Algorithms and Datastructures Levenshtein distance, Dynamic programming

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Bioinformatics Group / Department of Computer Science Algorithms and Datastructures, February 2018

Structure



Introduction

Edit distance

- Measurement for similarity of two words / strings
- Algorithm for efficient calculation
- General principle: dynamic programming

BioInfSearch

ejafjatlajökuk eyjafjallajökull eyjafjallajökull movie eyjafjallajälull trailer

Search!



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Wikipedia.org:

"Der Eyjafjallajökull (['eɪja,fjatla,jœ:kyt])][3], auf Deutsch Eyjafjöll-Gletscher, ist der sechstgrößte Gletscher Islands.

Er liegt an der äußersten Südküste, westlich des Gletschers Myrdalsjökull in der Gemeinde Rangárþing eystra, die größte Höhe beträgt 1651. m. Unter dem Gletscher befindet sich der Vulkan Eyjafjöll mit eigener Magmakammer, der seit der Besiedelung von Island in den Jahren 920, 1612 (oder 1613), 1821 bis 1823 und zuletzt im Jahr 2010 aktiv war."

A lot of applications where similar string are searched:

Duplicates in databases:

```
Hein Blöd 27568 Bremerhaven
Hein Bloed 27568 Bremerhafen
Hein Doof 27478 Cuxhaven
```

Product search:

memory stik

■ Websearch:

```
eyjaföllajaküll
uniwersität verien 2017
```

Bioinformatics: Similarity of DNA-sequences

Search of similar proteins:

- BLAST (Basic Local Alignment Search Tool)
- Changed life-science completely
- Cited 63437 times on Google Scholar (Sep. 2017)

Definition of edit distance: (Levenshtein-distance)

- Let x, y be two strings
- Edit distance ED(x,y) of x and y: The minimal number of operations to transform x into y
 - Insert a character
 - Replace a character with another
 - Delete a character

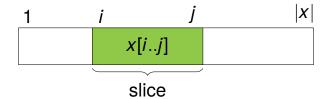
Example



```
12345
                           12345
                           BLOED
DOOF
        replace(1, B)
                                    replace(5, F)
                           BLOEF
BOOF
        replace(2, L)
                                    delete(4)
BLOF
                           BLOF
        insert(4, E)
                                    replace(2, 0)
BLOEF
                           BOOF
        replace(5, D)
                                    replace(1, D)
BLOED
                           DOOF
              ED=4
                                         ED=4
```

Notation:

- \blacksquare ε is the empty string
- |x| is the length of the string x (number of characters)
- x[i..j] is the slice of x from i to j where $1 \le i \le j \le |x|$



Trivial facts:

- \blacksquare ED(x, y) = ED(y, x)
- \blacksquare ED(x, ε) = |x|

■ ED(x,y) ≥ abs(|x|-|y|) abs(x) =
$$\begin{cases} x & \text{if } x \ge 0 \\ -x & \text{else} \end{cases}$$

■
$$ED(x,y) \le ED(x[1..n-1],y[1..m-1]) + 1$$
 $n = |x|, m = |y|$

Solutions based on examples:

- From VERIEN to FERIEN?
- From MEXIKO to AMERIKA?
- From AAEBEAABEAREEAEBA to RBEAAEEBAAAEBBAEAE?
- Searching biggest substrings can yield the solution but doesn't have to

Recursive approach:

■ Dividing in two halves? Not a good idea:

$$ED(GRAU, RAUM) = 2$$
 but $ED(GR, RA) + ED(AU, UM) = 4$

Finding "smaller" sub problems? Let's try it!

Terminology:

- \blacksquare Let x, y be two strings
- Let $\sigma_1, ..., \sigma_k$ be a sequence of k operations where $k = \mathrm{ED}(x, y)$ for $x \to y$ (transform x into y)

 (We do not know this sequence but we assume it exists)



Terminology:

■ We only consider monotonous sequences: The positition of σ_{i+1} is \geq the position of σ_i where we only allow the positions to be equal on a delete operation

```
12345
                          1234567
                          SAUDOOF
DOOF
        replace(1, B)
                                      delete(1)
                          AUDOOF
BOOF
        replace(2, L)
                                      delete(1)
BLOF
                          UDOOF
        insert(4, E)
                                      delete(1)
BLOEF
                          DOOF
        replace(5, D)
                                      insert(4, 0)
BI OFD
```



