

GENIOMHE

# Sequence algorithms

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# Contents

<b>1. Back to basics</b>	<b>3</b>
<b>2. Motif</b>	<b>5</b>
<b>3. Matrices</b>	<b>7</b>
3.1. Automata . . . . .	10
3.2. Suffix Automaton . . . . .	12
<b>4. Automata for motif search</b>	<b>14</b>
<b>5. Longest common subsequence</b>	<b>17</b>
<b>I. Sequence alignment</b>	<b>20</b>
5.1. Similarity between sequences . . . . .	21
<b>6. Section alignment</b>	<b>22</b>
6.1. Needleman - Wunsch algorithm . . . . .	22

# 1 Back to basics

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**Algorithm 1** Search an element in an array

---

```
1: function Search( $A$ : Array( $n$ ),  $E$ : element)
2:   for ( $i = 0$ ;  $i < n$ ;  $i++$ ) do
3:     if  $A[i] = E$  then
4:       return true
5:     end if
6:   end for
7:   return false
8: end function
```

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**Algorithm 2** Search an element in an array using a while loop

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```
1: function Search( $A$ : Array( $n$ ),  $E$ : element)
2:    $i \leftarrow 0$ 
3:   while  $i < n$  do
4:     if  $A[i] = E$  then
5:       return true
6:     end if
7:      $i \leftarrow i + 1$ 
8:   end while
9:   return false
10: end function
```

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**Algorithm 3** Search an element in an array using a while loop (bis)

---

```

1: function Search( $A$ : Array( $n$ ),  $E$ : element)
2:    $i \leftarrow 0$ 
3:   while  $i < n$  and  $A[i] \neq E$  do
4:      $i \leftarrow i + 1$ 
5:   end while
6:   if  $i = n$  then
7:     return false
8:   else
9:     return true
10:  end if
11: end function

```

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**Algorithm 4** Count the occurrences of an element in an array

---

```

1: function Search( $A$ : Array( $n$ ),  $E$ : element)
2:    $c \leftarrow 0$ 
3:   for ( $i = 0$ ;  $i < n$ ;  $i++$ ) do
4:     if  $A[i] = E$  then
5:        $c \leftarrow c + 1$ 
6:     end if
7:   end for
8:   return  $c$ 
9: end function

```

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# 2 Motif

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**Algorithm 5** Brute-force search of a motif in a sequence

---

```
1: function FindMotif( $S$ : Array( $n$ ),  $M$ : Array( $m$ ))
2:   returns a list of position
3:    $pos \leftarrow \{\}$ 
4:    $i \leftarrow 0$ 
5:   while  $i < n - m + 1$  do
6:      $j \leftarrow 0$ 
7:     while  $j < m$  and  $S[i + j] = M[j]$  do
8:        $j++$ 
9:     end while
10:    if  $j = m$  then
11:       $pos \leftarrow pos \cup \{i\}$ 
12:    end if
13:     $i++$ 
14:  end while
15:  return  $pos$ 
16: end function
```

---

**Algorithm 6** Knuth-Morris-Pratt algorithm

---

```

1: function KMP_Search( $S$ : Array( $n$ ),  $M$ : Array( $m$ ))
2:   returns Integer
3:    $table \leftarrow$  KMP_Table( $M$ )
4:    $c \leftarrow 0$   $\triangleright$  Count the number of matches
5:    $i \leftarrow 0$ 
6:    $j \leftarrow 0$ 
7:   while  $i < n$  do
8:     if  $S[i] = M[j]$  then
9:        $i \leftarrow i + 1$ 
10:       $j \leftarrow j + 1$ 
11:    end if
12:    if  $j = m$  then
13:       $c \leftarrow c + 1$ 
14:       $j \leftarrow table[j - 1]$ 
15:    else if  $j < n$  and  $M[j] \neq S[i]$  then
16:      if  $j \neq 0$  then
17:         $j \leftarrow table[j - 1]$ 
18:      else
19:         $i \leftarrow i + 1$ 
20:      end if
21:    end if
22:  end while
23:  return  $c$ 
24: end function
25: function KMP_Table( $M$ : Array( $m$ ))
26:   Returns Array( $m$ )
27:    $previous \leftarrow 0$ 
28:    $table \leftarrow$  array of zeros of size  $m$ 
29:   for  $i = 0; i < m; i ++$  do
30:     if  $M[i] = M[previous]$  then
31:        $previous \leftarrow previous + 1$ 
32:        $table[i] \leftarrow previous$ 
33:        $i \leftarrow i + 1$ 
34:     else
35:       if  $previous = 0$  then
36:          $previous \leftarrow table[previous - 1]$ 
37:       else
38:          $table[i] \leftarrow 0$ 
39:          $i \leftarrow 1$ 
40:       end if
41:     end if
42:   end for
43: end function

```

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# 3 Matrices

Let  $S_1$  and  $S_2$  be two sequences.

$S_1 = \text{ACGUUCC}$   $S_2 = \text{GUU}$

Let  $n = |S_1|$ ,  $m = |S_2|$  The complexity of this algorithm is  $\mathcal{O}(n \cdot m)$  to build the matrix, and it requires also to find the diagonals and thus it is a bit less efficient than the [Algorithm 5](#).

To find repetitions, we can use a comparison matrix with a single sequence against itself. A repetition would appear as a diagonal of ones, not on the main diagonal.

Let  $S = \text{ACGUUACGUU}$ . Let's write the comparison matrix.

---

**Algorithm 7** Construct a comparison matrix

---

