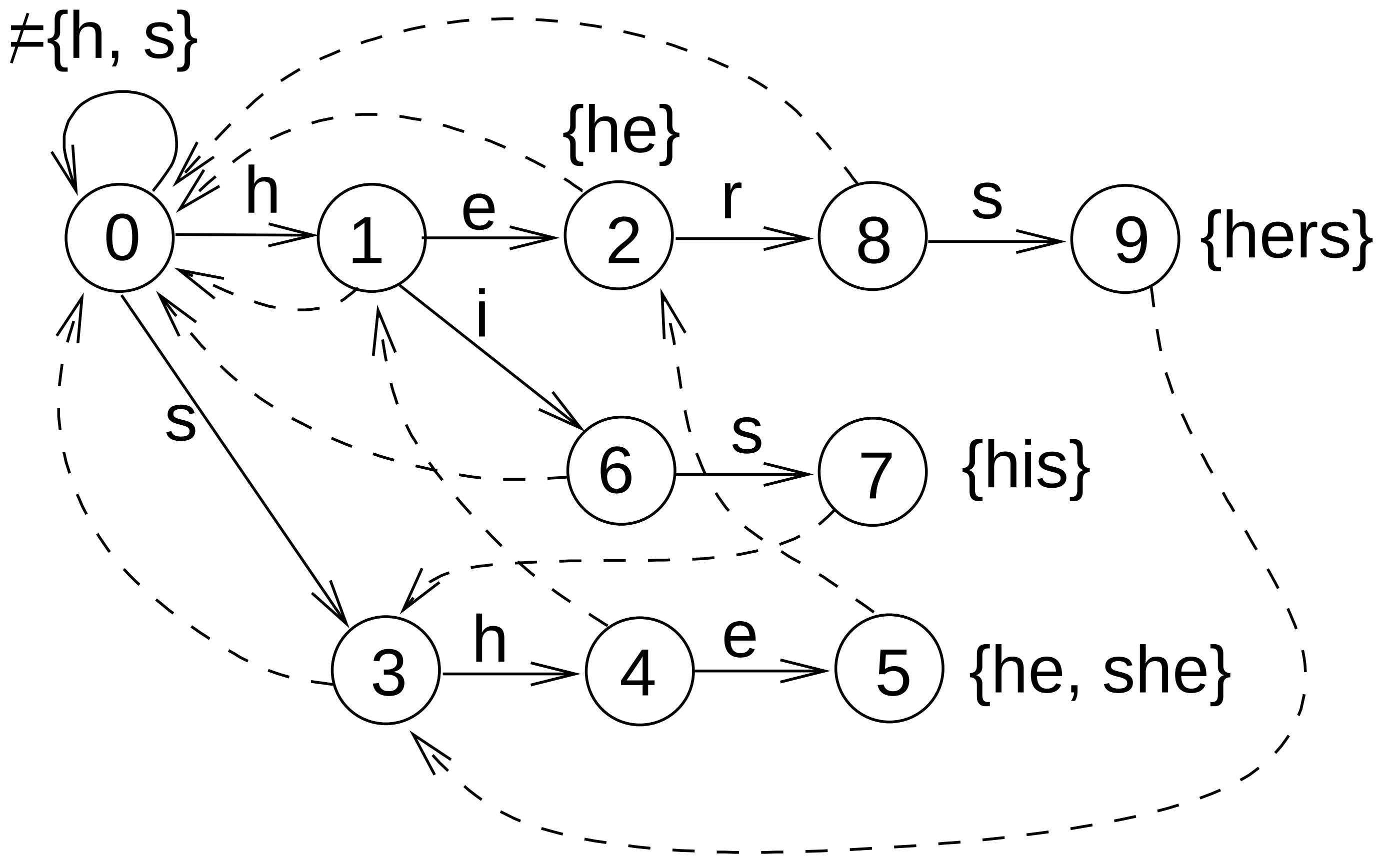
Actions are determined by three functions:

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
     $\leadsto$ 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** $\text{out}(q)$ 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 $i := 1$ **to** m **do**
  while $g(q, T[i]) = \emptyset$ **do**
    $q := f(q)$; // follow a fail
  $q := g(q, T[i])$; // follow a goto
  if $\text{out}(q) \neq \emptyset$ **then print** i, $\text{out}(q)$;
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) $\square$