Terminology:

- **Lemma:** For any x and y with k = ED(x,y) exists a monotonous sequence of k operations for $x \to y$
- Intuition: The order of our sequence is not relevant (Therefore we can also sort them monotonously)

Consider the last operation:

■ Solve blue part recursively

DOOF DOOF $\downarrow\downarrow\downarrow\downarrow\downarrow$ $\downarrow\downarrow\downarrow$ $\downarrow\downarrow\downarrow\downarrow\downarrow$ BLOE BLOED BLOED

Abbildung: Case 1a Abbildung: Case 1b

DOOF ↓↓↓↓↓ BLOEF

↓replace

BLOED

Abbildung: Case 1c

Consider the last operation:

■ Solve blue part recursively

WINTER $\downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow$ SOMMER $\downarrow \texttt{nothing}$ SOMMER

Abbildung: Case 2

Display of solution:

- Alignment
- Example:

Dynamic programming:

- Instances of Bellman's principle of optimality:
 - Shortest paths
 - Edit distance



Abbildung: Richard Bellman (1920 - 1984)

- Optimal solutions consist of optimal partial solutions
 - Shortest paths: Each partial path has to be optimal
 - Edit distance: Each partial alignment has to be optimal

 Always solvable through dynamic programming (Caching of optimal partial solutions)

Case analysis:

- We consider the last operation σ_k
 - $\sigma_1, ..., \sigma_{k-1} : x \to z$ and $\sigma_k : z \to y$ Example:

$$x = DOOF$$
, $z = SAUBLOEF$, $y = SAUBLOED$

- Let n = |x|, m = |y|, m' = |z|
- We note $m' \in \{m-1, m, m+1\}$ why?

Case analysis:

■ Case 1: σ_k does something at the outer end:

```
■ Case 1a: \sigma_k = \operatorname{insert}(m' + 1, y[m]) [then m' = m - 1]
■ Case 1b: \sigma_k = \operatorname{delete}(m') [then m' = m + 1]
■ Case 1c: \sigma_k = \operatorname{replace}(m', y[m]) [then m' = m]
```

■ Case 2: σ_k does nothing at the outer end:

```
■ Then z[m'] = y[m] and x[n'] = z[m'] and with that \sigma_1, ..., \sigma_{k-1} : x[1..n-1] \rightarrow y[1..m-1] and x[n] = y[m]
```



Case analysis:

- Case 1a (insert): $\sigma_1, \ldots, \sigma_{k-1}: X \rightarrow y[1..m-1]$
- Case 1b (delete): $\sigma_1, \ldots, \sigma_{k-1}$: $x[1..n-1] \rightarrow y$
- Case 1c (replace): $\sigma_1, \ldots, \sigma_{k-1}$: $x[1..n-1] \rightarrow y[1..m-1]$
- Case 2 (nothing): $\sigma_1, \ldots, \sigma_k$: $x[1..n-1] \rightarrow y[1..m-1]$

This results in the recursive formula:

- For |x| > 0 and |y| > 0 is ED(x, y) the minimum of
 - ED(x , y[1..m-1]) + 1 and
 - \blacksquare ED(x[1..n-1],y)+1 and
 - ED(x[1..n-1], y[1..m-1]) + 1 if $x[n] \neq y[m]$
 - ED(x[1..n-1],y[1..m-1]) + 0 if x[n] = y[m]
- For |x| = 0 is ED(x, y) = |y|
- For |y| = 0 is ED(x, y) = |x|



```
def edit_distance(x, y):
    if len(x) == 0:
        return len(y)
    if len(y) == 0:
        return len(x)
    ed1 = edit distance(x, y[:-1]) + 1
    ed2 = edit distance(x[:-1], y) + 1
    ed3 = edit_distance(x[:-1], y[:-1])
    if x[-1] != v[-1]:
        ed3 += 1
    return min(ed1, ed2, ed3)
```

Recursive program:

■ The algorithm results in the following recursive formular:

$$T(n,m) = T(n-1,m) + T(n,m-1) + T(n-1,m-1) + 1$$

$$\geq T(n-1,m-1) + T(n-1,m-1) + T(n-1,m-1)$$

$$= 3 \cdot T(n-1,m-1)$$

- This results in $T(n,n) \ge 3^n$
- ⇒ The runtime is at least exponential

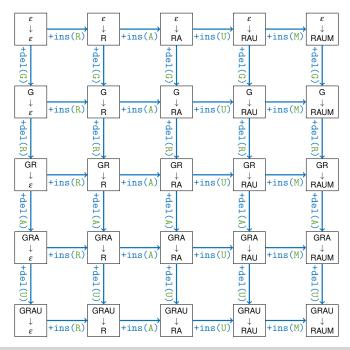
Dynamic programming:

- We create a table with all possible combination of substrings and save calculated entries
- This results in a runtime and space consumption of $O(n \cdot m)$

Visualization on the next slide:

- Operations always refer to the last position (indices are omitted)
- We also display the replaced character on a replace operation to visualize operations without costs

$$\Rightarrow$$
 repl(A, A)



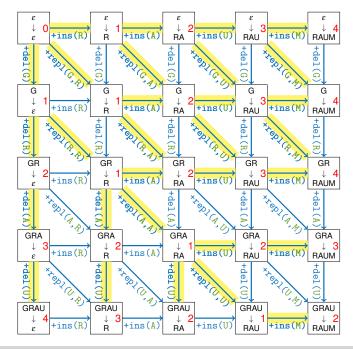
Fast algorithm

William St.

Z

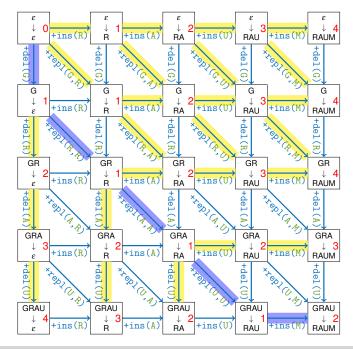
Fast algorithm:

We can determine the edit distance for all combination of partial strings from the top left to bottom right.



How to get the sequence of operations?

- We save at each recursion the most efficient previous entry (the highlighted arrows in our image)
- There can be more than one arrows to the three previous entries
- If we follow the highlighted path from (n,m) to (1,1) we get the optimum operations to transform x into y
 - If we can follow more than one path there exist more than one ideal sequence



General principle:

- Recursive computation of ...
 - ... the same reoccuring partial problems
 - a limited number of partial problems
- Computation of the solutions for all partial problems
- In a order that unsolved partial problems consist of already solved partial problems
- The "path" to our solution normally gets computed while searching the best solution
- Dijkstra algorithm is basically dynamic programming!

Additional applications:

- Edit distance: global alignment with $O(n^2)$ space and time consumption
- But: Model for deletition unrealistic
 - In evolution larger pieces are more likely
 - delete operation: first gap expensive (e.g. 2), remainding are cheaper (e.g. 0.5)

■ Solution in $O(n^3)$ time or $O(n^2)$ affine

Additional applications (II)



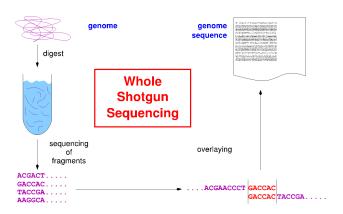
 $O(n^2)$ space consumption might be problematic:

Hirschberg algorithm:

- Divide-and-conquer approach
- O(n) space and $O(n^2)$ time consumption

Additional applications (III)





- Sequencing: $O(n^2)$ is too much
- Index: suffixtree, suffixarray, burrow-wheeler-transform

■ General

- [CRL01] Thomas H. Cormen, Ronald L. Rivest, and Charles E. Leiserson. Introduction to Algorithms. MIT Press, Cambridge, Mass, 2001.
- [MS08] Kurt Mehlhorn and Peter Sanders. Algorithms and data structures, 2008. https://people.mpi-inf.mpg.de/~mehlhorn/ftp/Mehlhorn-Sanders-Toolbox.pdf.

Dynamic programming

```
[Wik] Dynamic programming
    https:
    //en.wikipedia.org/wiki/Dynamic_programming
```

Edit distance

```
[Wik] Levenshtein distance
    https:
    //en.wikipedia.org/wiki/Levenshtein_distance
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