```
1: function ComparisonMatrix( $S$ : Array( $n$ ))
2:    $M \leftarrow$  Array( $n, n$ )
3:   for ( $i = 0; i < n; i++$ ) do
4:     for ( $j = 0; j < n; j++$ ) do
5:       if  $S[i] = S[j]$  then
6:          $M[i][j] = 1$ 
7:       else
8:          $M[i][j] = 0$ 
9:       end if
10:    end for
11:  end for
12:  return  $M$ 
13: end function
```

---

	A	C	G	U	U	C	C
G	0	0	1	0	0	0	0
U	0	0	0	1	1	0	0
U	0	0	0	1	1	0	0

**Table 3.1.** Comparison matrix

3. Matrices

	A	C	G	U	U	A	C	G	U	U	G	U	U
A	1	0	0	0	0	1	0	0	0	0	0	0	0
C	0	1	0	0	0	0	1	0	0	0	0	0	0
G	0	0	1	0	0	0	0	1	0	0	1	0	0
U	0	0	0	1	1	0	0	0	1	1	0	1	1
U	0	0	0	1	1	0	0	0	1	1	0	1	1
A	1	0	0	0	0	1	0	0	0	0	0	0	0
C	0	1	0	0	0	0	1	0	0	0	0	0	0
G	0	0	1	0	0	0	0	1	0	0	1	0	0
U	0	0	0	1	1	0	0	0	1	1	0	1	1
U	0	0	0	1	1	0	0	0	1	1	0	1	1
G	0	0	1	0	0	0	0	1	0	0	1	0	0
U	0	0	0	1	1	0	0	0	1	1	0	1	1
U	0	0	0	1	1	0	0	0	1	1	0	1	1



---

**Algorithm 8** Construct the top half of a comparison matrix
 

---

```

1: function ComparisonMatrix( $S$ : Array( $n$ ))
2:    $M \leftarrow$  Array( $n, n$ )
3:   for ( $i = 0; i < n; i++$ ) do
4:     for  $j=i; j < n; j++$  do
5:       if  $S[i] = S[j]$  then
6:          $M[i][j] = 1$ 
7:       else
8:          $M[i][j] = 0$ 
9:       end if
10:    end for
11:  end for
12:  return  $M$ 
13: end function

```

---



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**Algorithm 9** Find repetitions (with a set of visited segments)
 

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```

1: function FindRepetitions( $S$ : Array( $n$ ))
2:   returns A list of start and end positions for repeated sequences
3:    $M =$  ComparisonMatrix( $S$ )
4:    $pos = \{\}$ 
5:    $visited = \{\}$ 
6:   for ( $i_{start} = 0; i_{start} < n; i_{start}++$ ) do
7:     for ( $j_{start} = i_{start} + 1; j_{start} < n; j_{start}++$ ) do
8:       if  $M[i_{start}][j_{start}] = 1$  and  $(i_{start}, j_{start}) \notin visited$  then
9:          $i = i_{start}$ 
10:         $j = j_{start}$ 
11:        while  $M[i][j] = 1$  do
12:           $i++$ 
13:           $j++$ 
14:           $visited = visited \cup \{(i, j)\}$ 
15:        end while
16:         $pos = pos \cup \{(i_{start}, i), (j_{start}, j)\}$ 
17:      end if
18:    end for
19:  end for
20: end function

```

---

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**Algorithm 10** Find repetitions with an exploration of diagonals
 

