# UNI

# Entwurf, Analyse und Umsetzung von Algorithmen Levenshtein distance, Dynamic programming

The second secon

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Bioinformatics Group / Department of Computer Science Entwurf, Analyse und Umsetzung von Algorithmen



#### Structure



Introduction

Edit distance

#### Structure



Introduction

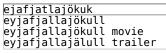
Edit distance

Measurement for similarity of two words / strings

- Measurement for similarity of two words / strings
- Algorithm for efficient calculation

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

### BioInfSearch



Search!



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#### Wikipedia.org:

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

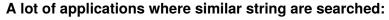
Er liegt an der äußersten Südküste, westlich des Gletschers Myrdalsjökull in der Gemeinde Rangárþing eystra, die größte Höhe beträgt 1651 m. Unter dem Gletscher befindet sich der Vulkan Eyjafjöll mit eigener Magmakammer, der seit der Besiedelung von Island in den Jahren 920, 1612 (oder 1613), 1821 bis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

## Introduction

Motivation



A lot of applications where similar string are searched:



Duplicates in databases:

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

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eyjaföllajaküll uniwersität verien 2017

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Bioinformatics: Similarity of DNA-sequences

#### Introduction

Example: Bioinformtics DNA-matching



#### Introduction

Example: Bioinformtics DNA-matching



#### Search of similar proteins:

■ BLAST (Basic Local Alignment Search Tool)

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- Alignment ê Edit distance

- BLAST (Basic Local Alignment Search Tool)
- Changed life-science completely

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- Changed life-science completely
- Cited 63437 times on Google Scholar (Sep. 2017)

#### Structure



Introduction

Edit distance





- Let x, y be two strings
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  The minimal number of operations to transform x into y
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  - Replace a character with another

- 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

# Edit distance Example



12345 DOOF

Example



```
12345
DOOF

↓ replace(1, B)
BOOF
```

```
12345

DOOF

↓ replace(1, B)

BOOF

↓ replace(2, L)

BLOF
```

Example

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

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

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

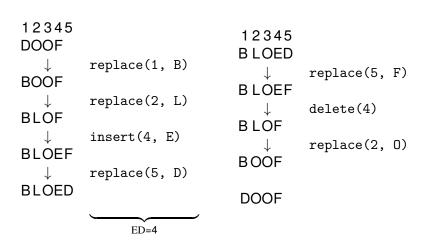
```
12345
DOOF
                                   12345
        replace(1, B)
                                  BLOED
BOOF
        replace(2, L)
BLOF
        insert(4, E)
BLOEF
                                  DOOF
        replace(5, D)
BLOED
             ED=4
```

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



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

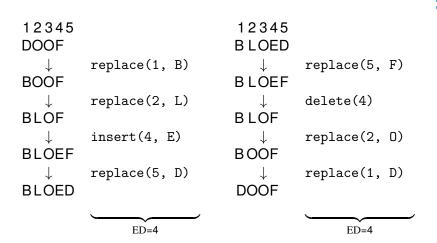






```
12345
                            12345
DOOF
                           BLOED
        replace(1, B)
                                    replace(5, F)
BOOF
                           BLOEF
        replace(2, L)
                                    delete(4)
BLOF
                           BLOF
   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







#### **Notation:**

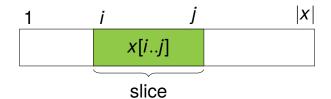
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$$\blacksquare \ \operatorname{ED}(x,y) = \operatorname{ED}(y,x)$$

- $\blacksquare$  ED(x,y) = ED(y,x)
- $\blacksquare$  ED $(x, \varepsilon) = |x|$



- $\blacksquare$  ED(x,y) = ED(y,x)
- $\blacksquare$  ED( $x, \varepsilon$ ) = |x|
- $\blacksquare$  ED $(x,y) \ge abs(|x|-|y|)$

$$abs(x) = \begin{cases} x & \text{if } x \ge 0 \\ -x & \text{else} \end{cases}$$

- $\blacksquare$  ED(x, y) = ED(y, x)
- $\blacksquare$  ED( $x, \varepsilon$ ) = |x|
- ED $(x,y) \ge abs(|x|-|y|)$  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|

■ From VERIEN to FERIEN?

- From VERIEN to FERIEN?
- From MEXIKO to AMERIKA?

- From VERIEN to FERIEN?
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- From AAEBEAABEAREEAEBA to RBEAAEEBAAAEBBAEAE?

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- Searching biggest substrings can yield the solution but doesn't have to



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#### Recursive approach:

# Solving examples

#### 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

- From VERIEN to FERIEN?
- From MEXIKO to AMERIKA?
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#### 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 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:** 



#### **Terminology:**

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



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```
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:

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

