

Homework 1: Pairwise Sequence Alignment

BCH4300B, Winter 2014

Assigned: March 5, 2014

Due: March 12, 2014

1. (i) By hand, construct the Needleman-Wunsch dynamic programming table for global alignment of the sequences $X = \text{GCGTC}$ and $Y = \text{ACGAC}$. Use the scoring matrix S below and the gap penalty $P = -1$. (These are the same as what we used in class.) (ii) What is the score of the best possible alignment? (iii) Is there only one possible best alignment, or are there more than one? Write out all optimal alignments. (Optional) If you are of the “programming” persuasion, you use a computer/programming to check your answers. But please do the exercise first by hand.

$$S = \begin{array}{c|cccc} & \text{A} & \text{C} & \text{G} & \text{T} \\ \hline \text{A} & 3 & -3 & -1 & -3 \\ \text{C} & -3 & 3 & -3 & -1 \\ \text{G} & -1 & -3 & 3 & -3 \\ \text{T} & -3 & -1 & -3 & 3 \end{array}$$

2. Do all the same things as in problem 1, but for an amino acid alignment problem. Align the sequences $X = \text{FKHM}$ and $Y = \text{FMDT}$, using the gap penalty $P = -1$ and BLOSUM62 scoring matrix below.

$$S = \begin{array}{c|cccccccccccccccccccc} & \text{A} & \text{R} & \text{N} & \text{D} & \text{C} & \text{Q} & \text{E} & \text{G} & \text{H} & \text{I} & \text{L} & \text{K} & \text{M} & \text{F} & \text{P} & \text{S} & \text{T} & \text{W} & \text{Y} & \text{V} \\ \hline \text{A} & 4 & -1 & -2 & -2 & 0 & -1 & -1 & 0 & -2 & -1 & -1 & -1 & -1 & -2 & -1 & 1 & 0 & -3 & -2 & 0 \\ \text{R} & -1 & 5 & 0 & -2 & -3 & 1 & 0 & -2 & 0 & -3 & -2 & 2 & -1 & -3 & -2 & -1 & -1 & -3 & -2 & -3 \\ \text{N} & -2 & 0 & 6 & 1 & -3 & 0 & 0 & 0 & 1 & -3 & -3 & 0 & -2 & -3 & -2 & 1 & 0 & -4 & -2 & -3 \\ \text{D} & -2 & -2 & 1 & 6 & -3 & 0 & 2 & -1 & -1 & -3 & -4 & -1 & -3 & -3 & -1 & 0 & -1 & -4 & -3 & -3 \\ \text{C} & 0 & -3 & -3 & -3 & 9 & -3 & -4 & -3 & -3 & -1 & -1 & -3 & -1 & -2 & -3 & -1 & -1 & -2 & -2 & -1 \\ \text{Q} & -1 & 1 & 0 & 0 & -3 & 5 & 2 & -2 & 0 & -3 & -2 & 1 & 0 & -3 & -1 & 0 & -1 & -2 & -1 & -2 \\ \text{E} & -1 & 0 & 0 & 2 & -4 & 2 & 5 & -2 & 0 & -3 & -3 & 1 & -2 & -3 & -1 & 0 & -1 & -3 & -2 & -2 \\ \text{G} & 0 & -2 & 0 & -1 & -3 & -2 & -2 & 6 & -2 & -4 & -4 & -2 & -3 & -3 & -2 & 0 & -2 & -2 & -3 & -3 \\ \text{H} & -2 & 0 & 1 & -1 & -3 & 0 & 0 & -2 & 8 & -3 & -3 & -1 & -2 & -1 & -2 & -1 & -2 & -2 & 2 & -3 \\ \text{I} & -1 & -3 & -3 & -3 & -1 & -3 & -3 & -4 & -3 & 4 & 2 & -3 & 1 & 0 & -3 & -2 & -1 & -3 & -1 & 3 \\ \text{L} & -1 & -2 & -3 & -4 & -1 & -2 & -3 & -4 & -3 & 2 & 4 & -2 & 2 & 0 & -3 & -2 & -1 & -2 & -1 & 1 \\ \text{K} & -1 & 2 & 0 & -1 & -3 & 1 & 1 & -2 & -1 & -3 & -2 & 5 & -1 & -3 & -1 & 0 & -1 & -3 & -2 & -2 \\ \text{M} & -1 & -1 & -2 & -3 & -1 & 0 & -2 & -3 & -2 & 1 & 2 & -1 & 5 & 0 & -2 & -1 & -1 & -1 & -1 & 1 \\ \text{F} & -2 & -3 & -3 & -3 & -2 & -3 & -3 & -3 & -1 & 0 & 0 & -3 & 0 & 6 & -4 & -2 & -2 & 1 & 3 & -1 \\ \text{P} & -1 & -2 & -2 & -1 & -3 & -1 & -1 & -2 & -2 & -3 & -3 & -1 & -2 & -4 & 7 & -1 & -1 & -4 & -3 & -2 \\ \text{S} & 1 & -1 & 1 & 0 & -1 & 0 & 0 & 0 & -1 & -2 & -2 & 0 & -1 & -2 & -1 & 4 & 1 & -3 & -2 & -2 \\ \text{T} & 0 & -1 & 0 & -1 & -1 & -1 & -1 & -2 & -2 & -1 & -1 & -1 & -1 & -2 & -1 & 1 & 5 & -2 & -2 & 0 \\ \text{W} & -3 & -3 & -4 & -4 & -2 & -2 & -3 & -2 & -2 & -3 & -2 & -3 & -1 & 1 & -4 & -3 & -2 & 11 & 2 & -3 \\ \text{Y} & -2 & -2 & -2 & -3 & -2 & -1 & -2 & -3 & 2 & -1 & -1 & -2 & -1 & 3 & -3 & -2 & -2 & 2 & 7 & -1 \\ \text{V} & 0 & -3 & -3 & -3 & -1 & -2 & -2 & -3 & -3 & 3 & 1 & -2 & 1 & -1 & -2 & -2 & 0 & -3 & -1 & 4 \end{array}$$