

align.py

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1: #####
2: # Implementation of the Needleman-Wunsch Global Pairwise Alignment algorithm
3: #####
4:
5: def buildTable(X, Y, score, gap):
6:
7:     # create table of zeros with dimension (1+|X|)-by-(1+|Y|)
8:     opt = [ [0] * (1+len(Y)) for _ in range(1+len(X))]
9:
10:    for k in range(1+len(Y)):
11:        opt[0][k] = k*gap        # initialize top row
12:    for j in range(1+len(X)):
13:        opt[j][0] = j*gap        # initialize left column
14:
15:    for j in range(1,1+len(X)):
16:        for k in range(1, 1+len(Y)):
17:            option1 = opt[j-1][k-1] + score(X[j-1],Y[k-1]) # align last chars
18:            option2 = opt[j-1][k] + gap                    # last of X with gap
19:            option3 = opt[j][k-1] + gap                    # last of Y with gap
20:            opt[j][k] = max(option1, option2, option3)
21:    return opt
22:
23: def optScore(X, Y, table):
24:     return table[len(X)][len(Y)] # bottom-right corner
25:
26: def reconstructSolution(X, Y, table, score, gap):
27:     first = '' # alignment for X
28:     second = '' # alignment for Y
29:     glue = '' # line showing matches/mismatches
30:
31:     # start reconstruction at bottom-right of table
32:     j = len(X)
33:     k = len(Y)
34:
35:     while j>0 or k>0:
36:
37:         if j>0 and k>0 and table[j][k] == table[j-1][k-1] + score(X[j-1],Y[k-1]):
38:             # option1 above; match X[j-1] with Y[k-1]
39:             first = X[j-1] + first
40:             second = Y[k-1] + second
41:             if X[j-1] == Y[k-1]:
42:                 glue = '|' + glue # designate match
43:             else:
44:                 glue = '.' + glue # designate mismatch
45:             j = j-1
46:             k = k-1
47:         elif j > 0 and table[j][k] == table[j-1][k] + gap:
48:             # option2 above; match X[j-1] with a gap in Y
49:             first = X[j-1] + first
50:             second = '-' + second
51:             glue = ' ' + glue
52:             j = j-1
53:         else:
54:             # option3 above; match gap in X with Y[k-1]
55:             first = '-' + first
56:             second = Y[k-1] + second
57:             glue = ' ' + glue
58:             k = k-1
59:
60:     return first,glue,second
61:
```