---

```

1: function FindRepetitions( $S$ : Array( $n$ ))
2:   returns A list of start and end positions for repeted sequences
3:    $M = \text{ComparisonMatrix}(S)$ 
4:    $pos = \{\}$ 
5:   for ( $diag = 1$ ;  $diag < n$ ;  $diag++$ ) do
6:      $j = diag$ 
7:      $i = 0$ 
8:     while  $i < n$  and  $j < n$  do
9:       if  $M[i][j] = 1$  then
10:         $i_{start} = i$ 
11:         $j_{start} = j$ 
12:        while  $i < n$  and  $j < n$  and  $M[i][j] = 1$  do
13:           $i++$ 
14:           $j++$ 
15:        end while
16:         $pos = pos \cup \{((i_{start}, i - 1), (j_{start}, j - 1))\}$ 
17:      end if
18:       $i++$ 
19:       $j++$ 
20:    end while
21:  end for
22: end function

```

---

## 3.1. Automata

An automaton is a tuple  $\langle S, s_0, T, \Sigma, f \rangle$

- $S$  the set of states
- $s_0$  the initial state
- $T$  the set of terminal states
- $\Sigma$  the alphabet
- $f$  the transition function  $f : (s_1, c) \rightarrow s_2$

**Example** Given the language  $L$  on the alphabet  $\Sigma = \{A, C, T\}$ ,  $L = \{A^*, CTT, CA^*\}$

### $\pi$ Definition 1: Deterministic automaton

An automaton is deterministic, if for each couple  $(p, a) \in S \times \Sigma$  it exists at most a state  $q$  such as  $f(p, a) = q$

### $\pi$ Definition 2: Complete automaton

An automaton is complete, if for each couple  $(p, a) \in S \times \Sigma$  it exists at least a state  $q$  such as  $f(p, a) = q$ .

**Algorithm 11** Find repetitions with an exploration of diagonals, without nested while

---

```

1: function FindRepetitions( $S$ : Array( $n$ ))
2:   returns A list of start positions for repeted sequences and match length
3:    $M = \text{ComparisonMatrix}(S)$ 
4:    $pos = \{\}$ 
5:   for ( $diag = 1$ ;  $diag < n$ ;  $diag ++$ ) do
6:      $j = diag$ 
7:      $i = 0$ 
8:      $l = 0$ 
9:     while  $i < n$  and  $j < n$  do
10:      if  $M[i][j] = 1$  then
11:         $l ++$ 
12:      else
13:        if  $l > 0$  then
14:           $pos = pos \cup \{(i - l, j - l, l)\}$ 
15:           $l = 0$ 
16:        end if
17:      end if
18:       $i ++$ 
19:       $j ++$ 
20:    end while
21:    if  $l > 0$  then
22:       $pos = pos \cup \{(i - l, j - l, l)\}$ 
23:    end if
24:  end for
25:  return  $pos$ 
26: end function

```

---

**Algorithm 12** Find repetitions

---

```

1: function FindRepetitions( $S$ : Array( $n$ ))
2:   returns A list of start and end positions for repeted sequences
3:    $M = \text{ComparisonMatrix}(S)$ 
4:    $pos = \{\}$ 
5:   for  $i_{start} = 0$ ;  $i_{start} < n$ ;  $i_{start} ++$  do
6:     for  $j_{start} = i_{start} + 1$ ;  $j_{start} < n$ ;  $j_{start} ++$  do
7:       if  $M[i_{start}][j_{start}] = 1$  then
8:          $i = i_{start}$ 
9:          $j = j_{start}$ 
10:        while  $M[i][j] = 1$  do
11:           $M[i][j] = 0$  ▷ Ensure that the segment is not explored again
12:           $i ++$ 
13:           $j ++$ 
14:        end while
15:         $pos = pos \cup \{(i_{start}, i - 1), (j_{start}, j - 1)\}$ 
16:      end if
17:    end for
18:  end for
19: end function

```

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**Algorithm 13** Check whether a word belongs to a language for which we have an automaton
 

