Departement Informatik

Programming and Problem-Solving

Dynamic Programming

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Spring 2021 – Mai 6, 2021

Recursive Sorting and Searching

$\mathcal{O}(n \log_2 n)$ Sorting Algorithms

Iterative Mergesort

8	3	1	5	6	2	4	7

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```
[8, 3, 1, 5, 6, 2, 4, 7]
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[[8], [3], [1], [5], [6], [2], [4], [7]]
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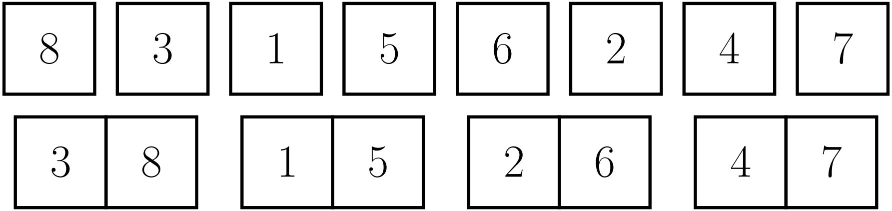
Iterative Mergesort



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[[3, 8], [1, 5], [2, 6], [4, 7]]
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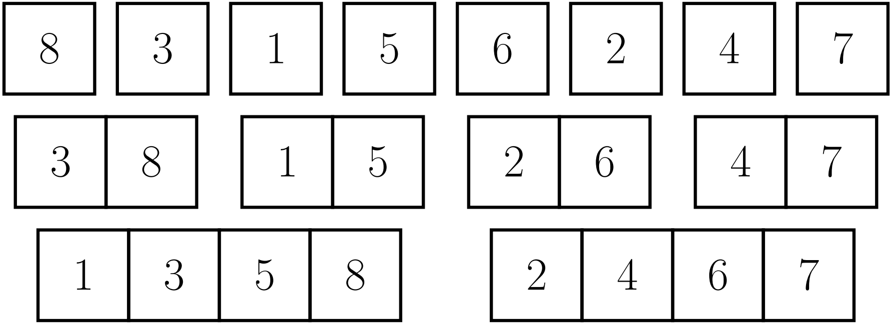

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```

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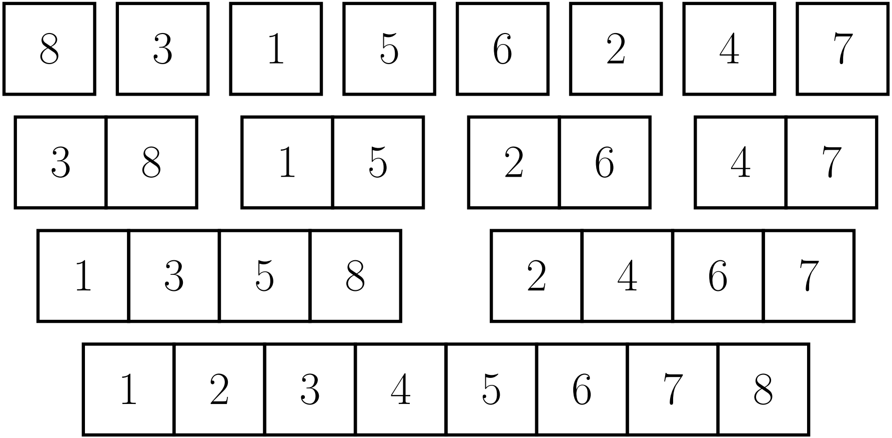

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Iterative Mergesort

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```
def merge(leftdata, rightdata):
    result = []
    while len(leftdata) > 0 and len(rightdata) > 0:
        if leftdata[0] > rightdata[0]:
            result.append(rightdata.pop(0))
        else:
            result.append(leftdata.pop(0))
    return result + leftdata + rightdata
```

Recursive Mergesort

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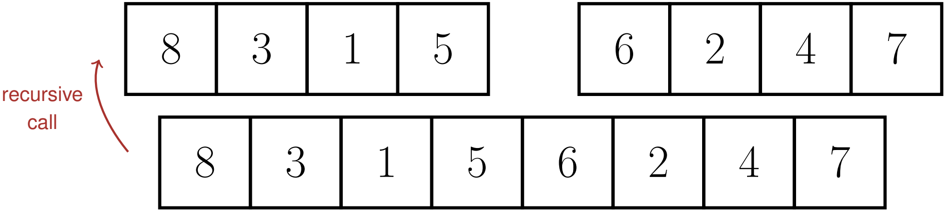
Recursive Mergesort



8	3	1	5

6	2	4	7

recursive call

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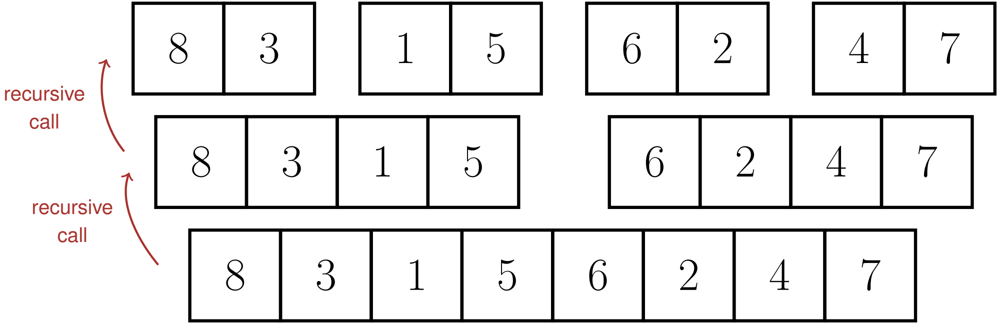
Recursive Mergesort



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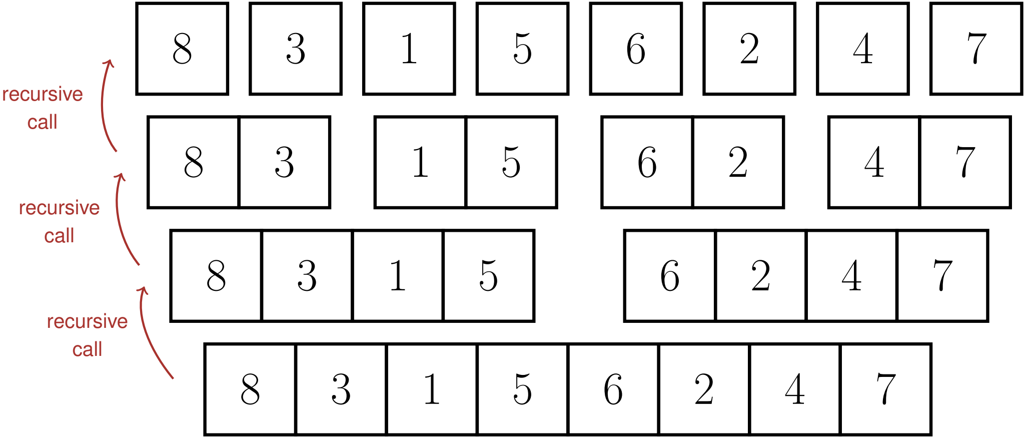

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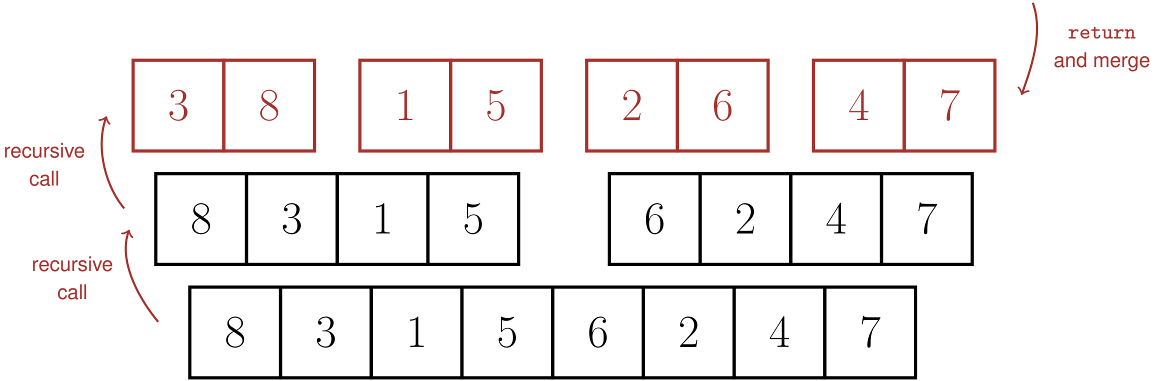

`return`
and merge

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recursive
call

8 3 1 5 | 6 2 4 7

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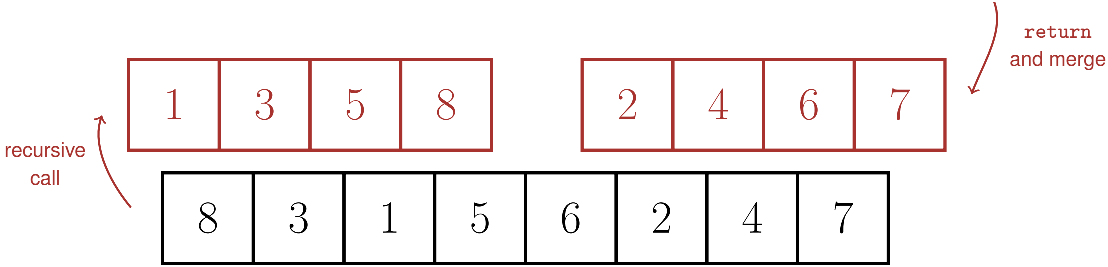
Recursive Mergesort



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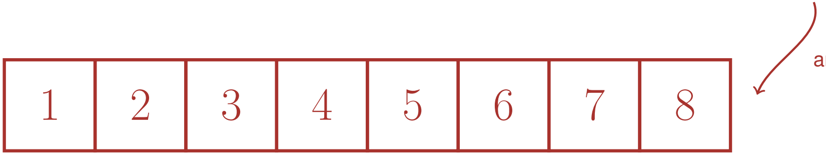

1	2	3	4	5	6	7	8

`return`
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Recursive Mergesort

Mergesort as a recursive Python function

- that takes a list as parameter
- splits it in the middle into two lists
- calls the algorithm recursively on these lists
- merges the lists that are sorted this way, and returns them

Recursive Mergesort

