# Theory I <br> Algorithm Design and Analysis 

(11 - Edit distance and approximate string matching)

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## Dynamic programming

- Algorithm design technique often used for optimization problems
- Generally usable for recursive approaches if the same partial solutions are required more than once
- Approach: store partial results in a table
- Advantage: improvement of complexity, often polynomial instead of exponential


## Two different approaches

## Bottom-up:

+ controlled efficient table management, saves time
+ special optimized order of computation, saves space
- requires extensive recoding of the original program
- possible computation of unnecessary values

Top-down: (Note-pad method)

+ original program changed only marginally or not at all
+ computes only those values that are actually required
- separate table management takes additional time
- table size often not optimal


## Problem: similarity of strings

## Edit distance

For two given $A$ and $B$, compute, as efficiently as possible, the edit distance $D(A, B)$ and a minimal sequence of edit operations which transforms $A$ into $B$.
$\begin{array}{llllllllllllll}i & n & f & - & - & - & o & r & m & a & t & i & k & - \\ i & n & t & e & r & p & o & 1 & - & a & t & i & o & n\end{array}$

## Problem: similarity of strings

Approximate string matching
For a given text $T$, a pattern $P$, and a distance $d$, find all substrings $P^{\prime}$ in $T$ with $D\left(P, P^{\prime}\right) \leq d$

## Sequence alignment

Find optimal alignments of DNA sequences

GAGCA-CTTGGATTCTCGG

-     - CACGTGG - - - - - -


## Edit distance

Given: two strings $A=a_{1} a_{2} \ldots . a_{m}$ and $B=b_{1} b_{2} \ldots b_{n}$

Wanted: minimal cost $D(A, B)$ for a sequence of edit operations to transform $A$ into $B$.

## Edit operations:

1. Replace one character in $A$ by a character from $B$
2. Delete one character from $A$
3. Insert one character from $B$

## Edit distance

Cost model:

$$
\begin{aligned}
& c(a, b)= \begin{cases}1 & \text { if } a \neq b \\
0 & \text { if } a=b\end{cases} \\
& a=\varepsilon, b=\varepsilon \text { possible }
\end{aligned}
$$

We assume the triangle inequality holds for $c$ :

$$
c(a, c) \leq c(a, b)+c(b, c)
$$

$\rightarrow$ Each character is changed at most once

## Edit distance

Trace as representation of edit sequences

or using indels


Edit distance (cost): 5
Division of an optimal trace results in two optimal sub-traces
$\rightarrow$ dynamic programming can be used

## Computation of the edit distance

Let $A_{i}=a_{1} \ldots a_{i}$ and $B_{j}=b_{1} \ldots b_{j}$

$$
D_{i, j}=D\left(A_{i j} B_{j}\right)
$$



B


## Computation of the edit distance

Three possibilities of ending a trace:

1. $a_{m}$ is replaced by $b_{n}$ :

$$
D_{m, n}=D_{m-1, n-1}+c\left(a_{m}, b_{n}\right)
$$

2. $a_{m}$ is deleted: $D_{m, n}=D_{m-1, n}+1$
3. $b_{n}$ is inserted: $D_{m, n}=D_{m, n-1}+1$

## Computation of the edit distance

Recurrence relation, if $m, n \geq 1$ :

$$
D_{m, n}=\min \left\{\begin{array}{ccc}
D_{m-1, n-1} & + & c\left(a_{m}, b_{n}\right) \\
D_{m-1, n} & + & 1 \\
D_{m, n-1} & + & 1
\end{array}\right\}
$$

$\rightarrow$ Computation of all $D_{i, j}$ is required, $0 \leq i \leq m, 0 \leq j \leq n$.


## Recurrence relation for the edit distance

## Base cases:

$$
\begin{aligned}
& D_{0,0}=D(\varepsilon, \varepsilon)=0 \\
& D_{0, j}=D\left(\varepsilon, B_{j}\right)=j \\
& D_{i, 0}=D\left(A_{i}, \varepsilon\right)=i
\end{aligned}
$$

Recurrence equation:

$$
D_{i, j}=\min \left\{\begin{array}{ccc}
D_{i-1, j-1} & +c\left(a_{i}, b_{j}\right) \\
D_{i-1, j} & + & 1 \\
D_{i, j-1} & + & 1
\end{array}\right\}
$$

## Order of computation for the edit distance



## Algorithm for the edit distance

Algorithm edit_distance
Input: two strings $A=a_{1} \ldots . a_{m}$ and $B=b_{1} \ldots b_{n}$
Output: the matrix $D=\left(D_{i j}\right)$
1 D[0,0]:= 0
2 for $i:=1$ to $m$ do $D[i, 0]=i$
3 for $j:=1$ to $n$ do $D[0, j]=j$
4 for $i:=1$ to $m$ do
5 for $j:=1$ to $n$ do
$\begin{array}{lc}6 & D[i, j]:=\min (D[i-1, j]+1, \\ 7 & D[i, j-1]+1, \\ 8 & \left.D[i-1, j-1]+c\left(a_{j} b_{j}\right)\right)\end{array}$