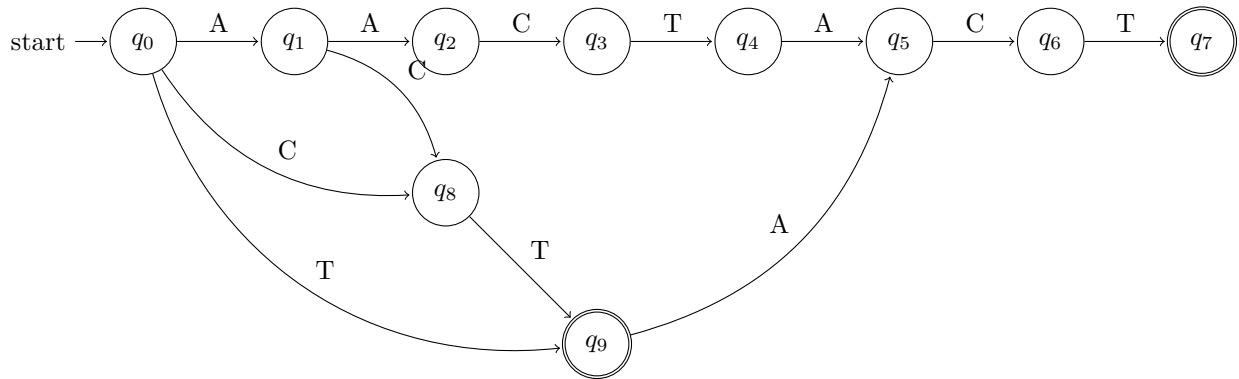
---

```

1: function WordInLanguage( $W$ : Array( $n$ ),  $A$ :  $\langle S, s_0, T, \Sigma, f \rangle$ )
2:   returns A Boolean valued to true if the word is recognized by the language automaton
3:    $s \leftarrow s_0$ 
4:    $i \leftarrow 0$ 
5:   while  $i < n$  do
6:      $a \leftarrow W[i]$ 
7:     if  $\exists f(s, a)$  then
8:        $s \leftarrow f(s, a)$ 
9:     else
10:      return false
11:    end if
12:     $i++$ 
13:  end while
14:  if  $s \in T$  then
15:    return true
16:  else
17:    return false
18:  end if
19: end function

```

---



**Figure 3.1.** Suffix automaton for  $S = AACTACT$

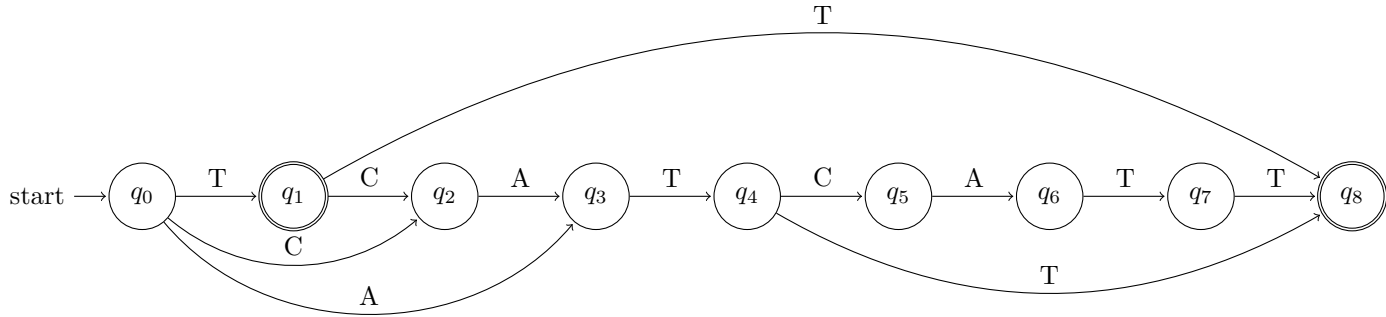
## 3.2. Suffix Automaton

Let  $S = AACTACT$

A suffix automata recognize all suffix of a given sequence.

The suffix language of  $S$  is  $\{S, ACTACT, CTA CT, TACT, ACT, CT, T\}$ .

The complexity of the pattern matching algorithm is  $\mathcal{O}(n + m)$ , because building the automaton is  $\mathcal{O}(m)$



**Figure 3.2.** Suffix automaton for  $S = \text{TCATCATT}$

---

**Algorithm 14** Check if a sequences matches a motif, from a suffix automaton  $\mathcal{O}(m)$ , built from the automaton

---

```

1: function CheckMotifInSuffixAutomaton( $W$ : Array( $m$ ),  $A$ :  $\langle S, s_0, T, \Sigma, f \rangle$ )
2:   returns Boolean valued to true if the motif is in the sequence
3:    $s \leftarrow s_0$ 
4:    $i \leftarrow 0$ 
5:   while  $i < m$  and  $\exists f(s, W[i])$  do
6:      $s \leftarrow f(s, W[i])$ 
7:      $i++$ 
8:   end while
9:   if  $i = n$  then
10:    return true
11:  else
12:    return false
13:  end if
14: end function

```

---

# 4 Automata for motif search

Let  $M$  be a motif  $M = ACAT$ .

