

Tutorial 2

February 23, 2019

1 Tutorial 2

1.1 Week 3-5

1.1.1 1) Write a program to implement Needleman-Wunsch for proteins

Importing blosum50 scoring matrix

```
In [2]: import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

# Importing blosum50 scoring matrix, adding column and row headers
header = ['A', 'R', 'N', 'D', 'C', 'Q', 'E', 'G', 'H', 'I', 'L', 'K', 'M', 'F', 'P', 'S', 'T', 'W', 'Y', 'V']
df=pd.read_csv('blosum50.txt', delim_whitespace = True, names = header, index_col = False)
df.rename(index = dict(zip(range(len(header)),header)),inplace =True)
df.head(21)
```

```
Out[2]:
```

	A	R	N	D	C	Q	E	G	H	I	L	K	M	F	P	S	T	W	Y	V
A	5	-2	-1	-2	-1	-1	-1	0	-2	-1	-2	-1	-1	-3	-1	1	0	-3	-2	0
R	-2	7	-1	-2	-4	1	0	-3	0	-4	-3	3	-2	-3	-3	-1	-1	-3	-1	-3
N	-1	-1	7	2	-2	0	0	0	1	-3	-4	0	-2	-4	-2	1	0	-4	-2	-3
D	-2	-2	2	8	-4	0	2	-1	-1	-4	-4	-1	-4	-5	-1	0	-1	-5	-3	-4
C	-1	-4	-2	-4	13	-3	-3	-3	-3	-2	-2	-3	-2	-2	-4	-1	-1	-5	-3	-1
Q	-1	1	0	0	-3	7	2	-2	1	-3	-2	2	0	-4	-1	0	-1	-1	-1	-3
E	-1	0	0	2	-3	2	6	-3	0	-4	-3	1	-2	-3	-1	-1	-1	-3	-2	-3
G	0	-3	0	-1	-3	-2	-3	8	-2	-4	-4	-2	-3	-4	-2	0	-2	-3	-3	-4
H	-2	0	1	-1	-3	1	0	-2	10	-4	-3	0	-1	-1	-2	-1	-2	-3	2	-4
I	-1	-4	-3	-4	-2	-3	-4	-4	-4	5	2	-3	2	0	-3	-3	-1	-3	-1	4
L	-2	-3	-4	-4	-2	-2	-3	-4	-3	2	5	-3	3	1	-4	-3	-1	-2	-1	1
K	-1	3	0	-1	-3	2	1	-2	0	-3	-3	6	-2	-4	-1	0	-1	-3	-2	-3
M	-1	-2	-2	-4	-2	0	-2	-3	-1	2	3	-2	7	0	-3	-2	-1	-1	0	1
F	-3	-3	-4	-5	-2	-4	-3	-4	-1	0	1	-4	0	8	-4	-3	-2	1	4	-1
P	-1	-3	-2	-1	-4	-1	-1	-2	-2	-3	-4	-1	-3	-4	10	-1	-1	-4	-3	-3
S	1	-1	1	0	-1	0	-1	0	-1	-3	-3	0	-2	-3	-1	5	2	-4	-2	-2
T	0	-1	0	-1	-1	-1	-1	-2	-2	-1	-1	-1	-1	-2	-1	2	5	-3	-2	0
W	-3	-3	-4	-5	-5	-1	-3	-3	-3	-3	-2	-3	-1	1	-4	-4	-3	15	2	-3
Y	-2	-1	-2	-3	-3	-1	-2	-3	2	-1	-1	-2	0	4	-3	-2	-2	2	8	-1
V	0	-3	-3	-4	-1	-3	-3	-4	-4	4	1	-3	1	-1	-3	-2	0	-3	-1	5

```
In [2]: m = 11
        n = 8

        # Creating a table to run HEAGAWGHEE versus PAWHEAE
        h = [' ', 'H', 'E', 'A', 'G', 'A', 'W', 'G', 'H', 'E', 'E']
        header2 = [' ', 'P', 'A', 'W', 'H', 'E', 'A', 'E']
        df1 = pd.DataFrame(data=[np.zeros(3)]*m]*n)
        df1.rename(index = dict(zip(range(len(header2)),header2)),inplace =True)
        df1.rename(columns=dict(zip(range(len(h)),h)), inplace = True)

        df1
```

```
Out [2]:
```

		H	E	A \
		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
P		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
A		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
W		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
H		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
E		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
A		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
E		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]

		G	A	W	G \
		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
P		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
A		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
W		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
H		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
E		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
A		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
E		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]

		H	E	E
		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
P		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
A		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
W		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
H		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
E		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
A		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
E		[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]

```
In [3]: # Filling the Global Alignment Table (array in row-column pair)
        #Forward Pass

        cost = -8 # Cost of insertion or delition

        # Calculating price of substitution when arrows moves diagonally
```

```

def blos(r, c):
    cname = df1.columns[c]
    rname = df1.index[r]
    if r == 0 or c == 0:
        return np.nan # Handling nan error when filling first row/column
    else:
        return int(df[rname][cname]) + int(df1.iloc[r-1,c-1][0])

arrow = []

# Loop to fill the table, deciding between if the upelement, leftelement or the diagelement
for r in range(0,8):
    for c in range(0,11):
        upelement = int(df1.iloc[r-1,c][0]) + cost if r >= 1 else np.nan # Handling nan
        leftelement = int(df1.iloc[r,c-1][0]) + cost if c >= 1 else np.nan # Handling nan
        diagelement = blos(r, c)
        if r == 0 and c == 0:
            upelement = 0
        list1 = np.array([diagelement, upelement, leftelement])
        re = np.nanargmax(list1)
        # Storing the location of the selected max element to find arrow direction during
        if list1[re] == diagelement:
            vec = [r-1,c-1]
            arrow.extend([r-1,c-1, r,c])
        elif list1[re] == upelement:
            vec = [r-1,c]
            arrow.extend([r-1,c, r,c])
        elif list1[re] == leftelement:
            vec = [r,c-1]
            arrow.extend([r,c-1, r,c])
        # Storing value, row and column coordinates in an array for each row-column pair
        df1.iloc[r,c] = np.array([list1[re], vec[0], vec[1]])

df1