```
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                          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
```

■ **Lemma:** For any x and y with k = ED(x,y) exists a monotonous sequence of k operations for  $x \to y$ 

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■ Solve blue part recursively

Solve blue part recursively

DOOF  $\downarrow \downarrow \downarrow \downarrow \downarrow$ **BLOE** ↓insert BLOED

Figure: Case 1a

**DOOF** 111111 **BLOEDF** √delete

**BLOED** 

Figure: Case 1b

**DOOF**  $\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow$ **BLOEF** 

↓replace

**BLOED** 

Figure: Case 1c

Solve blue part recursively

## Consider the last operation:

■ Solve blue part recursively

```
WINTER

↓↓↓↓↓↓

SOMMER

↓nothing

SOMMER
```

Figure: Case 2

## Display of solution:

- Alignment
- Example:

Instances of Bellman's principle of optimality:



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

- Instances of Bellman's principle of optimality:
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Figure: Richard Bellman (1920 - 1984)



- Instances of Bellman's principle of optimality:
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Figure: Richard Bellman (1920 - 1984)

Optimal solutions consist of optimal partial solutions

- Instances of Bellman's principle of optimality:
  - Shortest paths
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- Optimal solutions consist of optimal partial solutions
  - Shortest paths: Each partial path has to be optimal

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



Figure: 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

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



Figure: 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:

lacksquare We consider the last operation  $\sigma_k$ 

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

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

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■ Let 
$$n = |x|, m = |y|, m' = |z|$$

■ We consider the last operation  $\sigma_k$ 

■ 
$$\sigma_1, ..., \sigma_{k-1}$$
:  $x \to z$  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 1a: \sigma_k = \operatorname{insert}(m' + 1, y[m]) [then m' = m - 1]
```

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

■ Case 1:  $\sigma_k$  does something at the outer end:

```
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```

```
■ 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):  $\sigma_1, \dots, \sigma_{k-1}$ : X

$$\sigma_1,\ldots,\sigma_{k-1}:X$$

$$\rightarrow$$
  $y[1..m-1]$ 



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

```
■ Case 1a (insert): \sigma_1, \ldots, \sigma_{k-1}: X \rightarrow y[1..m-1]
```

■ Case 1b (delete): 
$$\sigma_1, ..., \sigma_{k-1}$$
:  $x[1..n-1] \rightarrow y$ 

■ Case 1c (replace): 
$$\sigma_1, \ldots, \sigma_{k-1}$$
:  $x[1..n-1] \rightarrow y[1..m-1]$ 

■ Case 2 (nothing): 
$$\sigma_1, \ldots, \sigma_k$$
:  $x[1..n-1] \rightarrow y[1..m-1]$ 



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- Case 1c (replace):  $\sigma_1, \ldots, \sigma_{k-1}$ :  $x[1..n-1] \rightarrow y[1..m-1]$
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#### This results in the recursive formula:

■ For |x| > 0 and |y| > 0 is ED(x, y) the minimum of



### Case analysis:

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- Case 2 (nothing):  $\sigma_1, \ldots, \sigma_k$ :  $x[1..n-1] \rightarrow y[1..m-1]$