```
def mergesort(data):
    if len(data) <= 1:
        return data
    mid = len(data) // 2
    leftdata = mergesort(data[:mid])
    rightdata = mergesort(data[mid:])
    result = []
    while len(leftdata) > 0 and len(rightdata) > 0:
        if leftdata[0] > rightdata[0]:
            result.append(rightdata.pop(0))
        else:
            result.append(leftdata.pop(0))

    return result + leftdata + rightdata
```

Recursive Sorting and Searching

$\mathcal{O}(n \log_2 n)$ Sorting Algorithms – Quicksort

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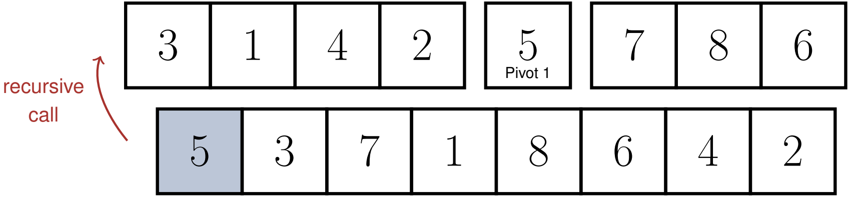
- Call algorithm recursively on these lists
- Concatenate lists that are sorted this way

Recursive Quicksort

5	3	7	1	8	6	4	2

Recursive Quicksort



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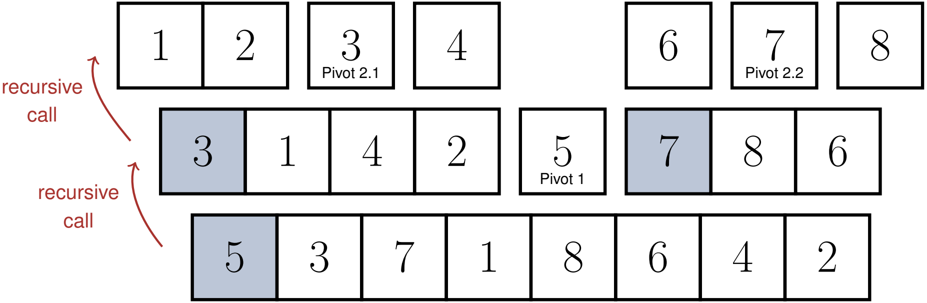

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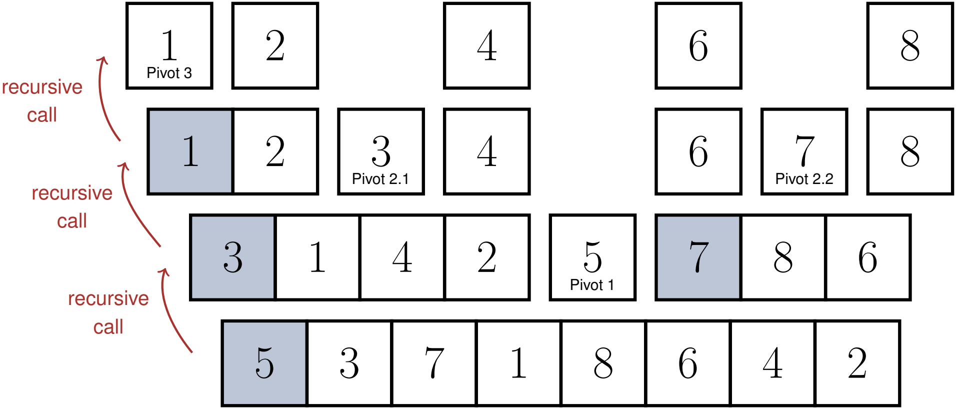

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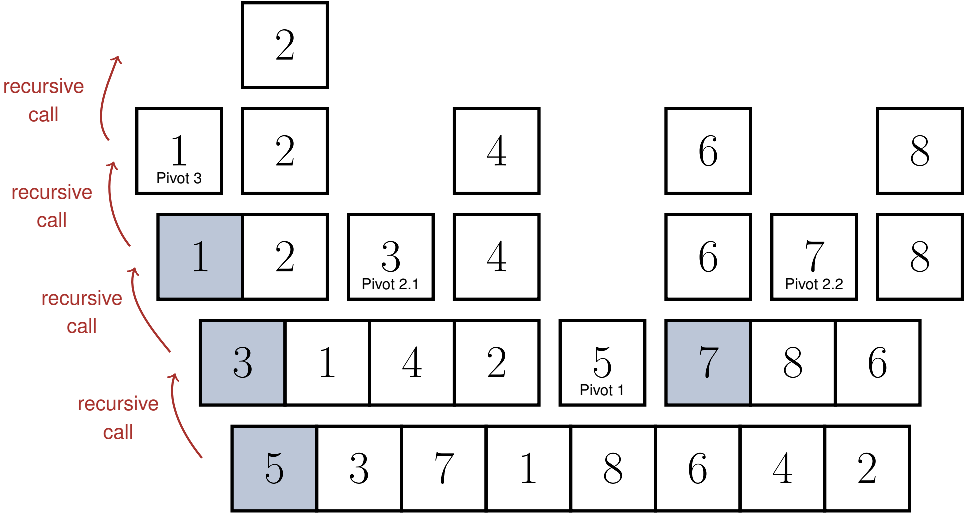

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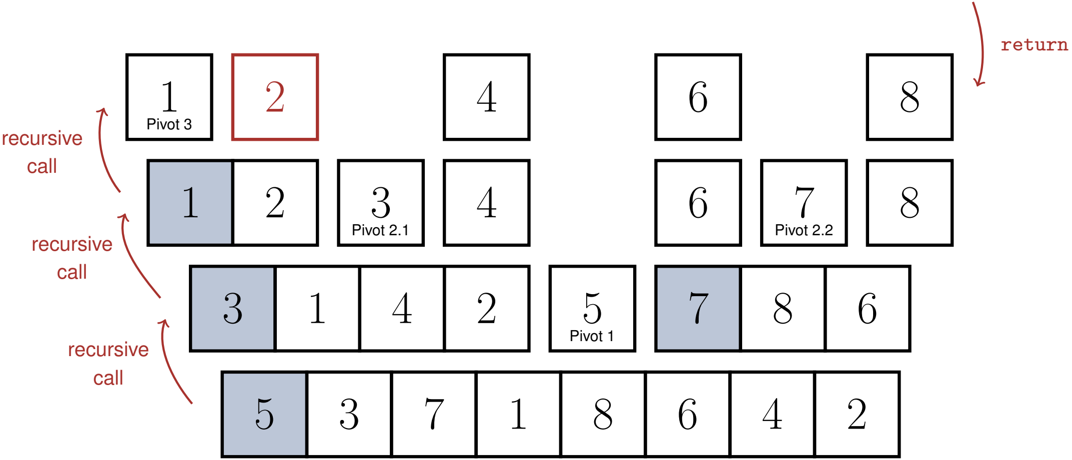

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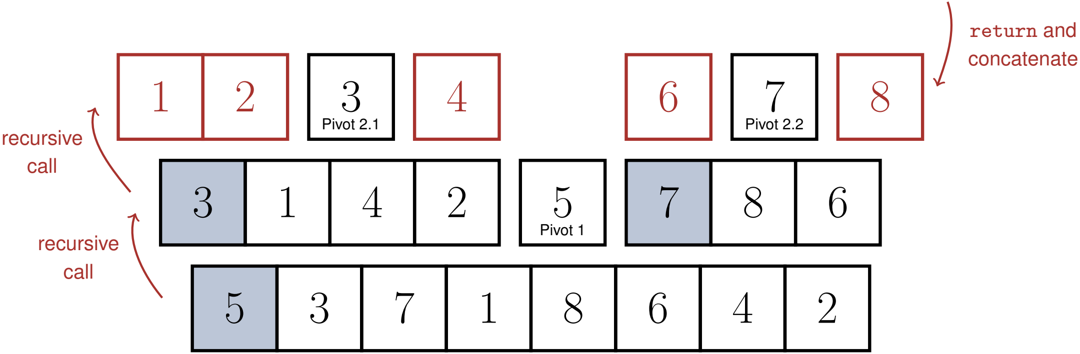

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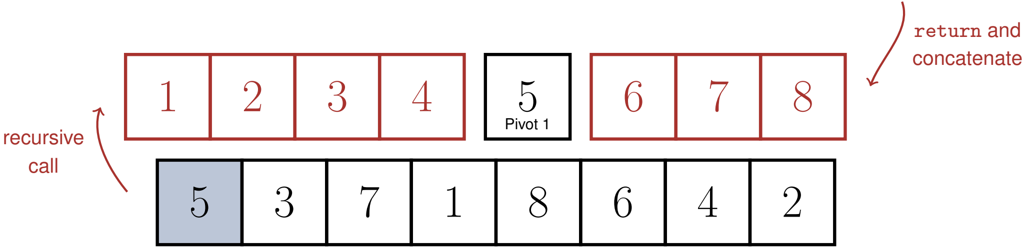

return and concatenate

1 2 3 4 | 5 Pivot 1 | 6 7 8

recursive call

5 3 7 1 8 6 4 2

Recursive Quicksort

`return` and concatenate

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Recursive Quicksort

Quicksort as a recursive Python function

- that takes a list `data`
- chooses the first element of `data` as pivot element
- creates a list with smaller and a list with larger elements
- calls the algorithm recursively on these lists
- concatenates and returns the lists that are sorted this way and the pivot element

Recursive Quicksort

```
def quicksort(data):
    if len(data) <= 1:
        return data
    else:
        pivot = data[0]
        leftdata = [i for i in data[1:] if i < pivot]
        rightdata = [i for i in data[1:] if i >= pivot]
        return quicksort(leftdata) + [pivot] + quicksort(rightdata)
```

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Restriction through access via index, e.g., if all data are associated with indices, but there is not data for all possible indices

Python Dictionaries

Key-Value pairs

Access not through index, but self-defined “key”

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- Keys and values are separated by colon

```
data = {10 : "Wert 1", 16 : "Wert 2", 39 : "Wert 3" }
data = {"eins" : "Wert 1", "zwei" : "Wert 2", "pi" : 3.14 }
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- Access value with key `key` with `[key]`

```
print(data[16])
```

Fibonacci Numbers

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- The sequence of Fibonacci numbers is defined as

$$1, 1, 2, 3, 5, 8, 13, 21, 34, \ldots,$$

- A number of the sequence is given by the sum of its two predecessors; the first two numbers are both 1

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- Can be found in many natural phenomena… or at Zurich main station

Fibonacci Numbers

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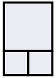

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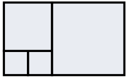

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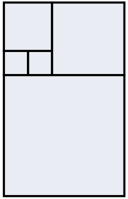