```

```

Out[3]:

```

		H	E	A \
	[0.0, -1.0, 0.0]	[-8.0, 0.0, 0.0]	[-16.0, 0.0, 1.0]	[-24.0, 0.0, 2.0]
P	[-8.0, 0.0, 0.0]	[-2, 0, 0]	[-9, 0, 1]	[-17, 0, 2]
A	[-16.0, 1.0, 0.0]	[-10, 1, 0]	[-3, 1, 1]	[-4, 1, 2]
W	[-24.0, 2.0, 0.0]	[-18, 2, 1]	[-11, 2, 2]	[-6, 2, 2]
H	[-32.0, 3.0, 0.0]	[-14, 3, 0]	[-18, 3, 1]	[-13, 3, 2]
E	[-40.0, 4.0, 0.0]	[-22, 4, 1]	[-8, 4, 1]	[-16, 5, 2]
A	[-48.0, 5.0, 0.0]	[-30, 5, 1]	[-16, 5, 2]	[-3, 5, 2]
E	[-56.0, 6.0, 0.0]	[-38, 6, 1]	[-24, 6, 1]	[-11, 6, 3]

	G	A	W	G \
	[-32.0, 0.0, 3.0]	[-40.0, 0.0, 4.0]	[-48.0, 0.0, 5.0]	[-56.0, 0.0, 6.0]
P	[-25, 1, 3]	[-33, 0, 4]	[-41, 1, 5]	[-49, 1, 6]

A	[-12, 2, 3]	[-20, 1, 4]	[-28, 2, 5]	[-36, 2, 6]
W	[-7, 2, 3]	[-15, 2, 4]	[-5, 2, 5]	[-13, 3, 6]
H	[-8, 3, 3]	[-9, 3, 4]	[-13, 3, 6]	[-7, 3, 6]
E	[-16, 4, 3]	[-9, 4, 4]	[-12, 4, 5]	[-15, 4, 7]
A	[-11, 6, 3]	[-11, 5, 4]	[-12, 5, 5]	[-12, 5, 6]
E	[-6, 6, 3]	[-12, 6, 4]	[-14, 6, 5]	[-15, 6, 6]

	H	E	E
	[-64.0, 0.0, 7.0]	[-72.0, 0.0, 8.0]	[-80.0, 0.0, 9.0]
P	[-57, 1, 7]	[-65, 0, 8]	[-73, 0, 9]
A	[-44, 2, 7]	[-52, 2, 8]	[-60, 2, 9]
W	[-21, 3, 7]	[-29, 3, 8]	[-37, 3, 9]
H	[-3, 3, 7]	[-11, 4, 8]	[-19, 4, 9]
E	[-7, 4, 7]	[3, 4, 8]	[-5, 4, 9]
A	[-15, 5, 8]	[-5, 5, 9]	[2, 5, 9]
E	[-12, 6, 7]	[-9, 6, 8]	[1, 6, 9]

```
In [4]: # Filling the Global Allignment Table (integer in row-column pair)
#Forward Pass
```

```
cost = -8 # Cost of insertion or delition
```

```
# Calculating price of substitution when arrows moves diagonally
```

```
def blos(r, c):
    cname = df1.columns[c]
    rname = df1.index[r]
    if r == 0 or c == 0:
        return np.nan # Handling nan error when filling first row/column
    else:
        return int(df[rname][cname]) + int(df1.iloc[r-1,c-1])
```

```
arrow = []
```

```
# Loop to fill the table, deciding between if the upelement, leftelement or the diagel
for r in range(0,8):
    for c in range(0,11):
        upelement = int(df1.iloc[r-1,c]) + cost if r >= 1 else np.nan # Handling nan e
        leftelement = int(df1.iloc[r,c-1]) + cost if c >= 1 else np.nan # Handling nan
        diagelement = blos(r, c)
        if r == 0 and c == 0:
            upelement = 0
        list1 = np.array([diagelement, upelement, leftelement])
        # Storing the max integer in row-column pair to fill table
        re = np.nanargmax(list1)
        df1.iloc[r,c] = list1[re]
        # Storing the location of the selected max element and of the corrisponding ad
        # to find arrow direction during the backward pass
        if list1[re] == diagelement:
```

```

        arrow.extend([r-1,c-1, r,c])
    elif list1[re] == upelement:
        arrow.extend([r-1,c, r,c])
    elif list1[re] == leftelement:
        arrow.extend([r,c-1, r,c])

df1

Out[4]:
      H    E    A    G    A    W    G    H    E    E
0   -8  -16  -24  -32  -40  -48  -56  -64  -72  -80
P  -8   -2   -9  -17  -25  -33  -41  -49  -57  -65  -73
A -16  -10   -3   -4  -12  -20  -28  -36  -44  -52  -60
W -24  -18  -11   -6   -7  -15   -5  -13  -21  -29  -37
H -32  -14  -18  -13   -8   -9  -13   -7   -3  -11  -19
E -40  -22   -8  -16  -16   -9  -12  -15   -7    3   -5
A -48  -30  -16   -3  -11  -11  -12  -12  -15   -5    2
E -56  -38  -24  -11   -6  -12  -14  -15  -12   -9    1

In [5]: # Backward pass

# Making empty lists where to append the backward pass elements and the two strings
back = []
letter1 = []
letter2 = []

# Starting from the last column-row pair in the table
K = arrow[len(arrow)-1] # Storing it's column coordinate
M = arrow[len(arrow)-1-1] # Storing it's row coordinate
h1 = arrow[len(arrow)-1-2] # Storing the column coordinate where the arrow in the block
h2 = arrow[len(arrow)-1-3] # Storing the row coordinate where the arrow in the block
back.append(df1.iloc[r,c]) # Storing the element corrisponding to the M,K coordinates
letter1.append(df1.index[r]) # Storing the letter corrisponding to the M row to form the string
letter2.append(df1.columns[c]) # Storing the letter corrisponding to the K column to form the string

i = len(arrow) -5 # Looping throught all the arrow array apart from all the initialization

while i > 0:
    if ((h1 <= arrow[i-2]) and (h2 <= arrow[i-3])): # If there are duplicates or coordinates
                                                    # in the arrow array, skip them
        i -=2
    elif ((arrow[i] == h1) and (arrow[i-1] == h2)): # If while going through the array
                                                    # are in is pointing at, store its
                                                    # coordinates this new element is
                                                    # corrispondent row/column letter
                                                    # respect to the previous element
                                                    # add - in the first string instead of the
                                                    # previous element the column number
                                                    # the second string instead of the