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



### Case analysis:

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- Case 2 (nothing):  $\sigma_1, \ldots, \sigma_k$ :  $x[1..n-1] \rightarrow y[1..m-1]$

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  - ED(x[1..n-1],y) + 1 and



## Case analysis:

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- 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  $x[n] \neq y[m]$

- Case 1a (insert):  $\sigma_1, \ldots, \sigma_{k-1}$ :  $X \rightarrow y[1..m-1]$
- Case 1b (delete):  $\sigma_1, ..., \sigma_{k-1}$ :  $x[1..n-1] \rightarrow y$
- Case 1c (replace):  $\sigma_1, \ldots, \sigma_{k-1}$ :  $x[1..n-1] \rightarrow y[1..m-1]$
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  - ED(x ,y[1..<math>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]

- Case 1a (insert):  $\sigma_1, \ldots, \sigma_{k-1}$ :  $X \rightarrow y[1..m-1]$
- Case 1b (delete):  $\sigma_1, ..., \sigma_{k-1}$ :  $x[1..n-1] \rightarrow y$
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  - $\blacksquare$  ED(x[1..n-1], y[1..m-1]) + 0 if x[n] = y[m]
- For |x| = 0 is ED(x, y) = |y|



#### Case analysis:

- Case 1a (insert):  $\sigma_1, \ldots, \sigma_{k-1}$ :  $X \rightarrow y[1..m-1]$
- Case 1b (delete):  $\sigma_1, ..., \sigma_{k-1}$ :  $x[1..n-1] \rightarrow y$
