Needleman-Wunsch

- Sequence alignment algorithm
- "How different/similar are two DNA/RNAsequences?"
- Gives optimal alignment, but there can be multiple ones
- Use of dynamic programming

- Input: Two sequences a and b
- |a| = m; |b| = n
- Data structure: A matrix with m * n
- Runtime and space complexity: O(m*n) ~ O(n^2)

	ϵ	b_0	b₁		bj		bn
ϵ	0	1	2		$D_{0,j}$		D _{0,n}
a0	1						
a1	2			$\int D_{z}$	$a_{i-1,j} + w(a_i, -)$		
а3	3		$D_{i,j} =$	$= \begin{cases} D_i \end{cases}$	$Q_{i-1,j} + w(a_i, -)$ $Q_{i-1,j-1} + w(a_i, b_j)$ $Q_{i,j-1} + w(-, b_j)$		
				$\bigcup D_i$			
ai	D _{i,0}						
am	$D_{m,0}$						$D_{m,n}$



$$D_{i,0} = D_{i-1,0} + w(a_i, -)$$



$$D_{0,j} = D_{0,j-1} + w(-,b_i)$$

Cost-function

$$w(a,b) = \begin{cases} 0, & a = b \\ 1, & a \neq b \end{cases}$$

$$w(a, -) = 1$$

$$w(-,b) = 1$$

Example

	ϵ	A	С
ϵ	0	1	2
Α	1		
G	2		
С	3		

$$D_{i,j} = \begin{cases} D_{i-1,j} + w(a_i, -) \\ D_{i-1,j-1} + w(a_i, b_j) \\ D_{i,j-1} + w(-, b_j) \end{cases}$$

Example

	ϵ	A	С
ϵ	0	1	2
Α	1	0	
G	2		
С	3		

$$D_{i,j} = \begin{cases} D_{i-1,j} + w(a_i, -) \\ D_{i-1,j-1} + w(a_i, b_j) \\ D_{i,j-1} + w(-, b_j) \end{cases}$$

Example

	ϵ	A	С
ϵ	0	1	2
Α	1	0	1
G	2	1	1
С	3	2	1

$$D_{i,j} = \begin{cases} D_{i-1,j} + w(a_i, -) \\ D_{i-1,j-1} + w(a_i, b_j) \\ D_{i,j-1} + w(-, b_j) \end{cases}$$

Example — Traceback

	ϵ	A	С
ϵ	0	1	2
Α	1	0	1
G	2	1	1
С	3	2 🐗	1

$$D_{i,j} = \begin{cases} D_{i-1,j} + w(a_i, -) \\ D_{i-1,j-1} + w(a_i, b_j) \\ D_{i,j-1} + w(-, b_j) \end{cases}$$

$$D_{3,2} = 1 \neq D_{3-1,2} + 1$$

 $D_{3,2} = 1 \neq D_{3,2-1} + 1$
 $D_{3,2} = 1 = D_{3-1,2-1} + 0$

Example — Traceback

	ϵ	Α	С
ϵ	0	1	2
Α	1	0	1
G	2	1	1
С	3	2	1

$$D_{i,j} = \begin{cases} D_{i-1,j} + w(a_i, -) \\ D_{i-1,j-1} + w(a_i, b_j) \\ D_{i,j-1} + w(-, b_j) \end{cases}$$

Insert gap in b Insert gap in a Alignment: A G C A - C

List of references

 Lecture Bioinformatics I, Number 3, Dr. Dominic Rose. http://www.bioinf.uni-freiburg.de//Lehre/ Courses/2014_SS/V_Bioinformatik_1/lecture3-1.pdf
 Date: 07/11/2014