## Example

|  | a |  | b | a | C |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | 0 | 1 | 2 | 3 | 4 |
| b | 1 |  |  |  |  |
| a | 2 |  |  |  |  |
| a | 3 |  |  |  |  |
| c | 4 |  |  |  |  |

## Computation of the edit operations

Algorithm edit_operations (i,j)
Input: matrix $D$ (computed)
1 if $i=0$ and $j=0$ then return
if $i \neq 0$ and $D[i, j]=D[i-1, j]+1$
3 then "delete $a[$ ] "
edit_operations ( $i-1, j$ )
5 else if $j \neq 0$ and $D[i, j]=D[i, j-1]+1$
6 then "insert $b[j]^{"}$
edit_operations (i, $j-1$ )
else

$$
\text { /* } D[i, j]=D[i-1, j-1]+c(a[i], b[j]) * /
$$

9
10 „replace a[i] by b[j] "
edit_operations ( $i-1, j-1$ )

Initial call: edit_operations( $m, n$ )

## Trace graph of the edit operations



## Sub-graph of the edit operations

Trace graph: Overview of all possible traces for the transformation of A into B , directed edges from vertex $(i, j)$ to $(i+1, j),(i, j+1)$ and ( $i+1, j+1$ ).
Weights of the edges represent the edit costs.

Costs are monotonic increasing along an optimal path.

Each path with monotonic increasing cost from the upper left corner to the lower right corner represents an optimal trace.

## Approximate string matching

Given: two strings $P=p_{1} p_{2} \ldots p_{m}$ (pattern) and

$$
T=t_{1} t_{2} \ldots t_{n} \text { (text) }
$$

Wanted: an interval $\left[j^{\prime}, j\right], 1 \leq j^{\prime} \leq j \leq n$, such that the substring $T_{j^{\prime}, j}=t_{j^{\prime}} \ldots t_{j}$ of $T$ is the one with the greatest similarity to pattern $P$, i.e. for all other intervals $\left[k^{\prime}, k\right], 1 \leq k^{\prime} \leq k \leq n$ :

$$
D\left(P, T_{j^{\prime}, j}\right) \leq D\left(P, T_{k^{\prime}, k}\right)
$$



## Approximate string matching

Naïve approach:

for all $1 \leq j^{\prime} \leq j \leq n$ do compute $D\left(P, T_{j^{\prime}, j}\right)$

choose minimum

## Approximate string matching

Consider a related problem:


For each text position $j$ and each pattern position $i$ compute the edit distance of the substring $T_{j^{\prime}, j}$ of $T$ $P \quad$ ending at $j$ which has the greatest similarity to $P_{i}$.

## Approximate string matching

Method:
for all $1 \leq j \leq n$ do
compute $j^{\prime}$ such that $D\left(P, T_{j^{\prime}, j}\right)$ is minimal

For $1 \leq i \leq m$ and $0 \leq j \leq n$ let:

$$
E_{i, j}=\min _{1 \leq j \backslash j+1} D\left(P_{i}, T_{j^{\prime}, j}\right)
$$

Optimal trace:

## Approximate string matching

Recurrence relation:

$$
E_{i, j}=\min \left\{\begin{array}{c}
E_{i-1, j-1}+c\left(p_{i}, t_{j}\right), \\
E_{i-1, j}+1, \\
E_{i, j-1}+1
\end{array}\right\}
$$

## Remark:

$j^{\prime}$ can be completely different for $E_{i-1, j-1}, E_{i-1, j}$ and $E_{i, j-1}$.
A subtrace of an optimal trace is an optimal subtrace.

## Approximate string matching

## Base cases:

$$
\begin{aligned}
& E_{0,0}=E(\varepsilon, \varepsilon)=0 \\
& E_{i, 0}=E\left(P_{j}, \varepsilon\right)=i
\end{aligned}
$$

but

$$
E_{0, j}=E\left(\varepsilon, T_{j}\right)=0
$$

Observation:
The optimal edit sequence from P to $T_{j^{\prime}, j}$ does not start with an insertion of $t_{j}$.

## Approximate string matching

## Dependency graph



## Approximate string matching

## Theorem

If there is a path from $E_{0, j^{-}-1}$ to $E_{i, j}$ in the dependency graph, then $T_{j^{\prime}, j}$ is a substring of $T$ ending in $j$ with the greatest similarity to $P_{i}$ and

$$
D\left(P_{i}, T_{j^{\prime}, j}\right)=E_{i, j}
$$