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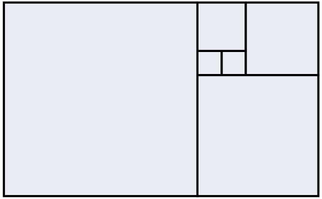

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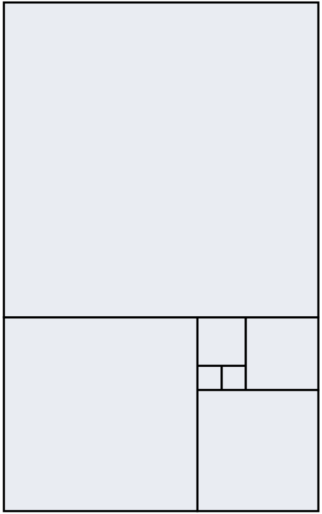

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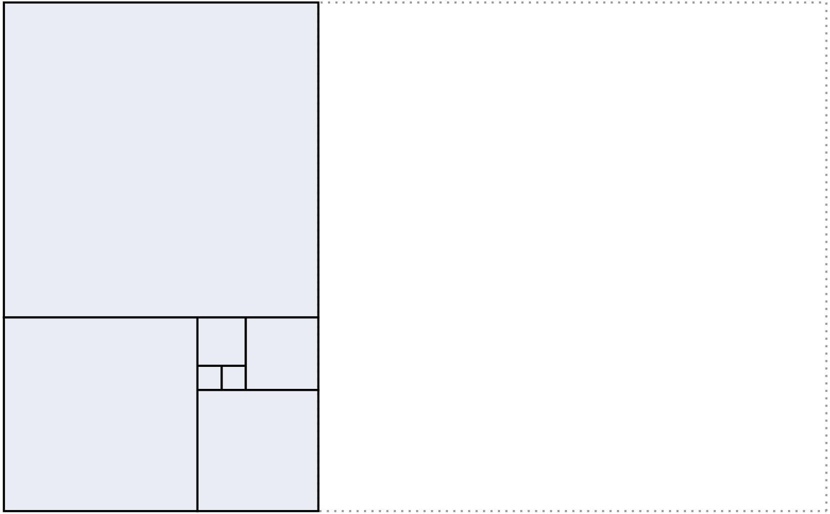

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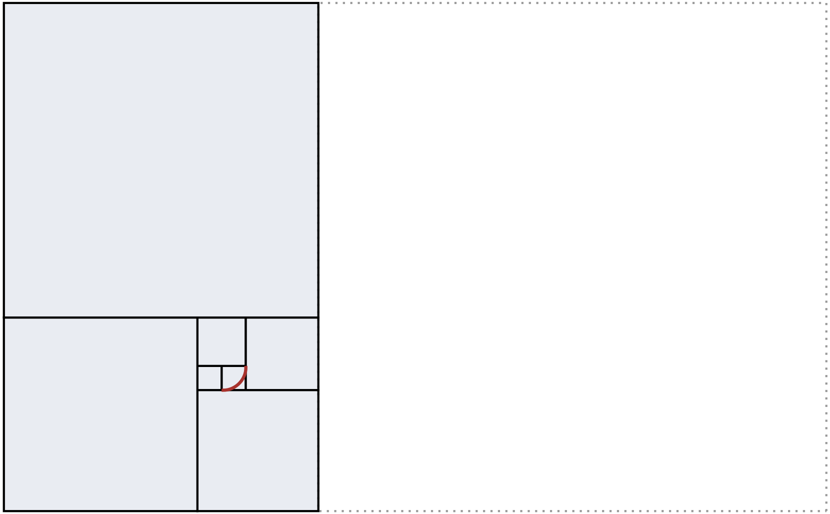

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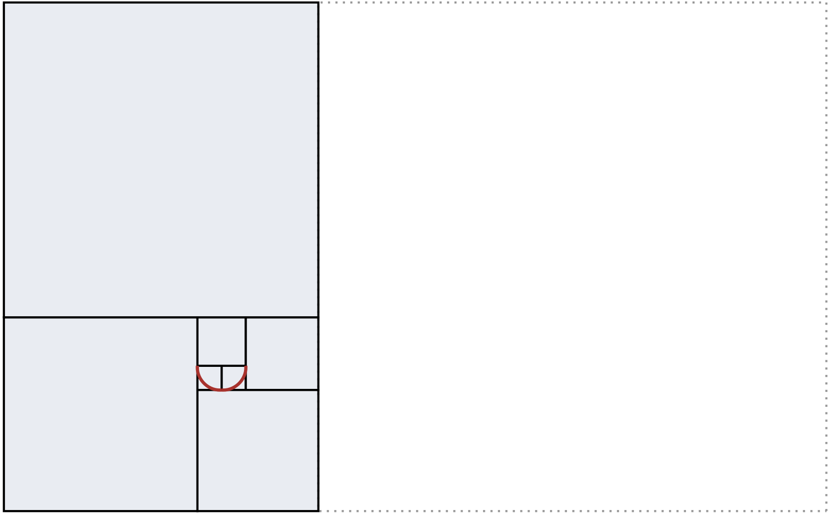

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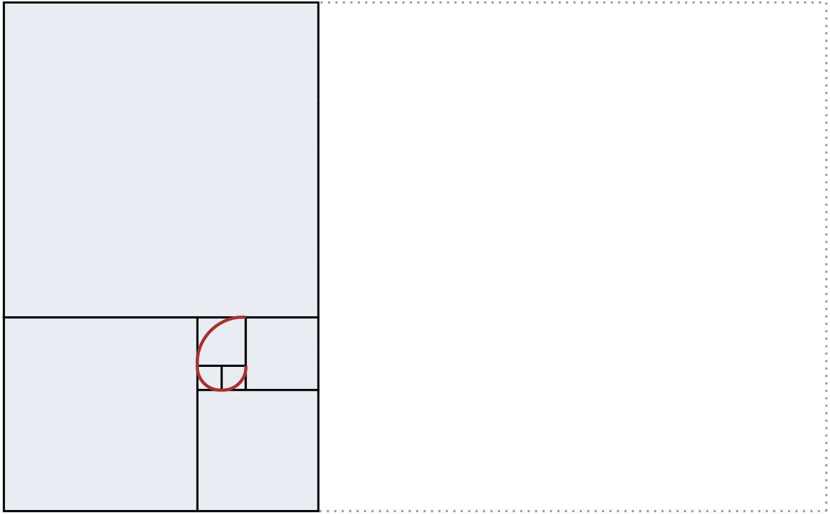

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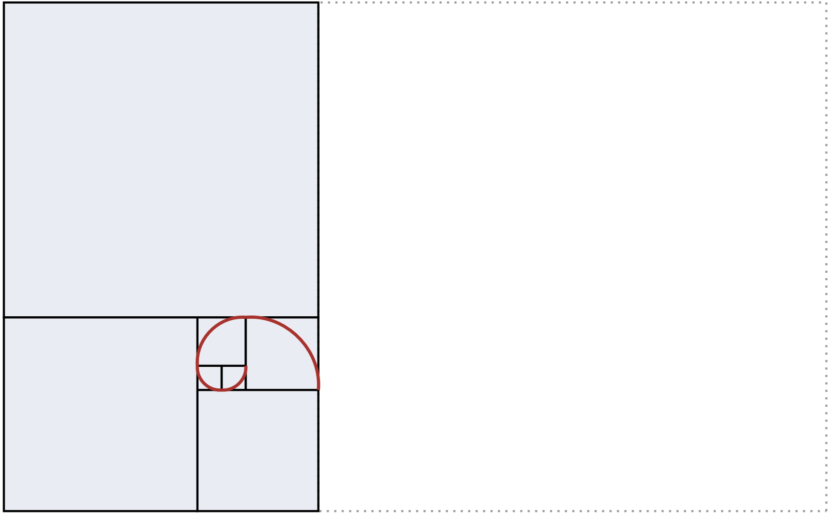

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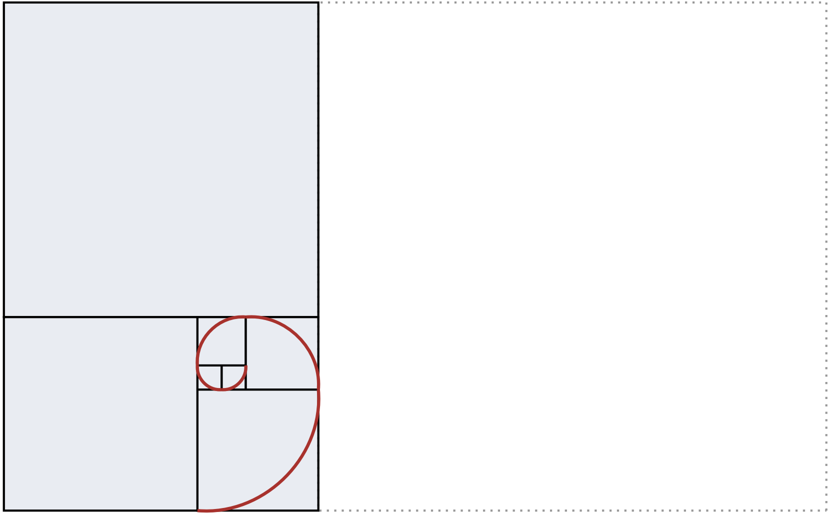

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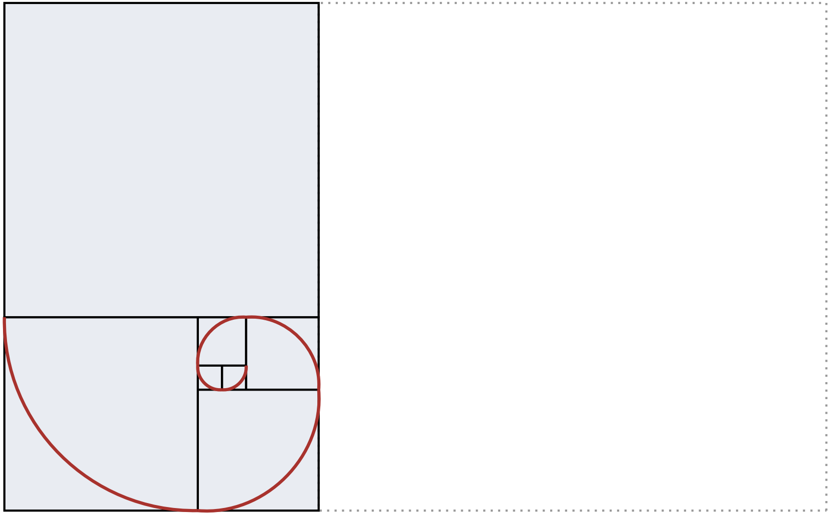

