Algorithms and Data Structures Levenshtein distance, Dynamic programming

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Bioinformatics Group / Department of Computer Science

Algorithms and Data Structures, February 2019

Structure

Introduction

Edit distance

Structure

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Edit distance

Edit distance:

Edit distance:

► Measurement for similarity of two words / strings

Edit distance:

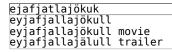
- ► Measurement for similarity of two words / strings
- ► Algorithm for efficient calculation

Edit distance:

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

Motivation: Error tolerant string comparison

BioInfSearch



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."

Motivation

A lot of applications where similar string are searched:

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

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Bioinformatics: Similarity of DNA-sequences

Example: Bioinformtics DNA-matching

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Search of similar proteins:

► BLAST (Basic Local Alignment Search Tool)

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Example: Bioinformtics DNA-matching

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

Example: Bioinformtics DNA-matching

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

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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

Example

12345 DOOF

BLOED

Example

```
12345
DOOF

↓ replace(1, B)
BOOF
```

BLOED

```
12345

DOOF

↓ replace(1, B)

BOOF

↓ replace(2, L)

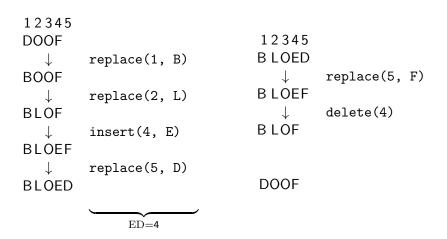
BLOF
```

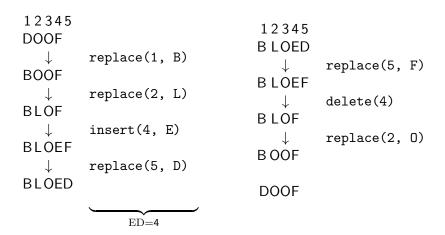
```
12345
DOOF
        replace(1, B)
BOOF
        replace(2, L)
BLOF
        insert(4, E)
BLOEF
        replace(5, D)
BLOED
             ED=4
```

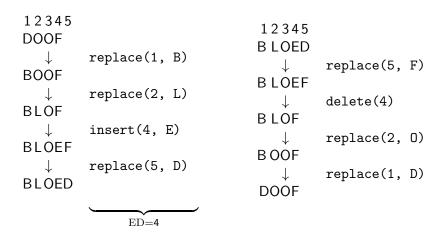
```
12345
DOOF
        replace(1, B)
                                      12345
                                     BLOED
BOOF
        replace(2, L)
BLOF
        insert(4, E)
BLOEF
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BLOED
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```
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DOOF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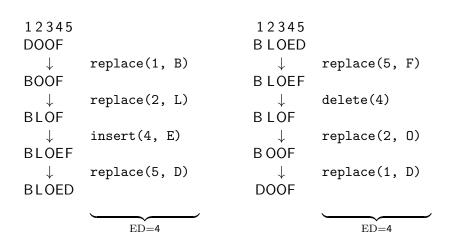
```
12345
DOOF
                              12345
        replace(1, B)
                              BLOED
BOOF
                                      replace(5, F)
        replace(2, L)
                              BLOEF
BLOF
        insert(4, E)
BLOEF
        replace(5, D)
                      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







Example



Notation:

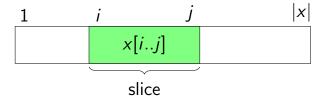
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Trivial facts:

 $\blacktriangleright \ \mathrm{ED}(x,y) = \mathrm{ED}(y,x)$

- ightharpoonup $\mathrm{ED}(x,y) = \mathrm{ED}(y,x)$
- ightharpoonup $\mathrm{ED}(x,\epsilon)=|x|$

- ightharpoonup $\mathrm{ED}(x,y) = \mathrm{ED}(y,x)$
- ightharpoonup ED(x, ϵ) = |x|
- ightharpoonup $\operatorname{ED}(x,y) \geq \operatorname{abs}(|x|-|y|)$

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

- ightharpoonup $\mathrm{ED}(x,y) = \mathrm{ED}(y,x)$
- ightharpoonup ED(x, ϵ) = |x|
- ► ED(x, y) ≥ abs(|x| |y|) abs $(x) = \begin{cases} x & \text{if } x \ge 0 \\ -x & \text{else} \end{cases}$
- ightharpoonup ED $(x,y) \le$ ED(x[1..n-1], y[1..m-1]) + 1 <math>n = |x|, m = |y|

Solving examples

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Solutions based on examples:

► From VERIEN to FERIEN?