```

```

K = arrow[i]
M = arrow[i-1]
h1 = arrow[i-2]
h2 = arrow[i-3]
back.append(df1.iloc[M,K])
if i>5:
    if((K==h1) and (M!=h2)):
        letter2.append('-')
        letter1.append(df1.index[M])
    elif((K!=h1) and (M==h2)):
        letter1.append('-')
        letter2.append(df1.columns[K])
    else:
        letter1.append(df1.index[M])
        letter2.append(df1.columns[K])
    i -=4
else:
    i -=1 # If no corrispondence if found go ahead to the next array element

back = np.asarray(back)
print(letter2[::-1]) # Reversing the string letter order
print(letter1[::-1]) # Reversing the string letter order
print(back)

['H', 'E', 'A', 'G', 'A', 'W', 'G', 'H', 'E', '-', 'E']
['-', '-', 'P', '-', 'A', 'W', '-', 'H', 'E', 'A', 'E']
[ 1. -5.  3. -3. -13. -5. -20. -25. -17. -16. -8.  0.]

```

In [6]: # Creating a table to Match the protein sequence SALPQPTTPVSSFTSGSMLGRTDALTNTYSAL with

```
m = 34
n = 35

# adding ' ' and , automatically to string
# import re
# st = 'S A L P Q P T T P V S S F T S G S M L G R T D T A L T N T Y S A L '
# print(re.findall(r"[\w']+", st))

# adding column and row headers
h = [' ', 'S', 'A', 'L', 'P', 'Q', 'P', 'T', 'T', 'P', 'V', 'S', 'S', 'F', 'T', 'S', 'G', 'S', 'M', 'L', 'G', 'R', 'T', 'D', 'T', 'A', 'L', 'T', 'N', 'T', 'Y', 'S', 'A', 'L']
header2 = [' ', 'P', 'S', 'P', 'T', 'M', 'E', 'A', 'V', 'T', 'S', 'V', 'E', 'A', 'S', 'P', 'H', 'S', 'T', 'S', 'S', 'Y', 'F', 'A', 'T', 'T', 'Y', 'Y', 'H', 'L']
df2 = pd.DataFrame(data=[np.zeros(1)]*m*n)
df2.rename(index = dict(zip(range(len(header2)),header2)),inplace =True)
```

df2

[illegible]

E	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
A	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
V	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
T	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
S	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
V	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
E	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
A	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
S	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
T	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
A	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
S	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
H	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
P	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
H	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
S	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
T	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
S	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
S	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
Y	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
F	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
A	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
T	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
T	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
Y	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
Y	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
H	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
L	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]
Y	...	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]	[0.0]

[35 rows x 34 columns]

```
In [7]: # Same as:
# Filling the Global Alignment Table (array in row-column pair)
#Forward Pass

cost = -8

def blos(r, c):
    cname = df2.columns[c]
    rname = df2.index[r]
    if r == 0 or c == 0:
        return np.nan
    else:
        return int(df[rname][cname]) + int(df2.iloc[r-1,c-1][0])

arrow = []
```



```

for r in range(0,35):
    for c in range(0,34):
        upelement = int(df2.iloc[r-1,c][0]) + cost if r >= 1 else np.nan
        leftelement = int(df2.iloc[r,c-1][0]) + cost if c >= 1 else np.nan
        diagelement = blos(r, c)
        if r == 0 and c == 0:
            upelement = 0
        list1 = np.array([diagelement, upelement, leftelement])
        re = np.nanargmax(list1)
        #df1.iloc[r,c] = list1[re]
        if list1[re] == diagelement:
            vec = [r-1,c-1]
            arrow.extend([r-1,c-1, r,c])
        elif list1[re] == upelement:
            vec = [r-1,c]
            arrow.extend([r-1,c, r,c])
        elif list1[re] == leftelement:
            vec = [r,c-1]
            arrow.extend([r,c-1, r,c])
        df2.iloc[r,c] = np.array([list1[re], vec[0], vec[1]])

```

df2

Out [7]:

		S	A \
	[0.0, -1.0, 0.0]	[-8.0, 0.0, 0.0]	[-16.0, 0.0, 1.0]
P	[-8.0, 0.0, 0.0]	[-1, 0, 0]	[-9, 0, 1]
S	[-16.0, 1.0, 0.0]	[-3, 1, 0]	[0, 1, 1]
P	[-24.0, 2.0, 0.0]	[-11, 2, 1]	[-4, 2, 1]
T	[-32.0, 3.0, 0.0]	[-19, 3, 1]	[-11, 3, 1]
M	[-40.0, 4.0, 0.0]	[-27, 4, 1]	[-19, 4, 2]
E	[-48.0, 5.0, 0.0]	[-35, 5, 1]	[-27, 5, 2]
A	[-56.0, 6.0, 0.0]	[-43, 6, 1]	[-30, 6, 1]
V	[-64.0, 7.0, 0.0]	[-51, 7, 1]	[-38, 7, 2]
T	[-72.0, 8.0, 0.0]	[-59, 8, 1]	[-46, 8, 2]
S	[-80.0, 9.0, 0.0]	[-67, 9, 0]	[-54, 9, 2]
V	[-88.0, 10.0, 0.0]	[-75, 10, 1]	[-62, 10, 2]
E	[-96.0, 11.0, 0.0]	[-83, 11, 1]	[-70, 11, 2]
A	[-104.0, 12.0, 0.0]	[-91, 12, 1]	[-78, 12, 1]
S	[-112.0, 13.0, 0.0]	[-99, 13, 0]	[-86, 13, 2]
T	[-120.0, 14.0, 0.0]	[-107, 14, 1]	[-94, 14, 2]
A	[-128.0, 15.0, 0.0]	[-115, 15, 1]	[-102, 15, 1]
S	[-136.0, 16.0, 0.0]	[-123, 16, 0]	[-110, 16, 2]
H	[-144.0, 17.0, 0.0]	[-131, 17, 1]	[-118, 17, 2]
P	[-152.0, 18.0, 0.0]	[-139, 18, 1]	[-126, 18, 2]
H	[-160.0, 19.0, 0.0]	[-147, 19, 1]	[-134, 19, 2]
S	[-168.0, 20.0, 0.0]	[-155, 20, 0]	[-142, 20, 2]
T	[-176.0, 21.0, 0.0]	[-163, 21, 1]	[-150, 21, 2]
S	[-184.0, 22.0, 0.0]	[-171, 22, 0]	[-158, 22, 2]

S	[-192.0, 23.0, 0.0]	[-179, 23, 0]	[-166, 23, 2]
Y	[-200.0, 24.0, 0.0]	[-187, 24, 1]	[-174, 24, 2]
F	[-208.0, 25.0, 0.0]	[-195, 25, 1]	[-182, 25, 2]
A	[-216.0, 26.0, 0.0]	[-203, 26, 1]	[-190, 26, 1]
T	[-224.0, 27.0, 0.0]	[-211, 27, 1]	[-198, 27, 2]
T	[-232.0, 28.0, 0.0]	[-219, 28, 1]	[-206, 28, 2]
Y	[-240.0, 29.0, 0.0]	[-227, 29, 1]	[-214, 29, 2]
Y	[-248.0, 30.0, 0.0]	[-235, 30, 1]	[-222, 30, 2]
H	[-256.0, 31.0, 0.0]	[-243, 31, 1]	[-230, 31, 2]
L	[-264.0, 32.0, 0.0]	[-251, 32, 1]	[-238, 32, 2]
Y	[-272.0, 33.0, 0.0]	[-259, 33, 1]	[-246, 33, 2]

	L	P	Q	P \
	[-24.0, 0.0, 2.0]	[-32.0, 0.0, 3.0]	[-40.0, 0.0, 4.0]	[-48.0, 0.0, 5.0]
P	[-17, 1, 2]	[-14, 0, 3]	[-22, 1, 4]	[-30, 0, 5]
S	[-8, 2, 2]	[-16, 2, 3]	[-14, 1, 4]	[-22, 2, 5]
P	[-4, 2, 2]	[2, 2, 3]	[-6, 3, 4]	[-4, 2, 5]
T	[-5, 3, 2]	[-5, 3, 3]	[1, 3, 4]	[-7, 3, 5]
M	[-8, 4, 2]	[-8, 4, 3]	[-5, 4, 4]	[-2, 4, 5]
E	[-16, 5, 3]	[-9, 5, 3]	[-6, 5, 4]	[-6, 5, 5]
A	[-24, 6, 3]	[-17, 6, 3]	[-10, 6, 4]	[-7, 6, 5]
V	[-29, 7, 2]	[-25, 7, 4]	[-18, 7, 5]	[-13, 7, 5]
T	[-37, 8, 3]	[-30, 8, 3]	[-26, 8, 4]	[-19, 8, 5]
S	[-45, 9, 3]	[-38, 9, 3]	[-30, 9, 4]	[-27, 9, 5]
V	[-53, 10, 2]	[-46, 10, 4]	[-38, 10, 5]	[-33, 10, 5]
E	[-61, 11, 3]	[-54, 11, 3]	[-44, 11, 4]	[-39, 11, 5]
A	[-69, 12, 3]	[-62, 12, 3]	[-52, 12, 5]	[-45, 12, 5]
S	[-77, 13, 3]	[-70, 13, 3]	[-60, 13, 5]	[-53, 13, 5]
T	[-85, 14, 3]	[-78, 14, 3]	[-68, 14, 5]	[-61, 14, 5]
A	[-93, 15, 3]	[-86, 15, 3]	[-76, 15, 5]	[-69, 15, 5]
S	[-101, 16, 3]	[-94, 16, 3]	[-84, 16, 5]	[-77, 16, 5]
H	[-109, 17, 3]	[-102, 17, 4]	[-92, 17, 5]	[-85, 17, 6]
P	[-117, 18, 3]	[-99, 18, 3]	[-100, 18, 5]	[-82, 18, 5]
H	[-125, 19, 3]	[-107, 19, 4]	[-98, 19, 4]	[-90, 19, 6]
S	[-133, 20, 3]	[-115, 20, 4]	[-106, 20, 5]	[-98, 20, 6]
T	[-141, 21, 3]	[-123, 21, 4]	[-114, 21, 5]	[-106, 21, 6]
S	[-149, 22, 3]	[-131, 22, 4]	[-122, 22, 5]	[-114, 22, 6]
S	[-157, 23, 3]	[-139, 23, 4]	[-130, 23, 5]	[-122, 23, 6]
Y	[-165, 24, 3]	[-147, 24, 4]	[-138, 24, 5]	[-130, 24, 6]
F	[-173, 25, 2]	[-155, 25, 4]	[-146, 25, 5]	[-138, 25, 6]
A	[-181, 26, 3]	[-163, 26, 4]	[-154, 26, 5]	[-146, 26, 6]
T	[-189, 27, 3]	[-171, 27, 4]	[-162, 27, 5]	[-154, 27, 6]
T	[-197, 28, 3]	[-179, 28, 4]	[-170, 28, 5]	[-162, 28, 6]
Y	[-205, 29, 3]	[-187, 29, 4]	[-178, 29, 5]	[-170, 29, 6]
Y	[-213, 30, 3]	[-195, 30, 4]	[-186, 30, 5]	[-178, 30, 6]
H	[-221, 31, 3]	[-203, 31, 4]	[-194, 31, 4]	[-186, 31, 6]
L	[-225, 32, 2]	[-211, 32, 4]	[-202, 32, 5]	[-194, 32, 6]
Y	[-233, 33, 3]	[-219, 33, 4]	[-210, 33, 5]	[-202, 33, 6]