Constructing an AC Automaton

The AC automaton can be constructed in two phases

Phase I:

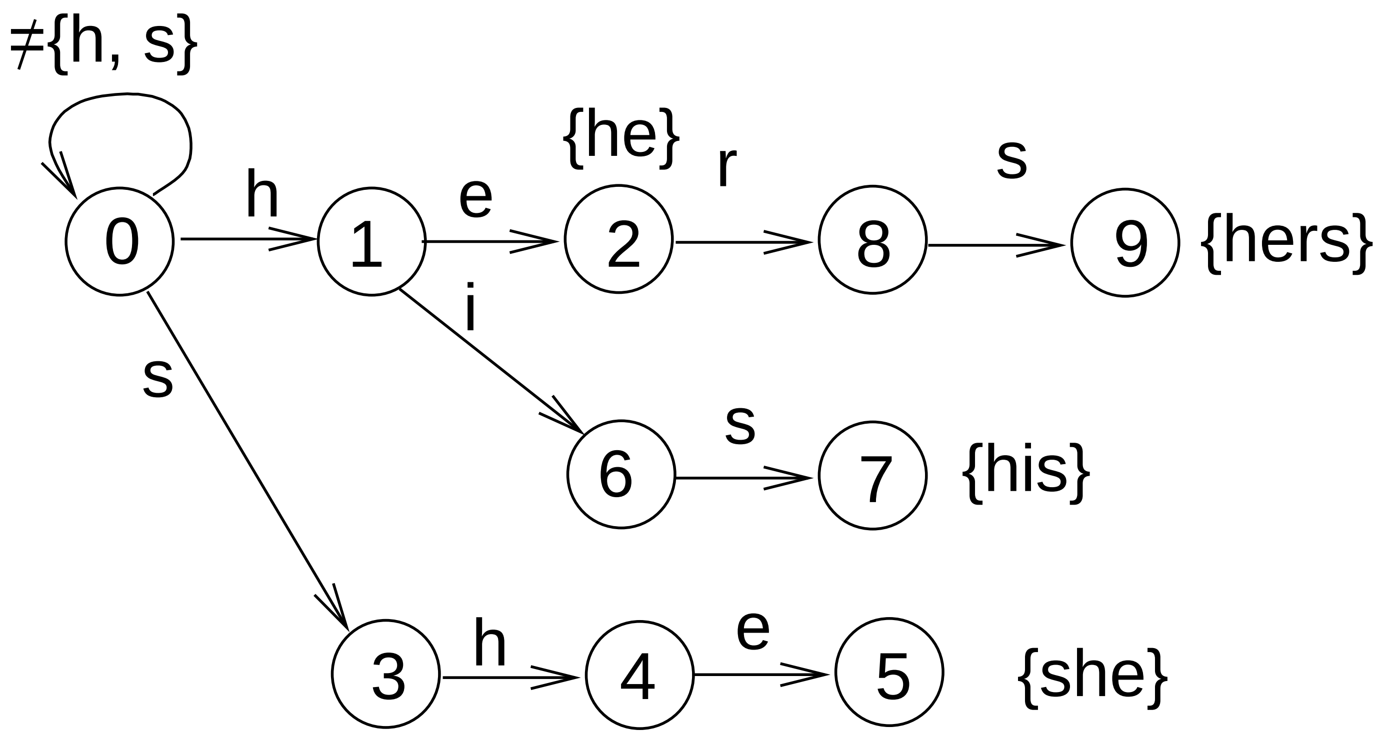
1. Construct the keyword tree for $\mathcal{P}$
   - for each $P \in \mathcal{P}$ added to the tree, set $\text{out}(v) := \{P\}$ for the node v labeled by P
2. complete the *goto* function for the root by setting