Solving examples

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

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- ► From AAEBEAABEAREEAEBA to RBEAAEEBAAAEBBAEAE?

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Recursive approach:

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Recursive approach:

Dividing in two halves? Not a good idea:

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

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Recursive approach:

Dividing in two halves? Not a good idea:

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

Terminology:

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- Let $\sigma_1, \ldots, \sigma_k$ 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)

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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

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12345		1234567	
DOOF		SAUDOOF	
\downarrow	replace(1, B)	\downarrow	delete(1)
BOOF		AUDOOF	
\downarrow	replace(2, L)	\downarrow	delete(1)
BLOF		UDOOF	
\downarrow	insert(4, E)	\downarrow	delete(1)
BLOEF		DOOF	
\downarrow	replace(5 , D)	\downarrow	insert(4, 0)
BLOED		DOOOF	

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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

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- ▶ **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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```
1 2 3 4 5 6 7 D O O F S A U D O O F B L O E D D O O O F
```

Recursive approach

Consider the last operation:

Recursive approach

Consider the last operation:

► Solve blue part recursively

Recursive approach

Consider the last operation:

► Solve blue part recursively

DOOF	DOOF	
$\downarrow\downarrow\downarrow\downarrow\downarrow$	$\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow$	
BLOE	BLOEDF	
\downarrow insert	\downarrow delete	
BLOED	BLOED	
Figure: Case 1a	Figure: Case 1b	

17/36

DOOF

BLOEF

BLOED

↓replace

Figure: Case 1c

Recursive approach

Consider the last operation:

Recursive approach

Consider the last operation:

► Solve blue part recursively

Recursive approach

Consider the last operation:

► Solve blue part recursively

```
WINTER

↓↓↓↓↓↓

SOMMER

↓nothing

SOMMER
```

Figure: Case 2

Display of solution:

- Alignment
- Example:

```
_ _ B L O E D S A U B L O E D
```

Dynamic programming

Dynamic programming

Dynamic programming:

Instances of Bellman's principle of optimality:

Dynamic programming

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

Dynamic programming

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

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Figure: Richard Bellman (1920 - 1984)

Optimal solutions consist of optimal partial solutions

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Figure: Richard Bellman (1920 - 1984)

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

Dynamic programming

- Instances of Bellman's principle of optimality:
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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

Dynamic programming

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

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

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

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► Let n = |x|, m = |y|, m' = |z|

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

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

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

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• Case 1b: $\sigma_k = \text{delete}(m')$ [then m' = m + 1]

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Case 1a: \sigma_k = \operatorname{insert}(m'+1, y[m]) [then m' = m-1]
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Case 1c: \sigma_k = \operatorname{replace}(m', y[m]) [then m' = m]
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► Case 2: σ_k does nothing at the outer end:

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```

- \triangleright Case 2: σ_k does nothing at the outer end:
 - ► Then z[m'] = y[m] and x[n'] = z[m'] and with that $\sigma_1, \ldots, \sigma_{k-1} \colon x[1..n-1] \to y[1..m-1]$ and x[n] = y[m]

Case analysis:

▶ Case 1a (insert): $\sigma_1, \ldots, \sigma_{k-1}$: \times $\rightarrow y[1..m-1]$

- ► 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 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

Case analysis:

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