	T	T	P \
	[-56.0, 0.0, 6.0]	[-64.0, 0.0, 7.0]	[-72.0, 0.0, 8.0]
P	[-38, 1, 6]	[-46, 1, 7]	[-54, 0, 8]
S	[-28, 1, 6]	[-36, 1, 7]	[-44, 2, 8]
P	[-12, 3, 6]	[-20, 3, 7]	[-26, 2, 8]
T	[1, 3, 6]	[-7, 3, 7]	[-15, 4, 8]
M	[-7, 4, 7]	[0, 4, 7]	[-8, 5, 8]
E	[-3, 5, 6]	[-8, 5, 7]	[-1, 5, 8]
A	[-6, 6, 6]	[-3, 6, 7]	[-9, 6, 8]
V	[-7, 7, 6]	[-6, 7, 7]	[-6, 7, 8]
T	[-8, 8, 6]	[-2, 8, 7]	[-7, 8, 8]
S	[-16, 9, 7]	[-6, 9, 7]	[-3, 9, 8]
V	[-24, 10, 7]	[-14, 10, 8]	[-9, 10, 8]
E	[-32, 11, 7]	[-22, 11, 8]	[-15, 11, 8]
A	[-39, 12, 6]	[-30, 12, 8]	[-23, 12, 8]
S	[-43, 13, 6]	[-37, 13, 7]	[-31, 13, 8]
T	[-48, 14, 6]	[-38, 14, 7]	[-38, 14, 8]
A	[-56, 15, 7]	[-46, 15, 8]	[-39, 15, 8]
S	[-64, 16, 7]	[-54, 16, 7]	[-47, 16, 8]
H	[-72, 17, 7]	[-62, 17, 8]	[-55, 17, 9]
P	[-80, 18, 7]	[-70, 18, 8]	[-52, 18, 8]
H	[-84, 19, 6]	[-78, 19, 8]	[-60, 19, 9]
S	[-88, 20, 6]	[-82, 20, 7]	[-68, 20, 9]
T	[-93, 21, 6]	[-83, 21, 7]	[-76, 21, 9]
S	[-101, 22, 7]	[-91, 22, 7]	[-84, 22, 8]
S	[-109, 23, 7]	[-99, 23, 7]	[-92, 23, 8]
Y	[-117, 24, 7]	[-107, 24, 8]	[-100, 24, 9]
F	[-125, 25, 7]	[-115, 25, 8]	[-108, 25, 9]
A	[-133, 26, 7]	[-123, 26, 8]	[-116, 26, 8]
T	[-141, 27, 6]	[-128, 27, 7]	[-124, 27, 8]
T	[-149, 28, 6]	[-136, 28, 7]	[-129, 28, 8]
Y	[-157, 29, 7]	[-144, 29, 8]	[-137, 29, 9]
Y	[-165, 30, 7]	[-152, 30, 8]	[-145, 30, 9]
H	[-173, 31, 7]	[-160, 31, 8]	[-153, 31, 9]
L	[-181, 32, 7]	[-168, 32, 8]	[-161, 32, 9]
Y	[-189, 33, 7]	[-176, 33, 8]	[-169, 33, 9]

	...	T	A \
	...	[-192.0, 0.0, 23.0]	[-200.0, 0.0, 24.0]
P	...	[-174, 1, 23]	[-182, 1, 24]
S	...	[-161, 2, 23]	[-169, 2, 24]
P	...	[-146, 3, 23]	[-154, 3, 24]
T	...	[-133, 3, 23]	[-141, 4, 24]
M	...	[-118, 5, 23]	[-126, 5, 24]
E	...	[-108, 6, 23]	[-116, 6, 24]
A	...	[-100, 6, 23]	[-103, 6, 24]
V	...	[-94, 7, 23]	[-100, 7, 24]