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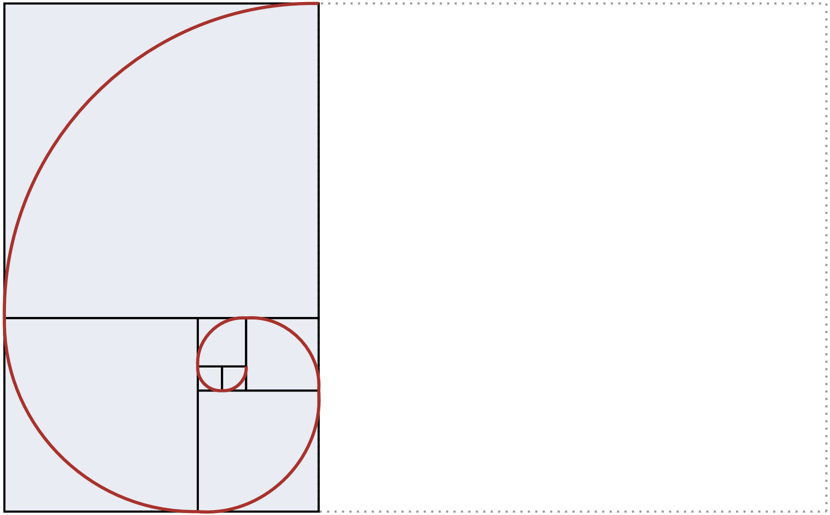

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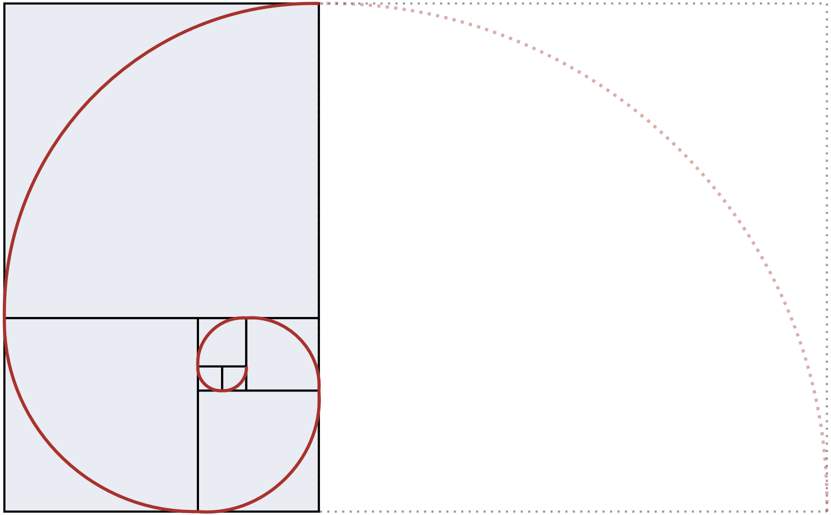

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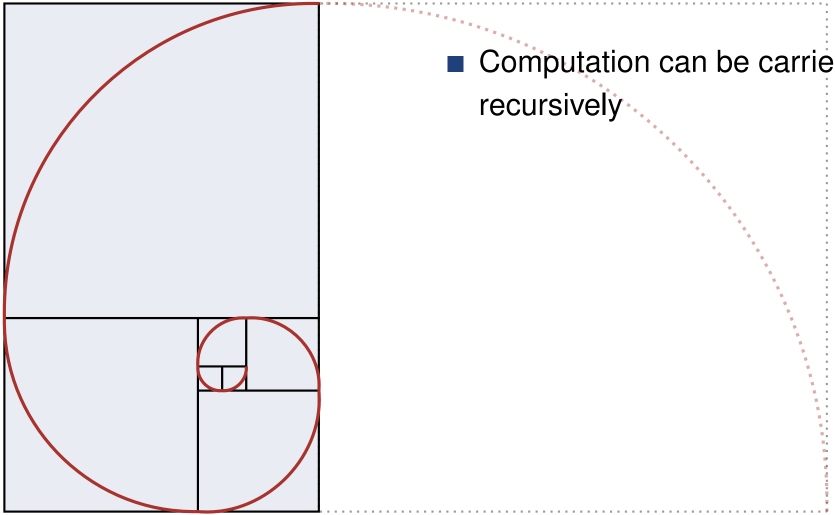
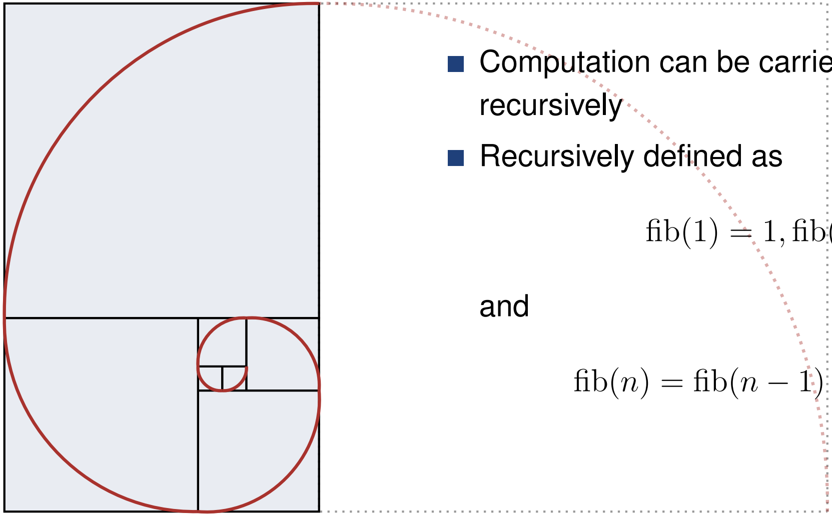


- Computation can be carried out iteratively or recursively

Fibonacci Numbers



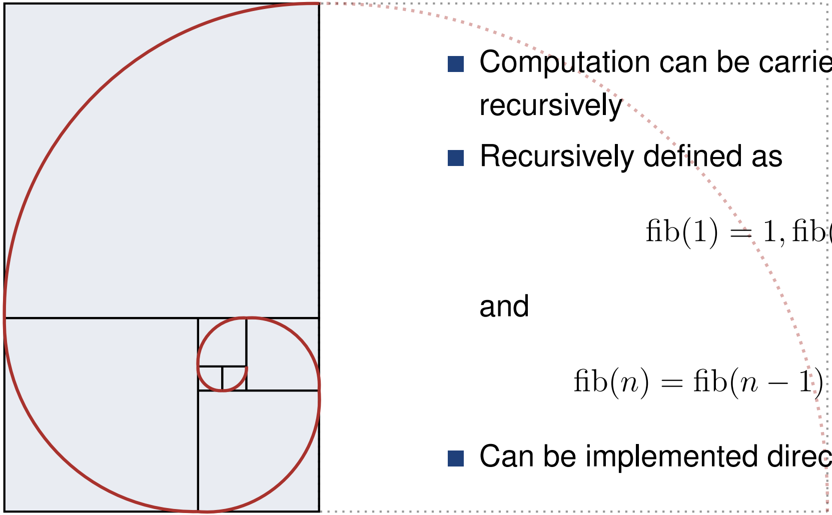
- Computation can be carried out iteratively or recursively
- Recursively defined as

$$\mathrm{fib}(1) = 1, \mathrm{fib}(2) = 1$$

and

$$\mathrm{fib}(n) = \mathrm{fib}(n-1) + \mathrm{fib}(n-2)$$

Fibonacci Numbers



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- Can be implemented directly in Python

Exercise – Computing Fibonacci Numbers Recursively

Implement a recursive function that

- takes a parameter `n`
- and returns the `n`th Fibonacci number

Then output the first 20 Fibonacci numbers

Computing Fibonacci Numbers Recursively

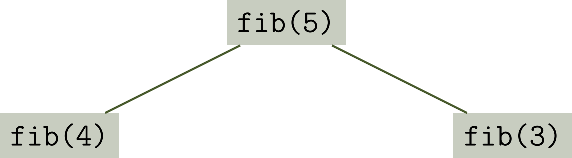
```
def fib(n):
    if n == 1 or n == 2:
        return 1
    else:
        return fib(n-1) + fib(n-2)

for i in range(1, 21):
    print(fib(i), end=" ")
```

Computing Fibonacci Numbers Recursively

`fib(5)`

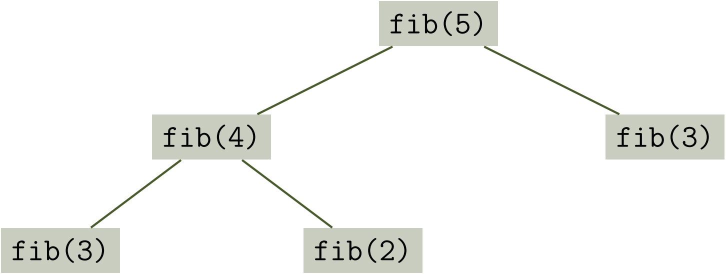
Computing Fibonacci Numbers Recursively



`fib(5)`

`fib(4)` `fib(3)`

Computing Fibonacci Numbers Recursively



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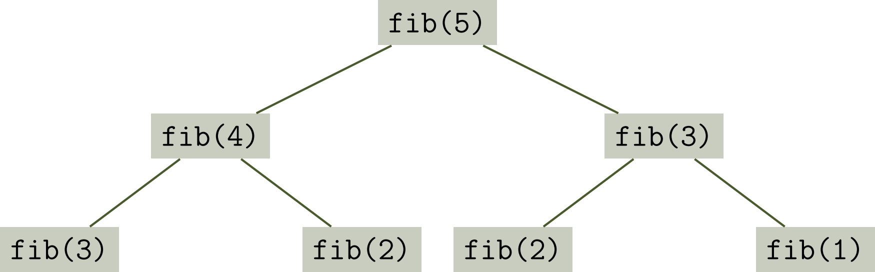
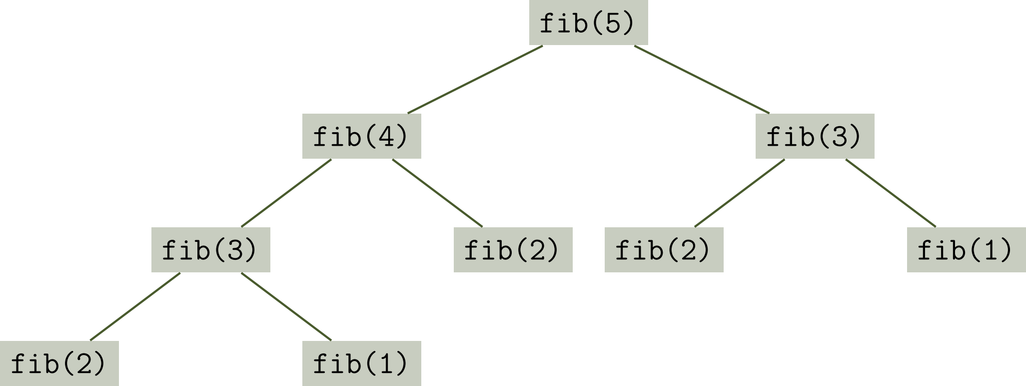