- Case 1c (replace):  $\sigma_1, \ldots, \sigma_{k-1}$ :  $x[1..n-1] \rightarrow y[1..m-1]$
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- For |x| > 0 and |y| > 0 is ED(x, y) the minimum of
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  - 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|
- $\blacksquare$  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)
```

# Edit distance Runtime analysis



**Recursive program:** 

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

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

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 Operations always refer to the last position (indices are omitted)

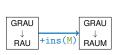
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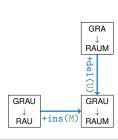
#### Visualization on the next slide:

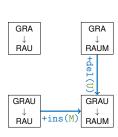
- Operations always refer to the last position (indices are omitted)
- We also display the replaced character on a replace operation to visualize operations without costs

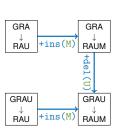
$$\Rightarrow$$
 repl(A, A)

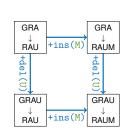
GRAU ↓ RAUM

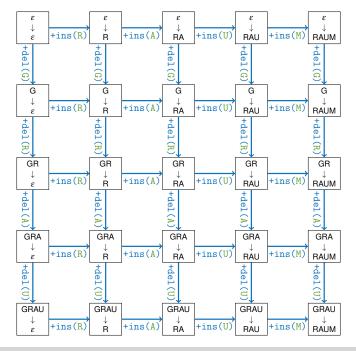












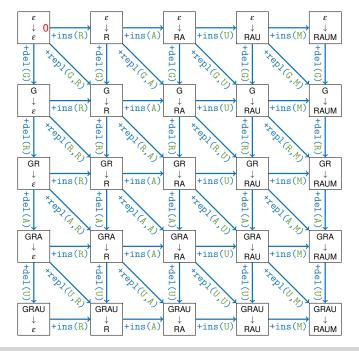
# Edit distance

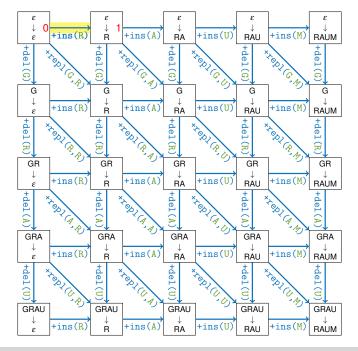
Fast algorithm