T	...	[-84, 8, 23]	[-92, 9, 24]
S	...	[-77, 9, 23]	[-83, 9, 24]
V	...	[-68, 11, 23]	[-76, 11, 24]
E	...	[-58, 12, 23]	[-66, 12, 24]
A	...	[-50, 12, 23]	[-53, 12, 24]
S	...	[-42, 13, 23]	[-49, 13, 24]
T	...	[-31, 14, 23]	[-39, 15, 24]
A	...	[-27, 15, 23]	[-26, 15, 24]
S	...	[-19, 16, 23]	[-26, 16, 24]
H	...	[-22, 17, 23]	[-21, 17, 24]
P	...	[-17, 18, 23]	[-23, 18, 24]
H	...	[-13, 20, 23]	[-19, 19, 24]
S	...	[-3, 20, 23]	[-11, 21, 24]
T	...	[-2, 21, 23]	[-3, 21, 24]
S	...	[-5, 22, 23]	[-1, 22, 24]
S	...	[2, 23, 23]	[-4, 23, 24]
Y	...	[-3, 24, 23]	[0, 24, 24]
F	...	[-10, 25, 23]	[-6, 25, 24]
A	...	[-16, 26, 23]	[-5, 26, 24]
T	...	[-14, 27, 23]	[-13, 27, 25]
T	...	[-19, 28, 23]	[-14, 28, 24]
Y	...	[-27, 29, 24]	[-21, 29, 24]
Y	...	[-28, 30, 23]	[-29, 30, 24]
H	...	[-36, 31, 23]	[-30, 31, 24]
L	...	[-41, 32, 23]	[-38, 32, 24]
Y	...	[-49, 33, 24]	[-43, 33, 24]

	L	T	N \
	[-208.0, 0.0, 25.0]	[-216.0, 0.0, 26.0]	[-224.0, 0.0, 27.0]
P	[-190, 1, 25]	[-198, 1, 26]	[-206, 1, 27]
S	[-177, 2, 25]	[-185, 2, 26]	[-193, 2, 27]
P	[-162, 3, 25]	[-170, 3, 26]	[-178, 3, 27]
T	[-149, 4, 25]	[-157, 3, 26]	[-165, 4, 27]
M	[-134, 5, 25]	[-142, 5, 26]	[-150, 5, 27]
E	[-124, 6, 25]	[-132, 6, 26]	[-140, 6, 27]
A	[-111, 7, 25]	[-119, 7, 26]	[-127, 7, 27]
V	[-102, 7, 25]	[-110, 8, 26]	[-118, 8, 27]
T	[-100, 9, 25]	[-97, 8, 26]	[-105, 9, 27]
S	[-91, 10, 25]	[-98, 9, 26]	[-96, 9, 27]
V	[-82, 10, 25]	[-90, 11, 26]	[-98, 11, 27]
E	[-74, 12, 25]	[-82, 12, 26]	[-90, 11, 27]
A	[-61, 13, 25]	[-69, 13, 26]	[-77, 13, 27]
S	[-56, 13, 25]	[-59, 13, 26]	[-67, 14, 27]
T	[-47, 15, 25]	[-51, 14, 26]	[-59, 14, 27]
A	[-34, 16, 25]	[-42, 16, 26]	[-50, 16, 27]
S	[-29, 16, 25]	[-32, 16, 26]	[-40, 17, 27]
H	[-29, 17, 25]	[-31, 17, 26]	[-31, 17, 27]
P	[-25, 18, 25]	[-30, 18, 26]	[-33, 18, 27]

H	[-26, 19, 25]	[-27, 19, 26]	[-29, 19, 27]
S	[-19, 21, 25]	[-24, 20, 26]	[-26, 20, 27]
T	[-11, 22, 25]	[-14, 21, 26]	[-22, 22, 27]
S	[-6, 22, 25]	[-9, 22, 26]	[-13, 22, 27]
S	[-4, 23, 25]	[-4, 23, 26]	[-8, 23, 27]
Y	[-5, 24, 25]	[-6, 24, 26]	[-6, 24, 27]
F	[1, 25, 25]	[-7, 25, 26]	[-10, 25, 27]
A	[-7, 26, 26]	[1, 26, 26]	[-7, 27, 27]
T	[-6, 27, 25]	[-2, 27, 26]	[1, 27, 27]
T	[-14, 28, 25]	[-1, 28, 26]	[-2, 28, 27]
Y	[-15, 29, 25]	[-9, 29, 27]	[-3, 29, 27]
Y	[-22, 30, 25]	[-17, 30, 26]	[-11, 30, 27]
H	[-30, 31, 26]	[-24, 31, 26]	[-16, 31, 27]
L	[-25, 32, 25]	[-31, 32, 26]	[-24, 32, 28]
Y	[-33, 33, 26]	[-27, 33, 26]	[-32, 33, 28]