- 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 1b (delete): $\sigma_1, \ldots, \sigma_{k-1}$: $x[1..n-1] \rightarrow y$
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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
 - ► ED(x[1..n-1], y) + 1 and

Case analysis:

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 - ► ED(x[1..n-1], y[1..m-1]) + 0 if x[n] = y[m]

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 - ightharpoonup ED(x[1..n-1], y[1..m-1]) + 0 if x[n] = y[m]
- ► For |x| = 0 is ED(x, y) = |y|

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- For |x| = 0 is ED(x, y) = |y|
- ► For |y| = 0 is ED(x, y) = |x|

Implementation - Python

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

Runtime analysis

Recursive program:

Runtime analysis

Recursive program:

▶ The algorithm results in the following recursive formular:

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

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

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

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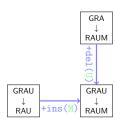
Visualization on the next slide:

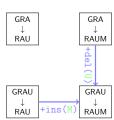
- Operations always refer to the last position (indices are omitted)
- We also display the replaced character on a replace operation to visualize operations without costs

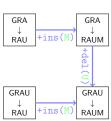
```
\Rightarrow repl(A, A)
```

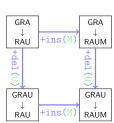


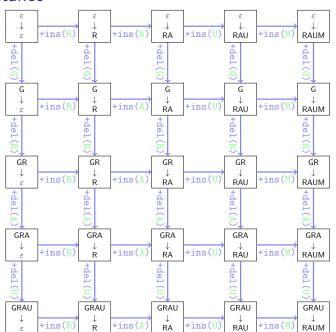








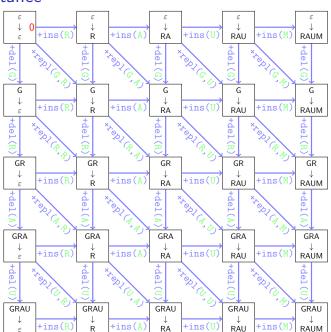


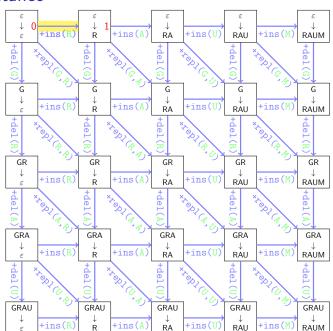


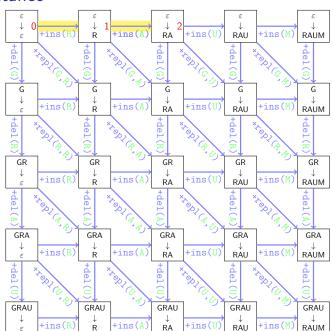
Fast algorithm

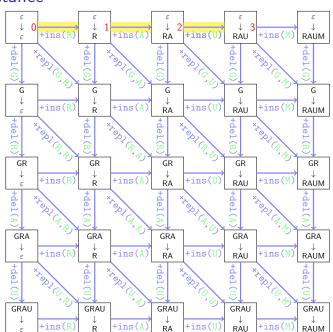
Fast algorithm:

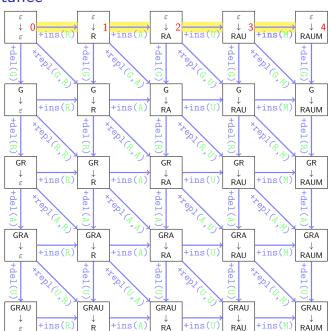
We can determine the edit distance for all combination of partial strings from the top left to bottom right.

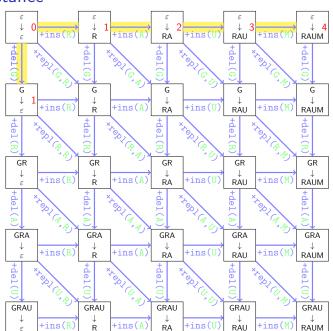


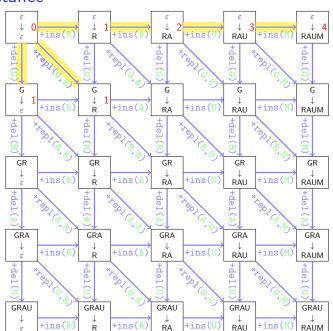


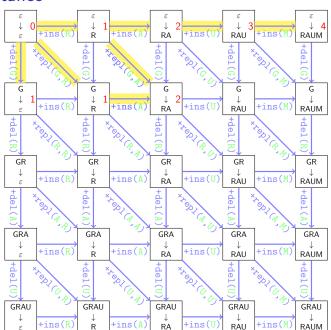


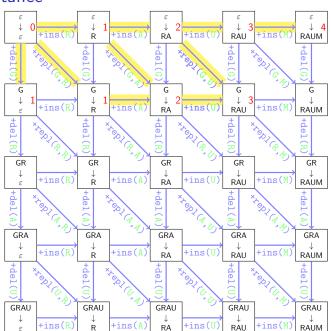


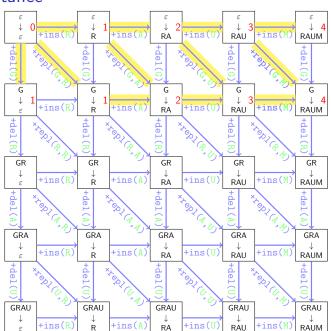


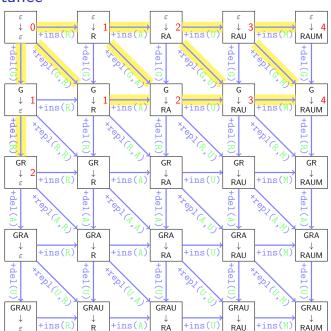


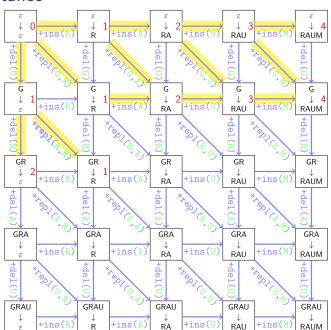


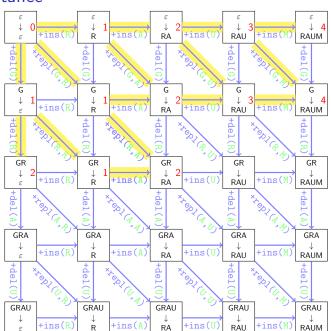