`fib(5)`

`fib(4)` `fib(3)`

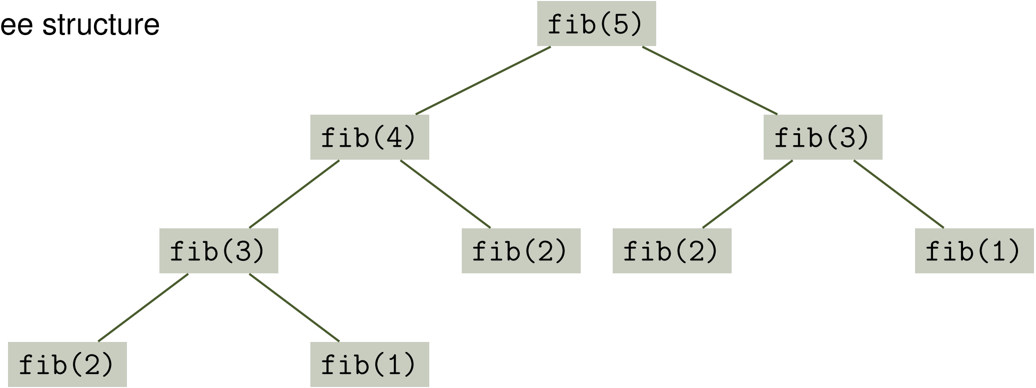
`fib(3)` `fib(2)` `fib(2)` `fib(1)`

Computing Fibonacci Numbers Recursively



Computing Fibonacci Numbers Recursively

Tree structure



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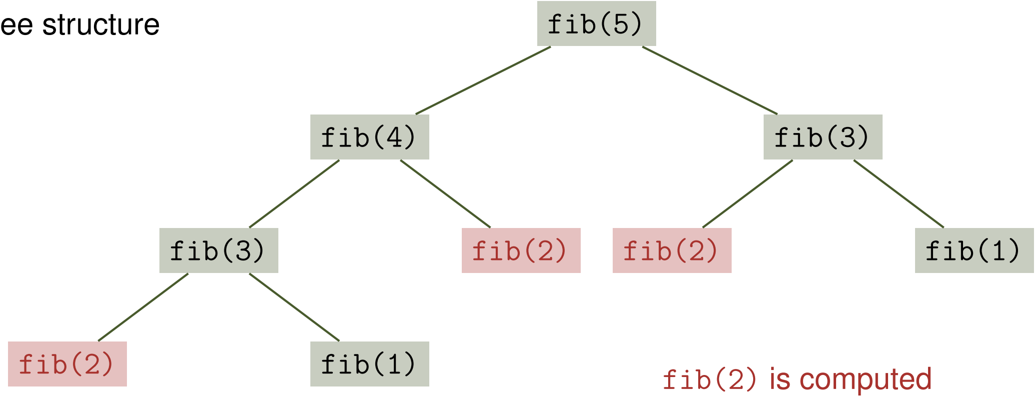

`fib(2)` is computed three times, for instance

Memoization

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- Function `fib` is called repeatedly with identical parameter values

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> - `fib(n)` calls `fib(n-1)` and `fib(n-2)`
> - `fib(n-1)` again calls `fib(n-2)`
> - `fib(n-2)` calls the whole subtree both times

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- Store values in dictionary
- This can be a global variable or passed as parameter

Exercise – Fibonacci Numbers with Memoization

Implement a recursive function that

- takes a parameter `n`
- and returns the `n`th Fibonacci number
- while using a dictionary to implement memoization, looking up the given value using `in`

Then output the first 200 Fibonacci numbers

Fibonacci Numbers with Memoization

```
memo = {1: 1, 2: 1}

def fib(n):
    if n in memo:
        return memo[n]
    else:
        memo[n] = fib(n-1) + fib(n-2)
        return memo[n]


for i in range(1, 201):
    print(fib(i))
```

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- Find data structure for molecules
- Define a reasonable similarity measure
- Design an algorithm to compute the similarity with respect to the measure efficiently

Modelling the Data – Molecules as Strings

Representation as strings

DNA are chainlike molecules that consist of repeated building blocks (cytosine, guanine, adenine, and thymine)

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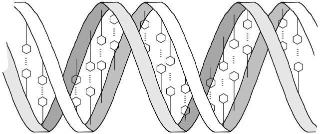

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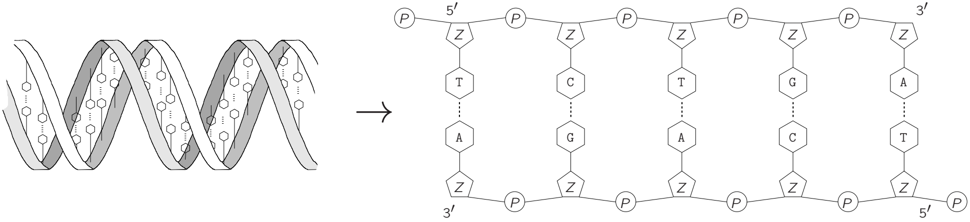

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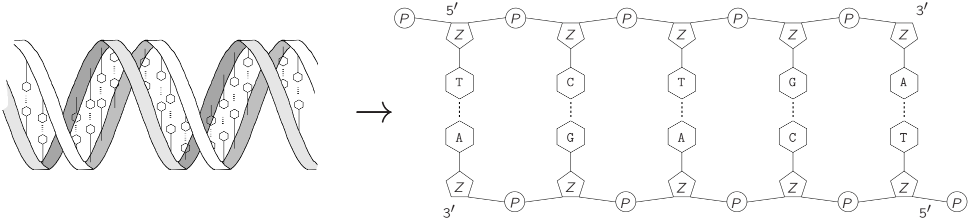

→ `TCTGA`

Alignments – Similarity Measure

Similarity measure should reflect **common changes** in DNA sequences

- Exchange of single bases of amino acids
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Two consecutive gaps do not make sense and are therefore assumed not appear

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Idea for penalties

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- **Goal:** Minimize penalty
- Example for penalties: **edit distance**

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Levenshtein, 1966

Count mismatches and gaps, i.e.,

- $g = 1$
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Edit distance: $d_{\text{edit}}(s', t') = 3 \quad d_{\text{edit}}(s'', t'') = 5 \quad d_{\text{edit}}(s''', t''') = 10$

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  - This already leads to 3^n alignments

Exponential Time Complexity

n	10	50	100	300	10 000
$10n$	100	500	1 000	3 000	100 000
$3n^2$	300	7 500	30 000	270 000	300 000 000
n^3	1 000	125 000	1 000 000	27 000 000	13 digits
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The Algorithm of Needleman and Wunsch

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- Memoization is closely related to dynamic programming
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- **Bellman equation:** Optimal solution can be computed from optimal solutions to subproblems

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Needleman and Wunsch, 1970

- All pairs of prefixes of the given strings are subproblems
- Compute alignments of longer prefixes from optimal alignments of shorter prefixes

Example for the Alignment of Prefixes

Compute optimal alignment of $s = \texttt{ATG}$ and $t = \texttt{TAG}$

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$$\underbrace{\begin{array}{|c|}\hline \texttt{AT} \\ \hline \texttt{TA} \\ \hline\end{array}}_{d_{\text{edit}}(\texttt{AT},\texttt{TA})}\underbrace{\begin{array}{c|}\hline \texttt{G} \\ \texttt{G} \\ \hline\end{array}}_{+0} \qquad \underbrace{\begin{array}{|c|}\hline \texttt{AT} \\ \hline \texttt{TAG} \\ \hline\end{array}}_{d_{\text{edit}}(\texttt{AT},\texttt{TAG})}\underbrace{\begin{array}{c|}\hline \texttt{G} \\ - \\ \hline\end{array}}_{+1} \qquad \underbrace{\begin{array}{|c|}\hline \texttt{ATG} \\ \hline \texttt{TA} \\ \hline\end{array}}_{d_{\text{edit}}(\texttt{ATG},\texttt{TA})}\underbrace{\begin{array}{c|}\hline - \\ \texttt{G} \\ \hline\end{array}}_{+1}$$

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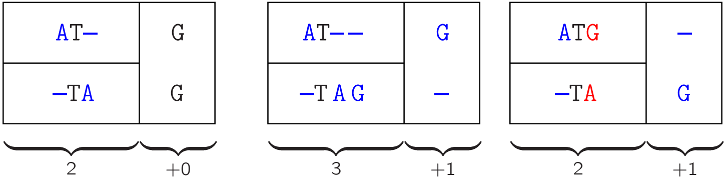

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Optimal alignment with edit distance $d_{\text{edit}}(s', t') = 2$:

$$\begin{aligned} s' &= \texttt{AT-G} \\ t' &= \texttt{-TAG} \end{aligned}$$

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- The **empty string** is a string of length 0
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Penalty: $d_{\text{edit}}(s_1 \ldots s_i, \lambda) = d_{\text{edit}}(\lambda, t_1 \ldots t_i) = i$

Filling out the Penalty Table

s \ t	0	C 1	C 2	T 3	G 4
0					
A 1					
C 2					
T 3					
T 4					
G 5					

Filling out the Penalty Table

s \ t	0	C 1	C 2	T 3	G 4
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Insert gap in t

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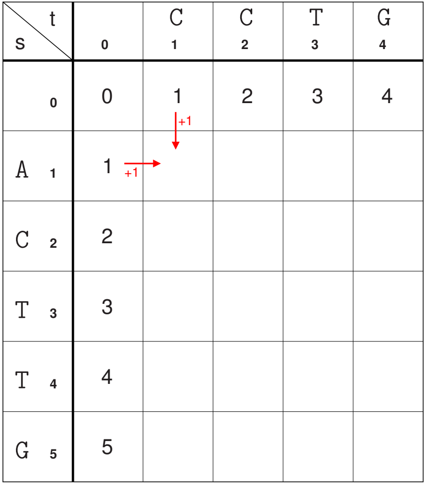
Compute $d_{\text{edit}}(s_1, t_1)$:

Filling out the Penalty Table



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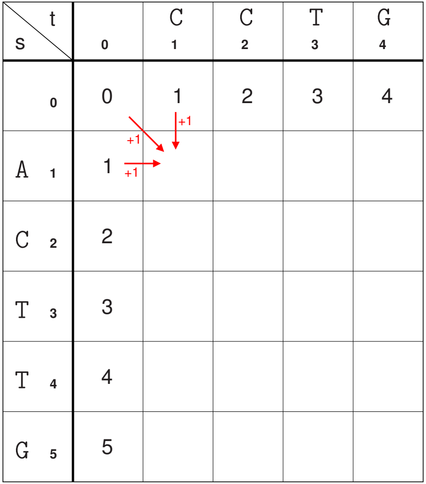

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Insert mismatch

$$\underbrace{\begin{matrix}\lambda\\ \lambda\end{matrix}}_{d_{\text{edit}}(\lambda,\lambda)} \;\Bigg|\; \underbrace{\begin{matrix}\texttt{A}\\ \texttt{C}\end{matrix}}_{+1}$$

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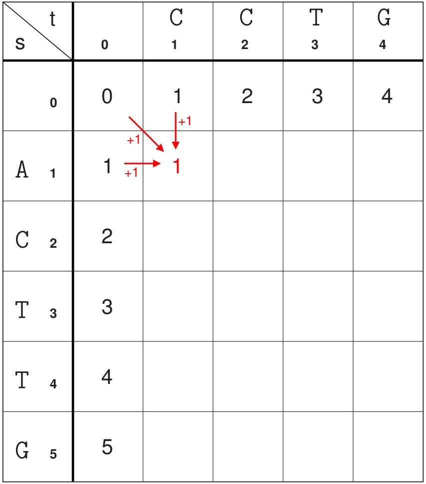

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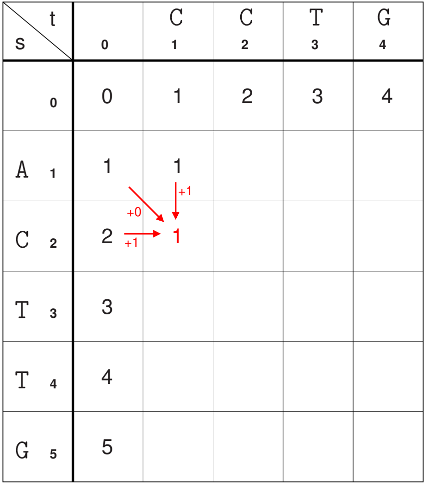

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Compute $d_{\text{edit}}(s_2, t_1)$

Filling out the Penalty Table

t s	0	C 1	C 2	T 3	G 4
0	0	1	2	3	4
A 1	1	1			
C 2	2	1			
T 3	3				
T 4	4				
G 5	5				

Compute $d_{\text{edit}}(s_2, t_1)$

Filling out the Penalty Table

s \ t	0	C 1	C 2	T 3	G 4
0	0	1	2	3	4
A 1	1	1			
C 2	2	1			
T 3	3	2			
T 4	4	3			
G 5	5	4			

Compute remainder of column 1

Filling out the Penalty Table

s \ t	0	C 1	C 2	T 3	G 4
0	0	1	2	3	4
A 1	1	1	2	3	4
C 2	2	1	1	2	3
T 3	3	2	2	1	2
T 4	4	3	3	2	2
G 5	5	4	4	3	2

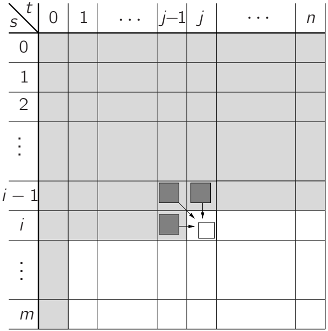
Compute remainder of table

Filling out the Penalty Table

t s	0	C 1	C 2	T 3	G 4
0	0	1	2	3	4
A 1	1	1	2	3	4
C 2	2	1	1	2	3
T 3	3	2	2	1	2
T 4	4	3	3	2	2
G 5	5	4	4	3	2

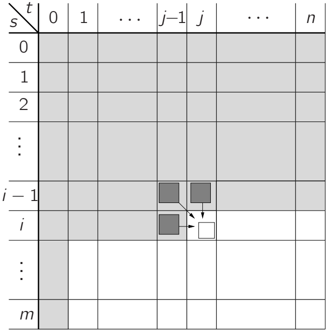
$$d_{\text{edit}}(s,t) = 2$$

Filling out the Penalty Table



↓	Gap in t	Case 1
→	Gap in s	Case 2
↘	Match resp. mismatch	Case 3

Filling out the Penalty Table



↓ Gap in t Case 1

→ Gap in s Case 2

↘ Match resp. mismatch Case 3

$$\begin{aligned} d_{\text{edit}}(s_1 \dots s_i, t_1 \dots t_j) = \min\{ & d_{\text{edit}}(s_1 \dots s_{i-1}, t_1 \dots t_j) + 1, \\ & d_{\text{edit}}(s_1 \dots s_i, t_1 \dots t_{j-1}) + 1, \\ & d_{\text{edit}}(s_1 \dots s_{i-1}, t_1 \dots t_{j-1}) + p(s_i, t_j)\} \end{aligned}$$

Dynamic Programming

Implementation in `numpy`

Alignment Algorithm – Initialization

- Use the module `numpy` that allows fast computations using matrices (tables)

```python
import numpy as np
```

Alignment Algorithm – Initialization

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- Input is given as two strings `seq1` and `seq2`

```
seq1 = "ACTAC"
seq2 = "AACTGATGA"
m = len(seq1)
n = len(seq2)
```

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- Input is given as two strings `seq1` and `seq2`

```
seq1 = "ACTAC"
seq2 = "AACTGATGA"
m = len(seq1)
n = len(seq2)
```

- Initialize penalty table

```
penal = np.zeros((m+1, n+1))
for j in range(0, n+1):
    penal[0][j] = j
for i in range(0, m+1):
    penal[i][0] = i
```

Alignment Algorithm – Initialization

- Use the module `numpy` that allows fast computations using matrices (tables)

```
import numpy as np
```

- Input is given as two strings `seq1` and `seq2`

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seq1 = "ACTAC"
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penal = np.zeros((m+1, n+1))
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```

First row (alignment with λ)

Alignment Algorithm – Initialization

- Use the module `numpy` that allows fast computations using matrices (tables)

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import numpy as np
```

- Input is given as two strings `seq1` and `seq2`

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seq1 = "ACTAC"
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m = len(seq1)
n = len(seq2)
```

- Initialize penalty table

```
penal = np.zeros((m+1, n+1))
for j in range(0, n+1):
    penal[0][j] = j
for i in range(0, m+1):
    penal[i][0] = i
```

First column (alignment with λ)

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
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      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

For every row

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

For every column

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

Same letter in current cell?

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

Then no penalty

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

Otherwise

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

There is a penalty

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

Consider three possibilities

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

Consider three possibilities

Insert gap in second string

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

Consider three possibilities

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```
for i in range(1, m+1):
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    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

Consider three possibilities

Insert match respectively mismatch

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

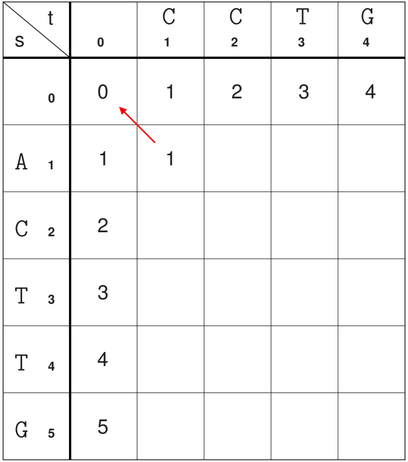
Compute minimum of these possibilities

Alignment Algorithm – Filling out the Penalty Table

```
for i in range(1, m+1):
  for j in range(1, n+1):
    if seq1[i-1] == seq2[j-1]:
      pij = 0
    else:
      pij = 1
    x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
    penal_min = np.amin(x)
    penal[i][j] = penal_min
```

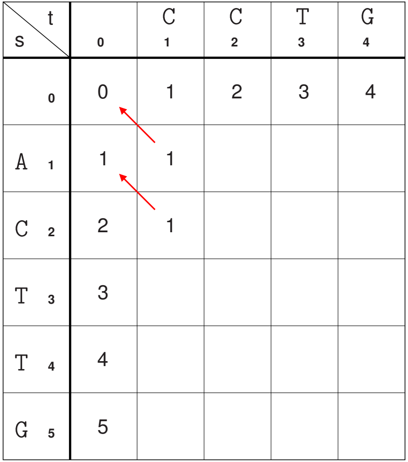
Store minimum value in penalty table

Computing the Optimal Alignment



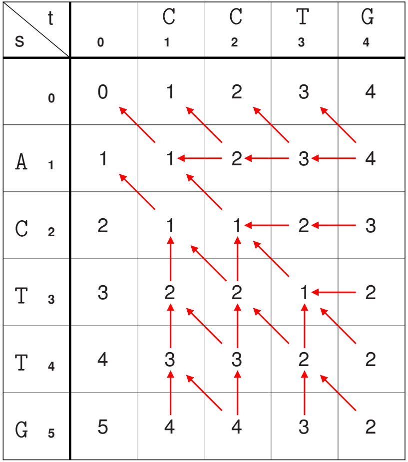
s \ t	0	C 1	C 2	T 3	G 4
0	0	1	2	3	4
A 1	1	1			
C 2	2				
T 3	3				
T 4	4				
G 5	5				

Computing the Optimal Alignment



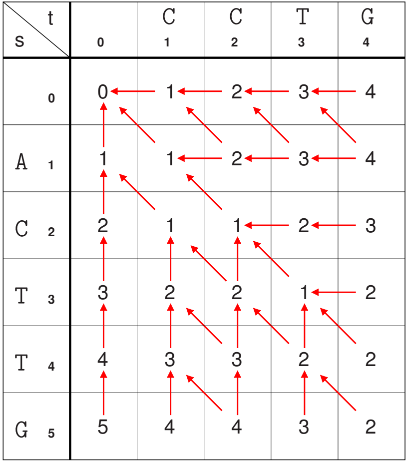
s \ t	0	C 1	C 2	T 3	G 4
0	0	1	2	3	4
A 1	1	1			
C 2	2	1			
T 3	3				
T 4	4				
G 5	5				