The alphabet of motif is the same as the alphabet of the sequence. The search automaton is complete. If there exists a letter  $c$  in the sequence that is not in the motif alphabet, we can make a virtual transition from each state to the initial state whenever we encounter an unknown letter.

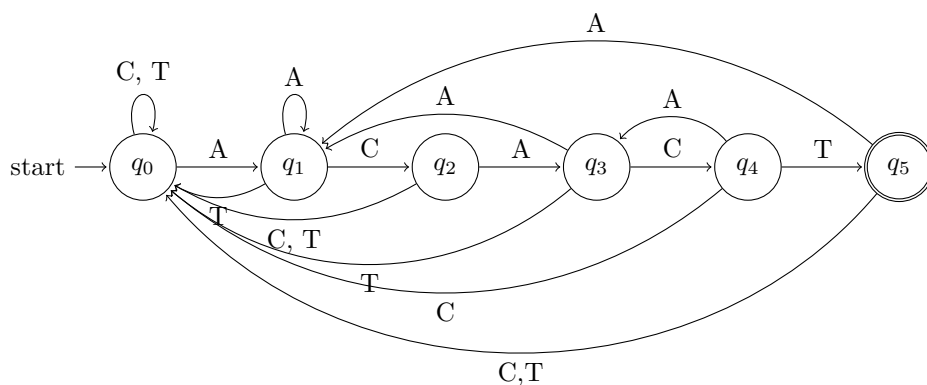


Figure 4.1. Motif search automaton for  $M = ACAT$

---

**Algorithm 15** Search a motif in a sequence with an automaton

---

```

1: function SearchMotif( $S$ : Array( $n$ ),  $A$ :  $\langle S, s_0, T, \Sigma, f \rangle$ ,  $P$ : Array( $m$ ))
2:   returns A set of positions where the motif has been found
3:    $s \leftarrow s_0$ 
4:    $i \leftarrow 0$ 
5:    $pos \leftarrow \{\}$ 
6:   while  $i < n$  do
7:     if  $s \in T$  then
8:        $pos \leftarrow pos \cup \{i - m\}$ 
9:     end if
10:     $s \leftarrow f(s, S[i])$ 
11:     $i++$ 
12:  end while
13:  return  $pos$ 
14: end function

```

---



---

**Algorithm 16** Check if the a motif automaton recognizes only the prefix of size  $m - 1$  of a motif  $P$  of size  $m$ 


---

```

1: function SearchMotifLastPrefix( $S$ : Array( $n$ ),  $A$ :  $\langle S, s_0, T, \Sigma, f \rangle$ ,  $P$ : Array( $m$ ))
2:   returns A set of positions where the motif has been found
3:    $s \leftarrow s_0$ 
4:    $i \leftarrow 0$ 
5:    $T_{new} \leftarrow \{\}$ 
6:   for  $s \in S$  do
7:     for  $a \in \Sigma$  do
8:       for  $t \in T$  do
9:         if  $\exists f(s, a)$  and  $f(s, a) = t$  then
10:           $T_{new} \leftarrow T_{new} \cup s$ 
11:        end if
12:      end for
13:    end for
14:  end for
15:  while  $i < n$  do
16:    if  $s \in T_{new}$  then
17:      return true
18:    end if
19:     $s \leftarrow f(s, S[i])$ 
20:     $i++$ 
21:  end while
22:  return false
23: end function

```

---

---

**Algorithm 17** Check if the a motif automaton recognizes only the prefix of size  $m - 1$  of a motif  $P$  of size  $m$ , knowing the sequence of the motif

---

```

1: function SearchMotifLastPrefix( $S$ : Array( $n$ ),  $A$ :  $\langle S, s_0, T, \Sigma, f \rangle$ ,  $P$ : Array( $m$ ))
2:   returns A set of positions where the motif has been found
3:    $s \leftarrow s_0$ 
4:    $i \leftarrow 0$ 
5:   while  $i < n$  and  $f(s, P[m - 1]) \notin T$  do
6:      $s \leftarrow f(s, S[i])$ 
7:      $i++$ 
8:   end while
9:   if  $f(s, P[m - 1]) \in T$  then
10:    return true
11:  else
12:    return false
13:  end if
14: end function

```

---



# 5 Longest common subsequence

Let  $S_1 = \text{ATCTGAT}$  and  $S_2 = \text{TGCATA}$ . In this case the longest common subsequence of  $S_1$  and  $S_2$  is  $TCTA$ .