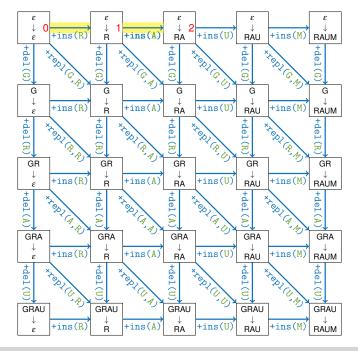


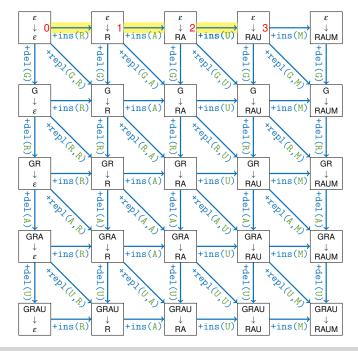
### Fast algorithm:

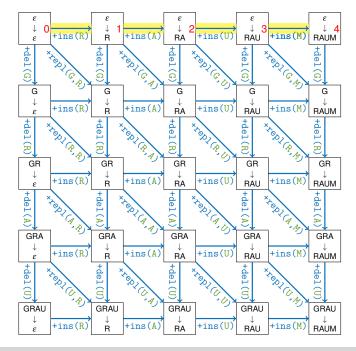
We can determine the edit distance for all combination of partial strings from the top left to bottom right.

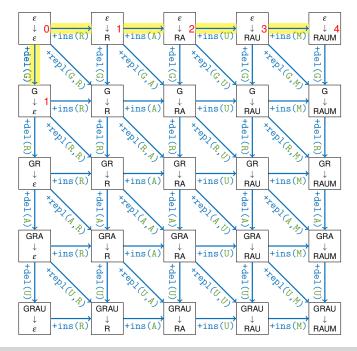


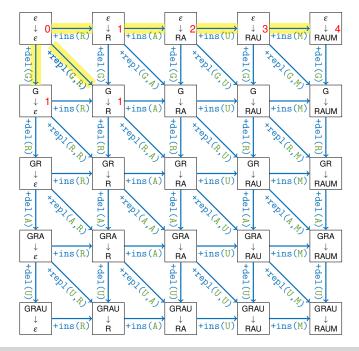


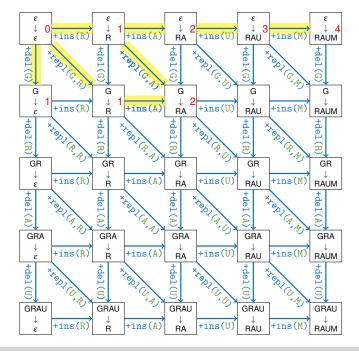


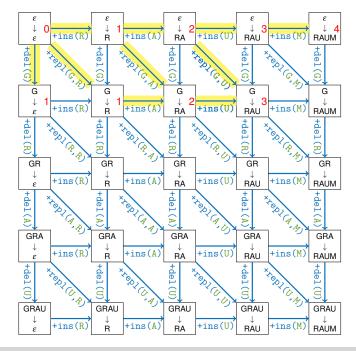


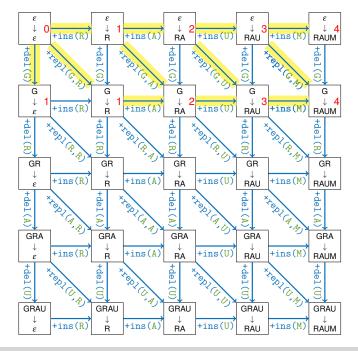


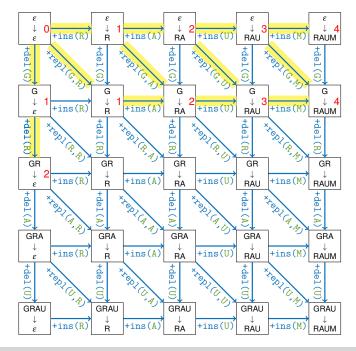


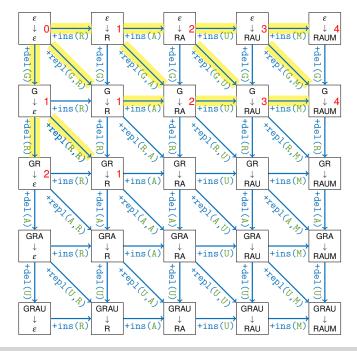


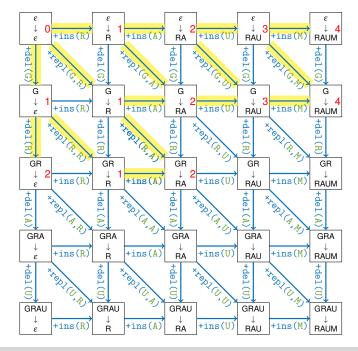


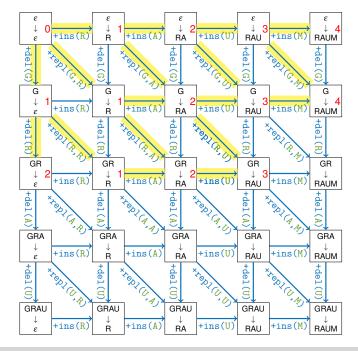


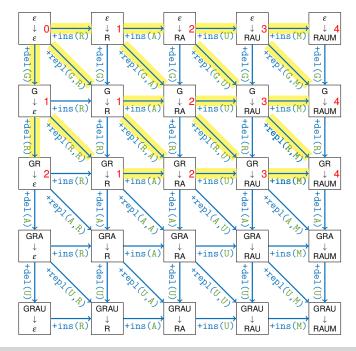


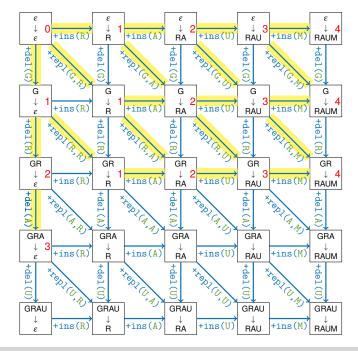


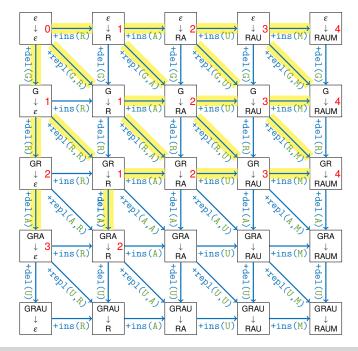


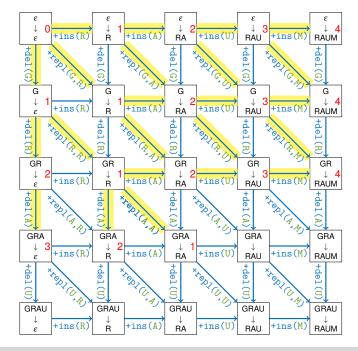




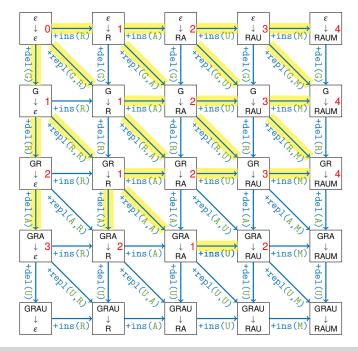




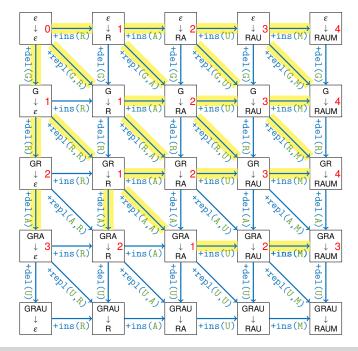




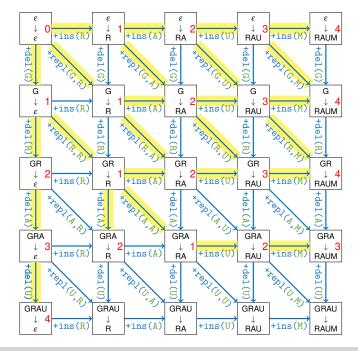
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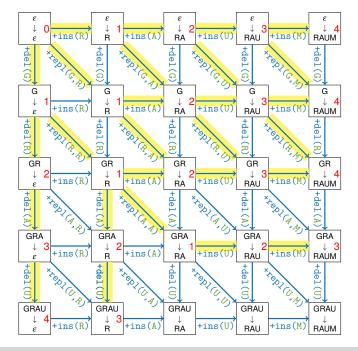
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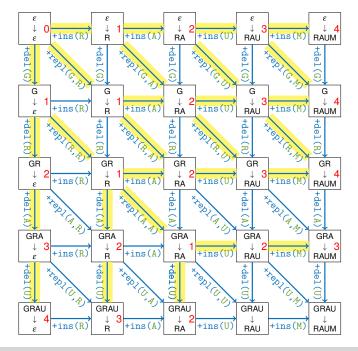


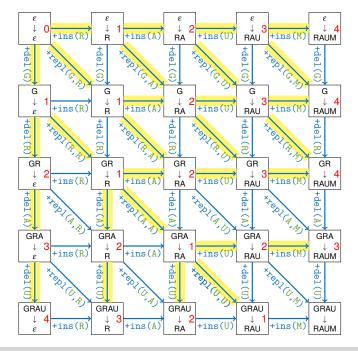
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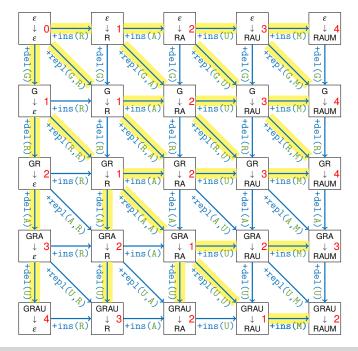


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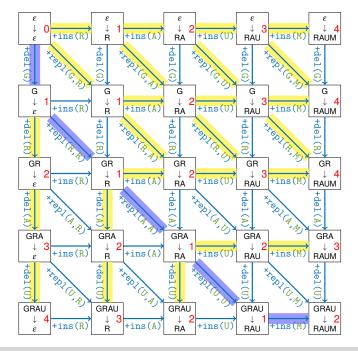