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

   for each $a \in \Sigma$ that doesn't label an edge out of the root

If the alphabet Σ 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**
  if $q(0, a) = q \neq 0$ **then**
    $f(q) := 0$; enqueue(q, Q);
while not isEmpty(Q) **do**
  r:= dequeue(Q);
  for $a \in \Sigma$ **do**
    if $g(r, a) = u \neq \emptyset$ **then**
      enqueue(u, Q); $v := f(r)$;
      while $g(v, a) = \emptyset$ **do** $v := f(v)$; // **(*)**
      $f(u) := g(v, a)$;
      out(u) := out$(u) \cup$ 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

$\leadsto$ 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

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

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 $df(u_1), \ldots, df(u_l)$ (all ≥ 0)

Now $df(u_{i+1}) \leq df(u_i) + 1 \Rightarrow$ the df values increase at most l times along the path. When locating $f(u_{i+1})$, each execution of line (*) takes v closer to the root, and thus makes value of $df(u_{i+1})$ *smaller* than $df(u_i) + 1$ *by one at least*

$\rightsquigarrow$ line (*) 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

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

No: Before the assignment, $\text{out}(u) = \emptyset$ or $\text{out}(u) = \{\mathcal{L}(u)\}$.
Any patterns in $\text{out}(f(u))$ 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

$\leadsto$ Ability to search for occurrences of patterns in time that is *independent of their number* is very useful

2. Matching with Wild Cards

Let ϕ be a **wild card** that matches any *single* character

For example, ab$\phi\phi$cϕ 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

$$C\phi\phi C\phi\phi\phi\phi\phi\phi\phi\phi\phi\phi\phi\phi H\phi\phi H$$

(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 $\mathcal{P} = \{P_1, \ldots, P_k\}$ 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

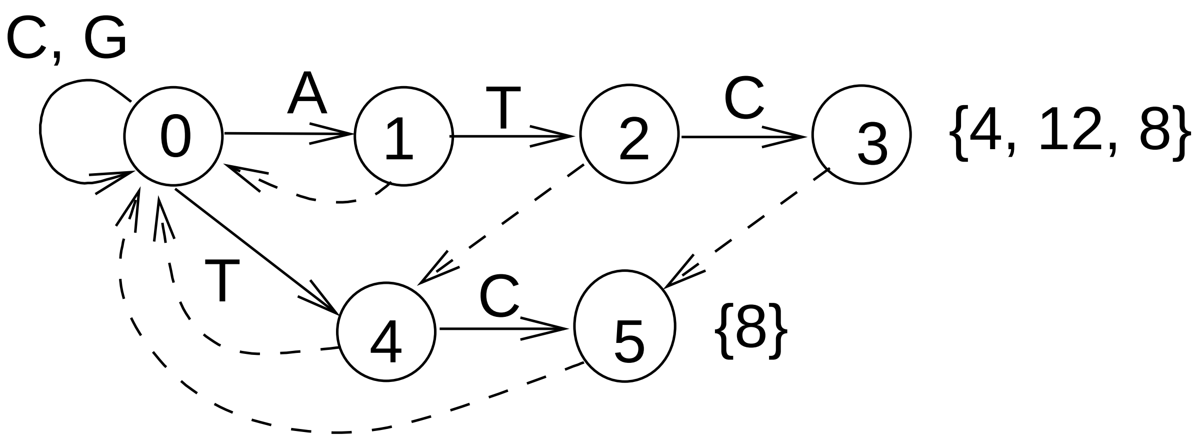
When pattern P_j is found to end at position $i \geq l_j$ of T, increment $C[i - l_j + 1]$ by one;

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

Example

Let $P = \phi ATC\phi\phi TC\phi ATC$

Then $\mathcal{P} = \{ATC, TC, ATC\}$ with $l_1 = 4$, $l_2 = 8$ and $l_3 = 12$



Search on

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i: 12345678901234...
T: ACGATCTCTCGATC...
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$\rightsquigarrow C[1] = C[7] = C[11] = 1$ and $C[3] = 3$ ($\sim$ occurrence)

Complexity of AC Wild-Card Matching

Let $|P| = n$ and $|T| = m$

Preprocessing: $O(n + m)$ ($\leftarrow \sum_{i=1}^{k} |P_i| \leq n$)

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
$\Rightarrow z \leq km$ ($= O(m)$ 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 $O(|P| + |T|)$ □