---

**Algorithm 18** Construct a longest common subsequence matrix

---

```
1: function LCSQ_Matrix( $S_1$ : Array( $n$ ),  $S_2$ : Array( $m$ ))
2:    $M \leftarrow$  Array( $m + 1$ ,  $n + 1$ )
3:   for ( $i = 0$ ;  $i < n + 1$ ;  $i++$ ) do
4:     for  $j = 0$ ;  $j < m + 1$ ;  $j++$  do
5:       if  $i = 0$  or  $j = 0$  then
6:          $M[i][j] = 0$ 
7:       else
8:         if  $S_1[i] = S_2[j]$  then
9:            $match = M[i - 1][j - 1] + 1$ 
10:        else
11:           $match = M[i - 1][j - 1]$ 
12:        end if
13:         $gap_1 = M[i - 1][j]$ 
14:         $gap_2 = M[i][j - 1]$ 
15:         $M[i][j] = \max\{match, gap_1, gap_2\}$ 
16:      end if
17:    end for
18:  end for
19:  return  $M$ 
20: end function
```

---

---

**Algorithm 19** Construct a longest common subsequence matrix keeping the path in memory
 

---

```

1: function LCSQ_Matrix_Path( $S_1$ : Array( $n$ ),  $S_2$ : Array( $m$ ))
2:    $M \leftarrow$  Array( $m + 1$ ,  $n + 1$ )
3:    $P \leftarrow$  Array( $m + 1$ ,  $n + 1$ )
4:   for ( $i = 0$ ;  $i < n + 1$ ,  $i++$ ) do
5:      $M[i][0] \leftarrow 0$ 
6:   end for
7:   for ( $j = 0$ ;  $j < m + 1$ ;  $j++$ ) do
8:      $M[0][j] \leftarrow 0$ 
9:   end for
10:  for ( $i = 1$ ;  $i < n + 1$ ;  $i++$ ) do
11:    for ( $j = 1$ ;  $j < m + 1$ ;  $j++$ ) do
12:      if  $i = 1$  or  $j = 0$  then
13:         $M[i][j] = 0$ 
14:      else
15:        if  $S_1[i - 1] = S_2[j - 1]$  then
16:           $M[i][j] \leftarrow M[i - 1][j - 1] + 1$ 
17:           $P[i][j] \leftarrow \backslash$ 
18:        else if  $M[i][j - 1] \geq M[i - 1][j]$  then
19:           $M[i][j] \leftarrow M[i][j - 1]$ 
20:           $P[i][j] \leftarrow \leftarrow$ 
21:        else
22:           $M[i][j] \leftarrow M[i - 1][j]$ 
23:           $P[i][j] \leftarrow \downarrow$ 
24:        end if
25:      end if
26:    end for
27:  end for
28:  return  $M, P$ 
29: end function

```

---

---

**Algorithm 20** Backtrack the longest common subsequence

---

```

1: function LCSQ( $S_1$ : Array( $n$ ),  $S_2$ : Array( $m$ ))
2:    $M, P \leftarrow$  LCSQ_Matrix( $S_1, S_2$ )
3:    $L \leftarrow$  Array( $M[n][m]$ )
4:    $k \leftarrow 0$ 
5:    $i \leftarrow n$ 
6:    $j \leftarrow m$ 
7:   while  $i > 0$  and  $j > 0$  do
8:     if  $P[i][j] = '\nwarrow'$  then
9:        $L[k] \leftarrow S_1[i]$ 
10:       $i --$ 
11:       $j --$ 
12:       $k ++$ 
13:     else if  $P[i][j] = '\leftarrow'$  then
14:        $j --$ 
15:     else
16:        $i --$ 
17:     end if
18:   end while
19:   return  $L$ 
20: end function

```

---

# Sequence alignment

# 5.1. Similarity between sequences

A function  $d$  is a distance between two sequences  $x$  and  $y$  in an alphabet  $\Sigma$  if

- $x, y \in \Sigma^*, d(x, x) = 0$
- $\forall x, y \in \Sigma^* d(x, y) = d(y, x)$
- $\forall x, y, z \in \Sigma^* d(x, z) \leq d(x, y) + d(x, z)$