Computing the Optimal Alignment



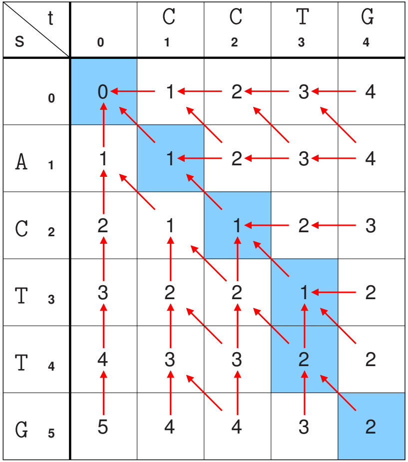
s \ t	0	C 1	C 2	T 3	G 4
0	0	1	2	3	4
A 1	1	1	2	3	4
C 2	2	1	1	2	3
T 3	3	2	2	1	2
T 4	4	3	3	2	2
G 5	5	4	4	3	2

Computing the Optimal Alignment



s \ t	0	C 1	C 2	T 3	G 4
0	0	1	2	3	4
A 1	1	1	2	3	4
C 2	2	1	1	2	3
T 3	3	2	2	1	2
T 4	4	3	3	2	2
G 5	5	4	4	3	2

Computing the Optimal Alignment



s \ t	0	C 1	C 2	T 3	G 4
0	0	1	2	3	4
A 1	1	1	2	3	4
C 2	2	1	1	2	3
T 3	3	2	2	1	2
T 4	4	3	3	2	2
G 5	5	4	4	3	2

$$s' = \mathtt{A\,C\,T\,T\,G}$$

$$t' = \mathtt{C\,C\,T\,-\,G}$$

Alignment Algorithm – Initialization of the Tracing Table

Tracing (Arrows in the penalty table)

Additionally store the index of the minimum element

Alignment Algorithm – Initialization of the Tracing Table

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Create table to store the way through the penalty table. . .

```
penal = np.zeros((m+1, n+1))
trace = np.zeros((m+1, n+1))
```

Alignment Algorithm – Initialization of the Tracing Table

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Additionally store the index of the minimum element

Create table to store the way through the penalty table. . .

```
penal = np.zeros((m+1, n+1))
trace = np.zeros((m+1, n+1))
```

Same size as penalty table

Alignment Algorithm – Initialization of the Tracing Table

Tracing (Arrows in the penalty table)

Additionally store the index of the minimum element

Create table to store the way through the penalty table…

```
penal = np.zeros((m+1, n+1))
trace = np.zeros((m+1, n+1))
```

```
for j in range(1, n+1):
  trace[0][j] = 1
for i in range(1, m+1):
  trace[i][0] = 0
```

Alignment Algorithm – Initialization of the Tracing Table

Tracing (Arrows in the penalty table)

Additionally store the index of the minimum element

Create table to store the way through the penalty table…

```
penal = np.zeros((m+1, n+1))
trace = np.zeros((m+1, n+1))
```

```
for j in range(1, n+1):
  trace[0][j] = 1
for i in range(1, m+1):
  trace[i][0] = 0
```

Only steps from left in first row

Alignment Algorithm – Initialization of the Tracing Table

Tracing (Arrows in the penalty table)

Additionally store the index of the minimum element

Create table to store the way through the penalty table…

```
penal = np.zeros((m+1, n+1))
trace = np.zeros((m+1, n+1))
```

```
for j in range(1, n+1):
  trace[0][j] = 1
for i in range(1, m+1):
  trace[i][0] = 0
```

Only steps from above in first column

Alignment Algorithm – Filling out the Tracing Table

Store index of minimum with `numpy` function **`argmin`**...

```
penal_min = np.amin(x)
index_min = np.argmin(x)
penal[i][j] = penal_min
trace[i][j] = index_min
```

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```

Compute minimum penalty

Alignment Algorithm – Filling out the Tracing Table

Store index of minimum with `numpy` function **`argmin`**…

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```

Compute index of the minimum

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Store index of minimum with `numpy` function **`argmin`**...

```
penal_min = np.amin(x)
index_min = np.argmin(x)
penal[i][j] = penal_min
trace[i][j] = index_min
```

Store value

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Store index of minimum with `numpy` function **`argmin`**...

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penal_min = np.amin(x)
index_min = np.argmin(x)
penal[i][j] = penal_min
trace[i][j] = index_min
```

Store index

Alignment Algorithm – Filling out the Tracing Table

Store index of minimum with `numpy` function **`argmin`**…

```
penal_min = np.amin(x)
index_min = np.argmin(x)
penal[i][j] = penal_min
trace[i][j] = index_min
```

- Run backwards through table `trace`
- Value gives index of the minimum

Alignment Algorithm – Filling out the Tracing Table

Store index of minimum with `numpy` function **`argmin`**...

```
penal_min = np.amin(x)
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penal[i][j] = penal_min
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```

- Run backwards through table `trace`
- Value gives index of the minimum
- Insert gap or match respectively mismatch accordingly

Alignment Algorithm – Filling out the Tracing Table

Store index of minimum with `numpy` function **`argmin`**...

```
penal_min = np.amin(x)
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penal[i][j] = penal_min
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```

- Run backwards through table `trace`
- Value gives index of the minimum
- Insert gap or match respectively mismatch accordingly
- Continue with previous column and row of `trace`

Alignment Algorithm – Filling out the Tracing Table

Store index of minimum with `numpy` function **`argmin`**…

```
penal_min = np.amin(x)
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```

- Run backwards through table `trace`
- Value gives index of the minimum
- Insert gap or match respectively mismatch accordingly
- Continue with previous column and row of `trace`
- For match respectively mismatch, this is the cell above-left
- `i = i-1` and `j = j-1`

Alignment Algorithm – Filling out the Tracing Table

Store index of minimum with `numpy` function **`argmin`**...

```
penal_min = np.amin(x)
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- Run backwards through table `trace`
- Value gives index of the minimum
- Insert gap or match respectively mismatch accordingly
- Continue with previous column and row of `trace`
- For match respectively mismatch, this is the cell above-left
- `i = i-1` and `j = j-1`
- Otherwise, only decrease `i` or `j`

Alignment Algorithm – Print the Result

- Result of algorithm is 2-dimensional list `result` with
  - one list for the first string
  - another list for the second string

Alignment Algorithm – Print the Result

- Result of algorithm is 2-dimensional list `result` with
    - one list for the first string
    - another list for the second string
- Start in the lower-right corner of the table
- Fill `result` with reversed alignment
- Result will be formatted more readable afterwards

Alignment Algorithm – Print the Result

- Result of algorithm is 2-dimensional list `result` with
  - one list for the first string
  - another list for the second string
- Start in the lower-right corner of the table
- Fill `result` with reversed alignment
- Result will be formatted more readable afterwards

```
result = [[], []]
i = m
j = n
```

Alignment Algorithm – Print the Result

```
while i > 0 or j > 0:
   if trace[i][j] == 0:
      result[0].append(seq1[i-1])
      result[1].append("-")
      i -= 1
   elif trace[i][j] == 1:
      result[0].append("-")
      result[1].append(seq2[j-1])
      j -= 1
   else:
      result[0].append(seq1[i-1])
      result[1].append(seq2[j-1])
      i -= 1
      j -= 1

for k in range(len(result[0])-1, -1, -1):
    print(result[0][k], " <-> ", result[1][k])
```

Alignment Algorithm – Print the Result

As long as we are not yet at the upper-left corner

```
while i > 0 or j > 0:
   if trace[i][j] == 0:
      result[0].append(seq1[i-1])
      result[1].append("-")
      i -= 1
   elif trace[i][j] == 1:
      result[0].append("-")
      result[1].append(seq2[j-1])
      j -= 1
   else:
      result[0].append(seq1[i-1])
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      j -= 1

for k in range(len(result[0])-1, -1, -1):
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Alignment Algorithm – Print the Result

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      i -= 1
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      result[0].append("-")
      result[1].append(seq2[j-1])
      j -= 1
   else:
      result[0].append(seq1[i-1])
      result[1].append(seq2[j-1])
      i -= 1
      j -= 1

for k in range(len(result[0])-1, -1, -1):
    print(result[0][k], " <-> ", result[1][k])
```

If step from above

Alignment Algorithm – Print the Result

```
while i > 0 or j > 0:
    if trace[i][j] == 0:
        result[0].append(seq1[i-1])
        result[1].append("-")
        i -= 1
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        result[0].append("-")
        result[1].append(seq2[j-1])
        j -= 1
    else:
        result[0].append(seq1[i-1])
        result[1].append(seq2[j-1])
        i -= 1
        j -= 1

for k in range(len(result[0])-1, -1, -1):
    print(result[0][k], " <-> ", result[1][k])
```

Insert gap in second string

Alignment Algorithm – Print the Result

```
while i > 0 or j > 0:
    if trace[i][j] == 0:
        result[0].append(seq1[i-1])
        result[1].append("-")
        i -= 1
    elif trace[i][j] == 1:
        result[0].append("-")
        result[1].append(seq2[j-1])
        j -= 1
    else:
        result[0].append(seq1[i-1])
        result[1].append(seq2[j-1])
        i -= 1
        j -= 1

for k in range(len(result[0])-1, -1, -1):
     print(result[0][k], " <-> ", result[1][k])
```

And continue in row above

Alignment Algorithm – Print the Result

```
while i > 0 or j > 0:
    if trace[i][j] == 0:
        result[0].append(seq1[i-1])
        result[1].append("-")
        i -= 1
    elif trace[i][j] == 1:
        result[0].append("-")
        result[1].append(seq2[j-1])
        j -= 1
    else:
        result[0].append(seq1[i-1])
        result[1].append(seq2[j-1])
        i -= 1
        j -= 1

for k in range(len(result[0])-1, -1, -1):
    print(result[0][k], " <-> ", result[1][k])
```

If step from left

Alignment Algorithm – Print the Result

```
while i > 0 or j > 0:
   if trace[i][j] == 0:
      result[0].append(seq1[i-1])
      result[1].append("-")
      i -= 1
   elif trace[i][j] == 1:
      result[0].append("-")
      result[1].append(seq2[j-1])
      j -= 1
   else:
      result[0].append(seq1[i-1])
      result[1].append(seq2[j-1])
      i -= 1
      j -= 1

for k in range(len(result[0])-1, -1, -1):
    print(result[0][k], " <-> ", result[1][k])
```

Insert gap in first string

Alignment Algorithm – Print the Result