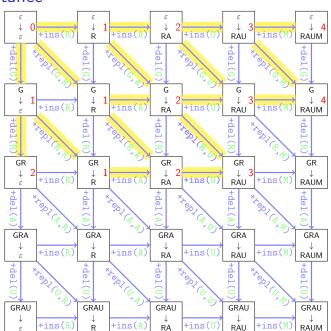


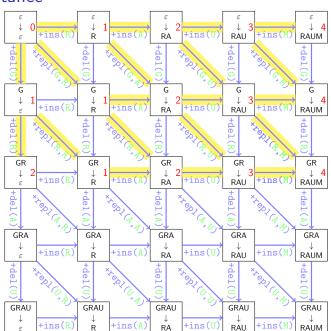


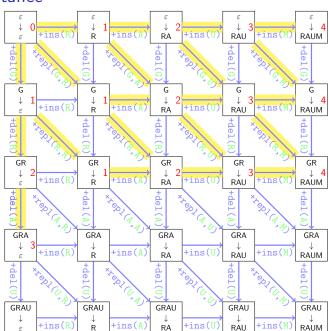


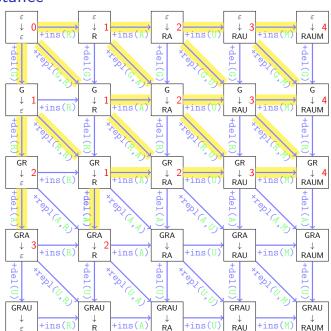


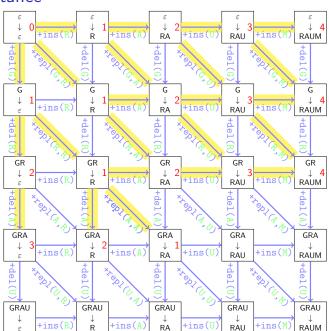


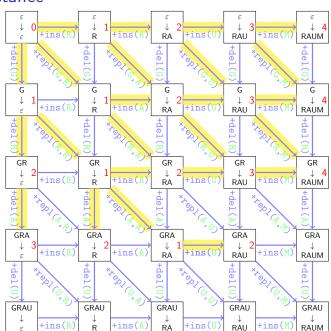


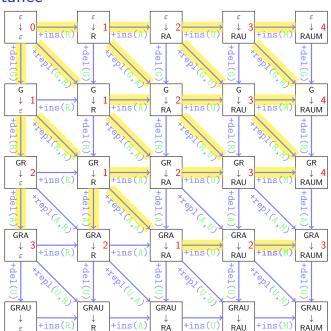


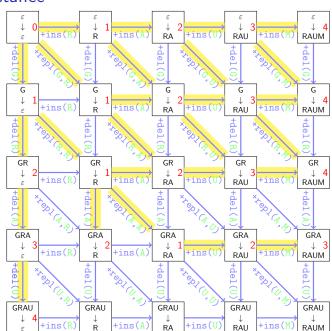


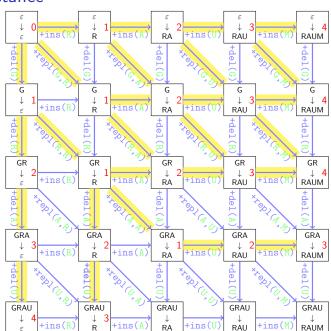


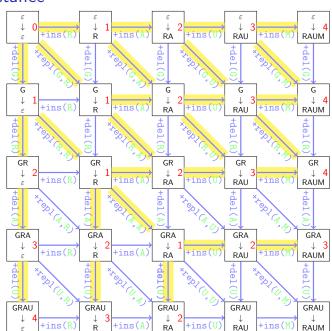


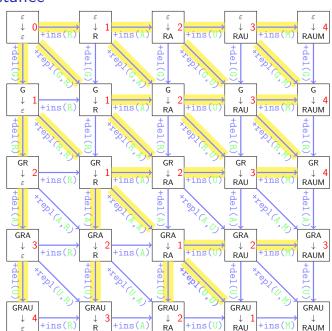


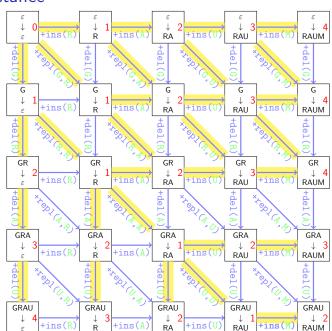












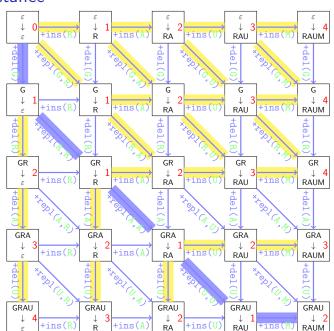
How to get the sequence of operations?

 We save at each recursion the most efficient previous entry (the highlighted arrows in our image)

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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



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

- ► Recursive computation of ...
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- 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 (I)

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Additional applications:

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

Additional applications (I)

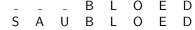
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▶ Solution in $O(n^3)$ time or $O(n^2)$ affine

Additional applications (II)

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

Hirschberg algorithm:

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

Hirschberg algorithm:

▶ Divide-and-conquer approach

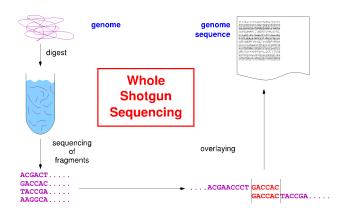
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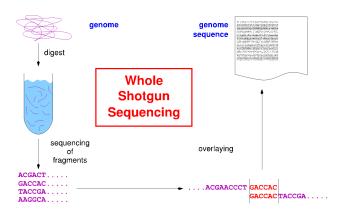
Hirschberg algorithm:

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

Additional applications (III)

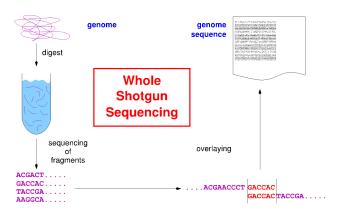


Additional applications (III)



▶ Sequencing: $O(n^2)$ is too much

Additional applications (III)



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

Further Literature

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.

Further Literature

Dynamic programming

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

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