Here we are interested by the distance that is able to represent the transformation of  $x$  to  $y$  using three types of basic operations:

- Substitution
- Insertion
- Deletion

Example:

- $sub(a, b) = \begin{cases} 0 & \text{if } a = b \\ 1 & \text{otherwise} \end{cases}$
- $del(a) = 1$
- $ins(a) = 1$

Let  $X = x_0x_1 \dots x_{m-1}, Y = y_0y_1 \dots y_{n-1}$

An alignment is noted as  $z = \begin{pmatrix} \bar{x}_0 \\ \bar{y}_0 \end{pmatrix} \dots \begin{pmatrix} \bar{x}_{p-1} \\ \bar{y}_{p-1} \end{pmatrix}$  of size  $p$ .  $n \leq p \leq n + m$

$\bar{x}_i = x_j$  or  $\bar{x}_i = \varepsilon$  for  $0 \leq i \leq p - 1$  and  $0 \leq j \leq m - 1$

$\bar{y}_i = y_j$  or  $\bar{y}_i = \varepsilon$  for  $0 \leq i \leq p - 1$  and  $0 \leq j \leq n - 1$

$X' = \bar{x}_0\bar{x}_1 \dots \bar{x}_i \dots \bar{x}_{p-1} Y' = \bar{y}_0\bar{y}_1 \dots \bar{y}_i \dots \bar{y}_{p-1}$  for  $0 \leq i \leq p - 1, \nexists i$ , such that  $\bar{x}_i = \bar{y}_i = \varepsilon$

# 6 Section alignment

## *6.1.* Needleman - Wunsch algorithm

**Algorithm 21** Needleman-Wunsch Algorithm

---

```

1: procedure FillMatrix( $S_1$ : Array( $m$ ),  $S_2$ : Array( $n$ ))  $\triangleright$  sub(a, b) is the substitution score, del(a) and
   ins(a) are the deletion and insertion penalty, in regard with the reference  $S_1$  sequence
2:    $M = \text{Array}(m + 1, n + 1)$   $\triangleright$  Initialize the matrix first column and first row
3:    $P = \text{Array}(m, n)$   $\triangleright$  Store the direction of the cell we chose to build the next cell up on.
4:    $M[0][0] = 0$ 
5:   for ( $i = 1; i < m + 1; i ++$ ) do
6:      $M[i][0] = M[i - 1][0] + \text{gap\_penalty}$ 
7:   end for
8:   for ( $j = 1; j < n + 1; j ++$ ) do
9:      $M[0][j] = M[0][j - 1] + \text{gap\_penalty}$ 
10:  end for  $\triangleright$  Fill the remaining matrix
11:  for ( $i = 1; i < m + 1; i ++$ ) do
12:    for ( $j = 1; j < n + 1; j ++$ ) do
13:       $\text{delete} = M[i - 1][j] + \text{gap\_penalty}$ 
14:       $\text{insert} = M[i][j - 1] + \text{gap\_penalty}$ 
15:       $\text{substitute} = M[i - 1][j - 1] + \text{sub}(S_1[i - 1], S_2[j - 1])$ 
16:       $\text{choice} = \min\{\text{delete}, \text{insert}, \text{substitute}\}$ 
17:      if  $\text{substitute} = \text{choice}$  then
18:         $P[i - 1][j - 1] = '\nwarrow'$ 
19:      else if  $\text{deletion} = \text{choice}$  then
20:         $P[i - 1][j - 1] = '\leftarrow'$ 
21:      else
22:         $P[i - 1][j - 1] = '\uparrow'$ 
23:      end if
24:       $M[i][j] = \text{choice}$ 
25:    end for
26:  end for
27: end procedure