	T	Y	S \
	[-232.0, 0.0, 28.0]	[-240.0, 0.0, 29.0]	[-248.0, 0.0, 30.0]
P	[-214, 1, 28]	[-222, 1, 29]	[-230, 1, 30]
S	[-201, 2, 28]	[-209, 2, 29]	[-217, 1, 30]
P	[-186, 3, 28]	[-194, 3, 29]	[-202, 3, 30]
T	[-173, 3, 28]	[-181, 4, 29]	[-189, 4, 30]
M	[-158, 5, 28]	[-166, 5, 29]	[-174, 5, 30]
E	[-148, 6, 28]	[-156, 6, 29]	[-164, 6, 30]
A	[-135, 7, 28]	[-143, 7, 29]	[-151, 7, 30]
V	[-126, 8, 28]	[-134, 8, 29]	[-142, 8, 30]
T	[-113, 8, 28]	[-121, 9, 29]	[-129, 9, 30]
S	[-103, 9, 28]	[-111, 10, 29]	[-116, 9, 30]
V	[-96, 10, 28]	[-104, 10, 29]	[-112, 11, 30]
E	[-98, 12, 28]	[-98, 11, 29]	[-105, 11, 30]
A	[-85, 13, 28]	[-93, 13, 29]	[-97, 12, 30]
S	[-75, 13, 28]	[-83, 14, 29]	[-88, 13, 30]
T	[-62, 14, 28]	[-70, 15, 29]	[-78, 15, 30]
A	[-58, 16, 28]	[-64, 15, 29]	[-69, 15, 30]
S	[-48, 16, 28]	[-56, 17, 29]	[-59, 16, 30]
H	[-39, 18, 28]	[-46, 17, 29]	[-54, 18, 30]
P	[-32, 18, 28]	[-40, 19, 29]	[-47, 18, 30]
H	[-35, 19, 28]	[-30, 19, 29]	[-38, 20, 30]
S	[-27, 20, 28]	[-35, 21, 29]	[-25, 20, 30]
T	[-21, 21, 28]	[-29, 21, 29]	[-33, 21, 30]
S	[-20, 22, 28]	[-23, 22, 29]	[-24, 22, 30]
S	[-11, 23, 28]	[-19, 24, 29]	[-18, 23, 30]
Y	[-10, 24, 28]	[-3, 24, 29]	[-11, 25, 30]
F	[-8, 25, 28]	[-6, 25, 29]	[-6, 25, 30]
A	[-10, 26, 28]	[-10, 26, 29]	[-5, 26, 30]
T	[-2, 27, 28]	[-10, 28, 29]	[-8, 27, 30]
T	[6, 28, 28]	[-2, 29, 29]	[-8, 28, 30]
Y	[-2, 29, 29]	[14, 29, 29]	[6, 30, 30]

Y	[-5, 30, 28]	[6, 30, 29]	[12, 30, 30]
H	[-13, 31, 28]	[-2, 31, 30]	[5, 31, 30]
L	[-17, 32, 28]	[-10, 32, 30]	[-3, 32, 31]
Y	[-25, 33, 29]	[-9, 33, 29]	[-11, 33, 31]

	A	L
	[-256.0, 0.0, 31.0]	[-264.0, 0.0, 32.0]
P	[-238, 1, 31]	[-246, 1, 32]
S	[-225, 2, 31]	[-233, 2, 32]
P	[-210, 3, 31]	[-218, 3, 32]
T	[-197, 4, 31]	[-205, 4, 32]
M	[-182, 5, 31]	[-190, 5, 32]
E	[-172, 6, 31]	[-180, 6, 32]
A	[-159, 6, 31]	[-167, 7, 32]
V	[-150, 8, 31]	[-158, 7, 32]
T	[-137, 9, 31]	[-145, 9, 32]
S	[-124, 10, 31]	[-132, 10, 32]
V	[-116, 10, 31]	[-123, 10, 32]
E	[-113, 11, 31]	[-119, 11, 32]
A	[-100, 12, 31]	[-108, 13, 32]
S	[-96, 13, 31]	[-103, 13, 32]
T	[-86, 15, 31]	[-94, 15, 32]
A	[-73, 15, 31]	[-81, 16, 32]
S	[-67, 17, 31]	[-75, 17, 32]
H	[-61, 17, 31]	[-69, 18, 32]
P	[-55, 18, 31]	[-63, 19, 32]
H	[-46, 20, 31]	[-54, 20, 32]
S	[-33, 21, 31]	[-41, 21, 32]
T	[-25, 21, 31]	[-33, 22, 32]
S	[-32, 22, 31]	[-28, 22, 32]
S	[-23, 23, 31]	[-31, 24, 32]
Y	[-19, 25, 31]	[-24, 24, 32]
F	[-14, 25, 31]	[-18, 25, 32]
A	[-1, 26, 31]	[-9, 27, 32]
T	[-5, 27, 31]	[-2, 27, 32]
T	[-8, 28, 31]	[-6, 28, 32]
Y	[-2, 30, 31]	[-9, 29, 32]
Y	[4, 30, 31]	[-3, 30, 32]
H	[10, 31, 31]	[2, 32, 32]
L	[3, 32, 31]	[15, 32, 32]
Y	[-5, 33, 31]	[7, 33, 33]

[35 rows x 34 columns]

```
In [8]: arrow2 = []
        letter1 = []
        letter2 = []
```

```

# Setting initial conditions, starting from the last element of the table
r =34
c =33
nextr = 34
nextc = 33
# Same as:
# Backward pass
if((c==nextc) and (r==nextr)):
    letter2.append('-')
    letter1.append(df2.index[r])
elif((c!=nextc) and (r==nextr)):
    letter1.append('-')
    letter2.append(df2.columns[c])
elif((c!=nextc) and (r!=nextr)):
    letter1.append(df2.index[r])
    letter2.append(df2.columns[c])

# Looping through the table to find the backward pass elements and their corresponding
for r in range(34, 0,-1):
    for c in range(33,-1,-1):
        if r == nextr and c == nextc: # Similar implementation as in Backward pass, the
                                        # direction has been stored in an array directly
                                        # in a separate list
            arrow2.append(df2.iloc[r,c][0])
            nextr = df2.iloc[r,c][1]
            nextc = df2.iloc[r,c][2]
            if c == 33 and r==34: # Handling starting condition
                letter2.append(df2.columns[c])
                letter1.append(df2.index[r-1])
            if c != 33 and r!=34:
                if((c==nextc) and (r==nextr)) or (nextr==0 and nextc==0)):
                    letter2.append('-')
                    letter1.append(df2.index[r])
                elif((c!=nextc) and (r==nextr)):
                    letter1.append('-')
                    letter2.append(df2.columns[c])
                else:
                    letter1.append(df2.index[r])
                    letter2.append(df2.columns[c])

arrow2.append(0)
arrow2 = np.asarray(arrow2)
print(letter2[::-1])
print(letter1[::-1])
print(arrow2)
# -SALPQPTTPVSSFTSGSMLGRTDTALNTYSAL-
# PSPTMEAVTSVEA-STASHPHSTSSYFATTYYHLY