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- If we follow the highlighted path from (n,m) to (1,1) we get the optimum operations to transform x into y
  - If we can follow more than one path there exist more than one ideal sequence



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- Recursive computation of ...
  - ... the same reoccuring partial problems
  - ... a limited number of partial problems

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- 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!

#### Edit distance

Additional applications (I)



■ Edit distance: global alignment with  $O(n^2)$  space and time consumption

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

#### Edit distance

Additional applications (II)



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

Hirschberg algorithm:

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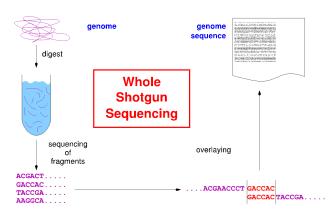
## Hirschberg algorithm:

Divide-and-conquer approach

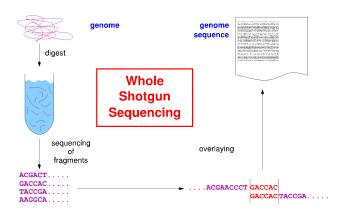
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## Hirschberg algorithm:

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





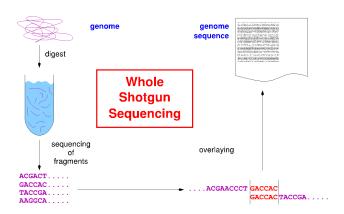


■ Sequencing:  $O(n^2)$  is too much

#### Edit distance

#### 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
```