3 Exercise solutions – Extension of global alignment

1. Affine gap penalty

Affine gap penalties are often preferable ways to calculate gap scores than linear penalties. A gap with length l can be calculated as: $g_l = g_{open} + (l-1) * g_{extend}$.

Use the following scoring scheme and gap penalties to answer the questions.

Scoring scheme:

$$R_{ab} = 1$$
 for $a = b$
 $R_{ab} = 0$ for $a \neq b$
 $g_{open} = 1$, $g_{extend} = 0.1$

(a) What is the gap penalty when l=2.

Solution:
$$g_{l=2} = 1 + (2-1) * 0.1 = 1.1$$

(b) Calculate the scores of the alignments.

1. q: CAGCT d: CT--T

Solution: 0.9

2. q: CAGCT d: C-T-T

Solution: 0

3. q: CCT-d: ---CT

Solution: -2.3

2. Affine gap with single DP table

You need to check extra cells in addition to the adjacent cells of H when finding an optimal alignment with affine gap penalties.

Scoring scheme:

$$R_{ab} = 1$$
 for $a = b$
 $R_{ab} = 0$ for $a \neq b$
 $g_{open} = 1$, $g_{extend} = 0.1$

		С	G
	0	-1	-1.1
С	-1	1	0
A	-1.1	0	

Assume we want to update $H_{2,2}$ and answer the following questions.

(a) Calculate $H_{1,1} + R_{q_2,d_2}$.

Solution: 1 + 0 = 1

(b) Calculate $\max_{1 \leq l \leq 2} (H_{2,2-l} - g_l)$.

Solution: $max(H_{2,1} - g_{l=1}, H_{2,0} - g_{l=2}) = max(01, -1.11.1) = -1$

(c) Calculate $\max_{1 \leq l \leq 2} (H_{2-l,2} - g_l)$.

Solution: $max(H_{1,2} - g_{l=1}, H_{0,2} - g_{l=2}) = max(01, -1.11.1) = -1$

(d) What is the score of $H_{2,2}$.

Solution: max(1, 1, -1) = 1

3. Initialization for affine gap penalty

Initialize the following tables when $g_{open} = 10$ and $g_{extend} = 1$.

	E				
		Т	G	С	
	0	-10	-11	-12	
A	-10				
A	-11				

		T	G	С
	0	-10	-11	-12
A	-11			
A	-12			

F

	G					
		Т	G	С		
	0	-10	-11	-12		
A	-10					
A	-11					

4. Affine gap with three DP tables

Use the following scoring scheme and gap penalties to find the optimal alignment score of two sequences q = AG and d = GGGC.

Scoring scheme:

$$R_{ab} = 1$$
 for $a = b$

$$R_{ab} = 0$$
 for $a \neq b$

$$g_{open} = 1, g_{extend} = 0.1$$

(a) Fill all blank cells in the DP tables E, F, and G.

	E					
		G	G	G	С	
	0	-1	-1.1	-1.2	-1.3	
A	-1	-2	-2.1	-2.2	-2.3	
G	-1.1	-1	-2	-2.1	-2.2	

		G	G	G	С
	0	-1	-1.1	-1.2	-1.3
A	-1	-2	-1	-1.1	-1.2
G	-1.1	-2.1	-1	0	-0.1

F

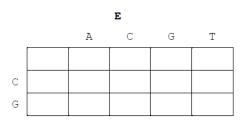
			G		
		G	G	G	C
	0	-1	-1.1	-1.2	-1.3
A	-1	0	-1	-1.1	-1.2
G	-1.1	0	1	0	-1.1

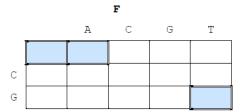
(b) What is the optimal score?

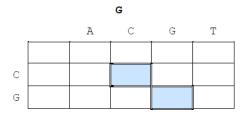
Solution: -0.1

5. Trackback with affine gap penalty

Perform backtracking on E, F, and G tables to find the optimal alignment. The cells with double border should be visited during backtracking.







(a) Write the optimal alignment.

Solution:

- q: -CG-
- d: ACGT

6. Sequence distance with DP DP can be used to calculate the edit distance (Levenshtein distance) between two sequences.

Scoring scheme:

$$R_{ab} = 0$$
 for $a = b$
 $R_{ab} = -1$ for $a \neq b$
 $g = 1$

With the scoring scheme above, the edit distance d is calculated as 1 * T where T is the optimal score of the DP.

Find the edit distance between two sequences q = AG and d = ACG.

(a) Fill the DP table.

q/d		A	С	T
	0	-1	-2	-3
A	-1	0	-1	-2
G	-2	-1	-1	-2

(b) What is the edit distance between q and d?

Solution:

2