```
while i > 0 or j > 0:
   if trace[i][j] == 0:
      result[0].append(seq1[i-1])
      result[1].append("-")
      i -= 1
   elif trace[i][j] == 1:
      result[0].append("-")
      result[1].append(seq2[j-1])
      j -= 1
   else:
      result[0].append(seq1[i-1])
      result[1].append(seq2[j-1])
      i -= 1
      j -= 1

for k in range(len(result[0])-1, -1, -1):
    print(result[0][k], " <-> ", result[1][k])
```

And continue in column to the left

Alignment Algorithm – Print the Result

```
while i > 0 or j > 0:
   if trace[i][j] == 0:
      result[0].append(seq1[i-1])
      result[1].append("-")
      i -= 1
   elif trace[i][j] == 1:
      result[0].append("-")
      result[1].append(seq2[j-1])
      j -= 1
   else:
      result[0].append(seq1[i-1])
      result[1].append(seq2[j-1])
      i -= 1
      j -= 1

for k in range(len(result[0])-1, -1, -1):
    print(result[0][k], " <-> ", result[1][k])
```

If step from above-left

Alignment Algorithm – Print the Result

```
while i > 0 or j > 0:
   if trace[i][j] == 0:
      result[0].append(seq1[i-1])
      result[1].append("-")
      i -= 1
   elif trace[i][j] == 1:
      result[0].append("-")
      result[1].append(seq2[j-1])
      j -= 1
   else:
      result[0].append(seq1[i-1])
      result[1].append(seq2[j-1])
      i -= 1
      j -= 1

for k in range(len(result[0])-1, -1, -1):
    print(result[0][k], " <-> ", result[1][k])
```

Insert match respectively mismatch
(Print both letters)

Alignment Algorithm – Print the Result

```
while i > 0 or j > 0:
   if trace[i][j] == 0:
      result[0].append(seq1[i-1])
      result[1].append("-")
      i -= 1
   elif trace[i][j] == 1:
      result[0].append("-")
      result[1].append(seq2[j-1])
      j -= 1
   else:
      result[0].append(seq1[i-1])
      result[1].append(seq2[j-1])
      i -= 1
      j -= 1

for k in range(len(result[0])-1, -1, -1):
    print(result[0][k], " <-> ", result[1][k])
```

And continue in cell above-left

Alignment Algorithm – Time Complexity

- There are two parts
  1. Filling out the tables
  2. Output of the result

Alignment Algorithm – Time Complexity

- There are two parts
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- Filling out the matrices takes more time since every cell is considered

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```
for i in range(1, m+1):
    for j in range(1, n+1):
        if seq1[i-1] == seq2[j-1]
        ...
        x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
        penalty_min = amin(x)
        ...
```

Alignment Algorithm – Time Complexity

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        x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
        penalty_min = amin(x)
        ...
```

For every row

Alignment Algorithm – Time Complexity

- There are two parts
  1. Filling out the tables
  2. Output of the result
- Filling out the matrices takes more time since every cell is considered

```
for i in range(1, m+1):
    for j in range(1, n+1):
        if seq1[i-1] == seq2[j-1]
        ...
        x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
        penalty_min = amin(x)
        ...
```

For every column

Alignment Algorithm – Time Complexity

- There are two parts
  1. Filling out the tables
  2. Output of the result
- Filling out the matrices takes more time since every cell is considered

```
for i in range(1, m+1):
    for j in range(1, n+1):
        if seq1[i-1] == seq2[j-1]
        ...
        x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
        penalty_min = amin(x)
        ...
```

One comparison

Alignment Algorithm – Time Complexity

- There are two parts
    1. Filling out the tables
    2. Output of the result
- Filling out the matrices takes more time since every cell is considered

```
for i in range(1, m+1):
    for j in range(1, n+1):
        if seq1[i-1] == seq2[j-1]
        ...
        x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
        penalty_min = amin(x)
        ...
```

Two comparisons

Alignment Algorithm – Time Complexity

- There are two parts
  1. Filling out the tables
  2. Output of the result
- Filling out the matrices takes more time since every cell is considered

```
for i in range(1, m+1):
    for j in range(1, n+1):
        if seq1[i-1] == seq2[j-1]
        ...
        x = [penal[i-1][j] + 1, penal[i][j-1] + 1, penal[i-1][j-1] + pij]
        penalty_min = amin(x)
        ...
```

$3 \cdot m \cdot n$ comparisons

Alignment Algorithm – Time Complexity

Time complexity: Roughly $3n^2$ for two strings of equal length n

Alignment Algorithm – Time Complexity

Time complexity: Roughly $3n^2$ for two strings of equal length n

n	10	50	100	300	10 000
$10n$	100	500	1 000	3 000	100 000
$3n^2$	300	7 500	30 000	270 000	300 000 000
n^3	1 000	125 000	1 000 000	27 000 000	13 digits
3^n	59 049	24 digits	48 digits	143 digits	4 772 digits

Alignment Algorithm – Time Complexity

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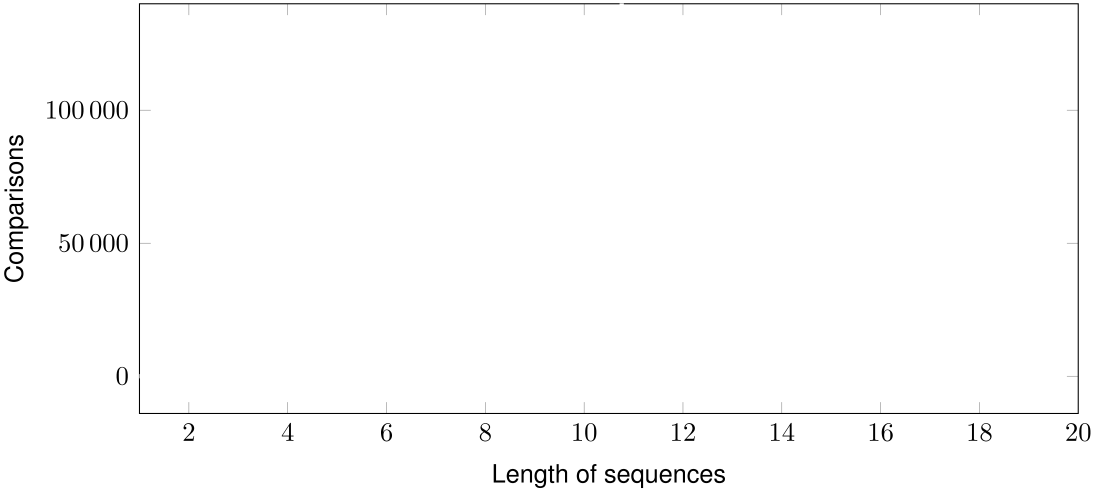
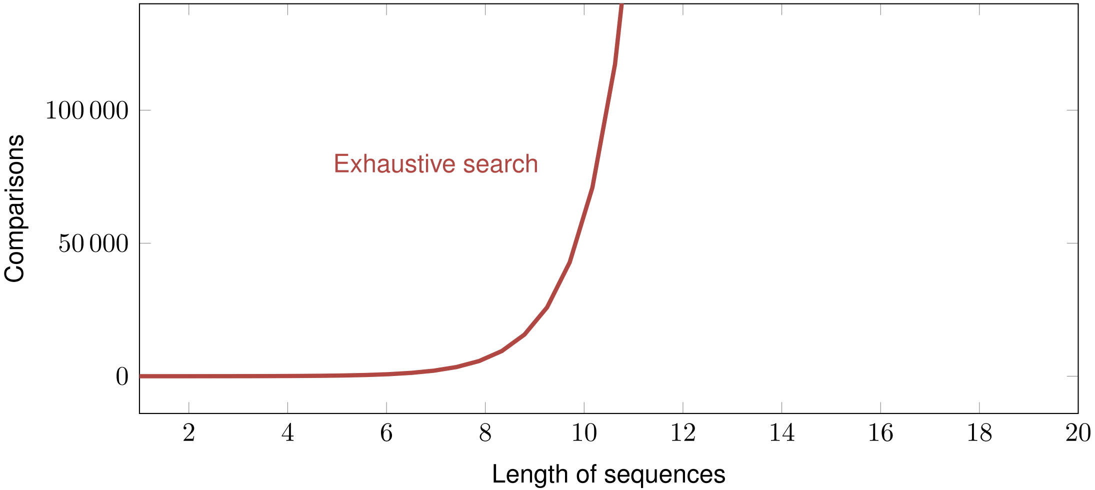
Comparison of two genes (size of $n \approx 10\,000$) takes

- **100 MB** of space and
- **less than 1 minute** of time

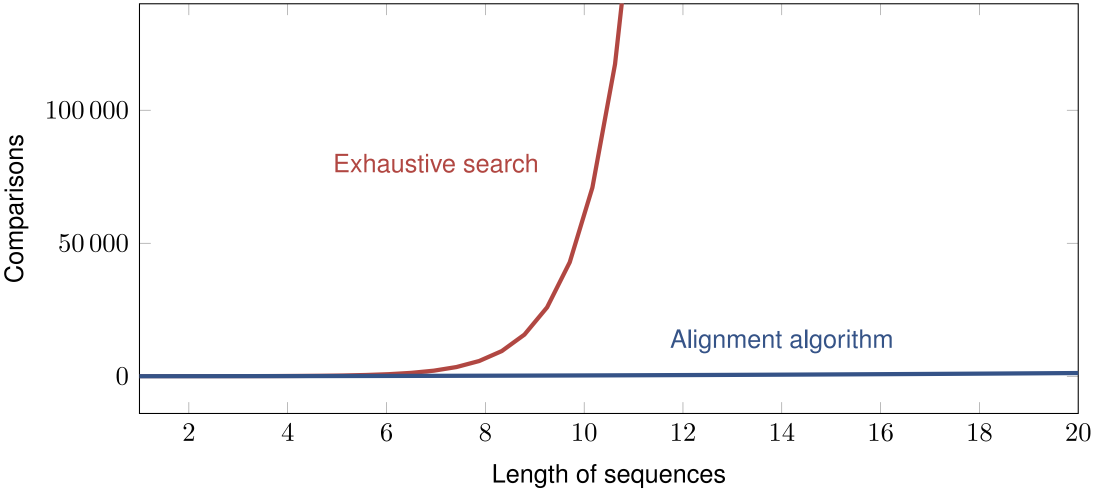
Alignment Algorithm – Time Complexity



Alignment Algorithm – Time Complexity



Alignment Algorithm – Time Complexity



Thanks for your attention