Exercise sheet 5: Probalign

For the following exercises on Probalign, we use an affine gap penalty with $g(k) = \alpha + \beta k = -0.5 - 0.25k$, there temperature $T = 1$ and the similarity function $\sigma(x_i, y_j)$:

$$\sigma(x_i, y_j) = \begin{array}{c} \\ A \\ C \\ G \\ T \end{array} \begin{array}{c} \begin{array}{cccc} A & C & G & T \end{array} \\ \begin{pmatrix} 2 & -1 & -1 & -1 \\ -1 & 2 & -1 & -1 \\ -1 & -1 & 2 & -1 \\ -1 & -1 & -1 & 2 \end{pmatrix} \end{array}$$

Exercise 1

Question 1A Compute the Boltzmann-weighted score for the following alignments:

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(a)  x: --AGCGG          (b) x: AGCGG------
          ||:||                     :
     y: ACAGGGG               y: ----ACAGGGG
```

Hint 1 : Formulae

$$S(a) = \sum_{x_i \sim y_j \in a} \sigma(x_i, y_j) + \sum \text{gap penalties} \qquad e^{\frac{S(a)}{T}} = \left(\prod_{x_i \sim y_j \in a} e^{\frac{\sigma(x_i, y_j)}{T}} \right) \times e^{\frac{\sum \text{gap penalties}}{T}}$$

Hint 2 For each alignment you only need to calulate e^x once.

Hint 3: Calculations

(a) $e^{\sigma(A,A)} \times e^{3\sigma(G,G)} \times e^{\sigma(C,G)} \times e^{g(2)} = e^2 \times e^6 \times e^{-1} \times e^{-0.5+(-0.25\times 2)} = e^6$

(b) $e^{\sigma(G,A)} \times e^{g(4)} \times e^{g(6)} = e^{-1} \times e^{0.5+(-0.25\times 4)} \times e^{0.5+(-0.25\times 6)} = e^{-4.5}$

Solution

$$e^6 = 403.43$$
$$e^{-4.5} = 0.011$$

Exercise 2

Question 2A Derive the recursion formula for $Z^I_{i,j}$. Allow insertions after deletions and vice versa.

Hint 1 : Formulae

$$Z^I_{i,j} = Z^I_{i,j-1} \times e^{\frac{\beta}{T}} + Z^M_{i,j-1} \times e^{\frac{g(1)}{T}} + Z^D_{i,j-1} \times e^{\frac{g(1)}{T}}$$

Hint 2 t

Hint 3: Calculations t

Solution t