```

---

---

**Algorithm 22** Needleman-Wunsch Algorithm (Backtrack)

---

```

1: procedure ShowAlignment( $S_1$ : Array( $m$ ),  $S_2$ : Array( $n$ ))
2:    $extend_1 = ""$ 
3:    $extend_2 = ""$ 
4:    $i = m$ 
5:    $j = n$ 
6:   while  $i > 0$  and  $j > 0$  do
7:     if  $P[i - 1][j - 1] = '\swarrow'$  then
8:        $extend_1 = S_1[i - 1] \circ extend_1$ 
9:        $extend_2 = S_2[j - 1] \circ extend_2$ 
10:       $i --$ 
11:       $j --$ 
12:     else if  $P[i - 1][j - 1] = '\uparrow'$  then
13:        $extend_1 = S_1[i - 1] \circ extend_1$ 
14:        $extend_2 = '-' \circ extend_2$ 
15:        $i --$ 
16:     else
17:        $extend_1 = '-' \circ extend_1$ 
18:        $extend_2 = S_2[j - 1] \circ extend_2$ 
19:        $j --$ 
20:     end if
21:   end while
22:   while  $i > 0$  do
23:      $extend_1 = S_1[i - 1] \circ extend_1$ 
24:      $extend_2 = '-' \circ extend_2$ 
25:      $i --$ 
26:     Insert(0,  $alignment, tuple$ )
27:   end while
28:   while  $j > 0$  do
29:      $extend_1 = '-' \circ extend_1$ 
30:      $extend_2 = S_2[j - 1] \circ extend_2$ 
31:      $j --$ 
32:   end while
33:   print( $extend_1$ )
34:   print( $extend_2$ )
35: end procedure
36: FillMatrix( $S_1, S_2$ )
37: ShowAlignment( $S_1, S_2$ )

```

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**Algorithm 23** Needleman-Wunsch Algorithm (Backtrack)

---

```

1: procedure FillMatrix( $S_1$ : Array( $m$ ),  $S_2$ : Array( $n$ ))
2:    $M$  = Array( $m + 1$ ,  $n + 1$ )
3:    $P$  = Array( $m$ ,  $n$ )            $\triangleright$  Store the direction of the cell we chose to build the next cell up on.
4:    $M[0][0] = 0$ 
5:   for ( $i = 1$ ;  $i < m + 1$ ;  $i++$ ) do
6:      $M[i][0] = M[i - 1][0] + \text{gap\_penalty}$ 
7:   end for
8:   for ( $j = 1$ ;  $j < n + 1$ ;  $j++$ ) do
9:      $M[0][j] = M[0][j - 1] + \text{gap\_penalty}$ 
10:  end for
11:  for ( $i = 1$ ;  $i < m + 1$ ;  $i++$ ) do
12:    for ( $j = 1$ ;  $j < n + 1$ ;  $j++$ ) do
13:       $\text{delete} = M[i - 1][j] + \text{gap\_penalty}$ 
14:       $\text{insert} = M[i][j - 1] + \text{gap\_penalty}$ 
15:       $\text{substitute} = M[i - 1][j - 1] + \text{sub}(S_1[i - 1], S_2[j - 1])$ 
16:       $M[i][j] = \min\{\text{substitute}, \text{insert}, \text{delete}\}$ 
17:    end for
18:  end for
19: end procedure

```

---

**Algorithm 24** Needleman-Wunsch Algorithm, using proper notation (Backtrack)

---

```

1: procedure BacktrackAlignment( $S_1$ : Array( $m$ ),  $S_2$ : Array( $n$ ))
2:    $alignment = LinkedList$ 
3:    $i = m$ 
4:    $j = n$ 
5:   while  $i > 0$  and  $j > 0$  do
6:     if  $M[i-1][j-1] = M[i][j] - sub(S_1[i-1], S_2[j-1])$  then
7:        $tuple = \begin{pmatrix} S_1[i-1] \\ S_2[j-1] \end{pmatrix}$ 
8:        $i --$ 
9:        $j --$ 
10:    else if  $M[i-1][j-1] = M[i][j-1] - gap\_penalty$  then
11:       $tuple = \begin{pmatrix} S_1[i-1] \\ \varepsilon \end{pmatrix}$ 
12:       $i --$ 
13:    else
14:       $tuple = \begin{pmatrix} \varepsilon \\ S_2[j-1] \end{pmatrix}$ 
15:       $j --$ 
16:    end if
17:    Insert(0,  $alignment, tuple$ )
18:  end while
19:  while  $i > 0$  do
20:     $tuple = \begin{pmatrix} S_1[i-1] \\ \varepsilon \end{pmatrix}$ 
21:     $i --$ 
22:    Insert(0,  $alignment, tuple$ )
23:  end while
24:  while  $j > 0$  do
25:     $tuple = \begin{pmatrix} \varepsilon \\ S_2[j-1] \end{pmatrix}$ 
26:     $j --$ 
27:    Insert(0,  $alignment, tuple$ )
28:  end while
29: end procedure
30: FillMatrix( $S_1, S_2$ )
31: BacktrackAlignment( $S_1, S_2$ )

```

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