```

```
['-', 'S', 'A', 'L', 'P', 'Q', 'P', 'T', 'T', 'P', 'V', 'S', 'S', 'F', 'T', 'S', 'G', 'S', 'M',
['P', 'S', 'P', 'T', 'M', 'E', 'A', 'V', 'T', 'S', 'V', 'E', 'A', '-', 'S', 'T', 'A', 'S', 'H',
[ 7. 15. 10. 12. 14.  6.  1.  1.  1.  0.  2.  0.  0. -5. -4. -2.  2.  3.
-2. -2. -4. -6.  2.  1.  2. -3. -2. -7. -7. -6. -8. -5. -4. -3. -8.  0.]
```

1.1.2 2) Modify your program to implement the Smith-Waterman algorithm

Again run this on HEAGAWGHEE versus PAWHEAE

```
In [9]: m = 11
        n = 8

        # Creating a table to run HEAGAWGHEE versus PAWHEAE
        h = [' ', 'H', 'E', 'A', 'G', 'A', 'W', 'G', 'H', 'E', 'E']
        header2 = [' ', 'P', 'A', 'W', 'H', 'E', 'A', 'E']
        df3 = pd.DataFrame(data=[np.zeros(3)]*m]*n)
        df3.rename(index=dict(zip(range(len(header2)),header2)),inplace=True)
        df3.rename(columns=dict(zip(range(len(h)),h)), inplace=True)

        # Filling the Global Allignment Table (array in row-column pair)
        #Forward Pass

        cost = -8 # Cost of insertion or delition

        # Calculating price of substitution when arrows moves diagonally
        def blos(r, c):
            cname = df3.columns[c]
            rname = df3.index[r]
            if r == 0 or c == 0:
                return np.nan # Handling nan error when filling first row/column
            else:
                return int(df[rname][cname]) + int(df3.iloc[r-1,c-1][0])

        arrow = []
        maxf = []

        # Loop to fill the table, deciding between if the upelement, leftelement or the diagelement
        for r in range(0,8):
            for c in range(0,11):
                zero = 0
                upelement = int(df3.iloc[r-1,c][0]) + cost if r >= 1 else np.nan # Handling nan
                leftelement = int(df3.iloc[r,c-1][0]) + cost if c >= 1 else np.nan # Handling nan
                diagelement = blos(r, c)
                if r == 0 and c == 0:
                    upelement = 0
                list1 = np.array([zero, diagelement, upelement, leftelement])
                re = np.nanargmax(list1)
```



```

# Storing the location of the selected max element to find arrow direction dur
if list1[re] == zero:    # Added condition of 0 with priority 1 between the opt
    vec = [0,0]
    vec2 = [r,c] # Added vec2 to find the index of the max element in the tab
    arrow.extend([0,0, r,c])
elif list1[re] == diagelement:
    vec = [r-1,c-1]
    vec2 = [r,c]
    arrow.extend([r-1,c-1, r,c])
elif list1[re] == upelement:
    vec = [r-1,c]
    vec2 = [r,c]
    arrow.extend([r-1,c, r,c])
elif list1[re] == leftelement:
    vec = [r,c-1]
    arrow.extend([r,c-1, r,c])
# Storing value, row and column coordinates in an array for each row-column pa
df3.iloc[r,c] = np.array([list1[re], vec[0], vec[1]])
maxf.append([list1[re],vec[0], vec[1], vec2[0], vec2[1]]) # Array for later fi
# table

```

df3

Out [9]:

	H	E	A \
	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
P	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]
A	[0.0, 0.0, 0.0]	[0, 0, 0]	[5, 1, 2]
W	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]
H	[0.0, 0.0, 0.0]	[10, 3, 0]	[2, 4, 1]
E	[0.0, 0.0, 0.0]	[2, 4, 1]	[16, 4, 1]
A	[0.0, 0.0, 0.0]	[0, 0, 0]	[8, 5, 2]
E	[0.0, 0.0, 0.0]	[0, 0, 0]	[6, 6, 1]

	G	A	W	G \
	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
P	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
A	[0, 0, 0]	[5, 1, 4]	[0, 0, 0]	[0, 0, 0]
W	[2, 2, 3]	[0, 0, 0]	[20, 2, 5]	[12, 3, 6]
H	[0, 0, 0]	[0, 0, 0]	[12, 3, 6]	[18, 3, 6]
E	[0, 0, 0]	[0, 0, 0]	[4, 4, 6]	[10, 4, 7]
A	[13, 6, 3]	[5, 5, 4]	[0, 0, 0]	[4, 5, 6]
E	[18, 6, 3]	[12, 6, 4]	[4, 7, 5]	[0, 0, 0]

	H	E	E
	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
P	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
A	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
W	[4, 3, 7]	[0, 0, 0]	[0, 0, 0]
H	[22, 3, 7]	[14, 4, 8]	[6, 4, 9]

E	[18, 4, 7]	[28, 4, 8]	[20, 4, 9]
A	[10, 5, 8]	[20, 5, 9]	[27, 5, 9]
E	[4, 6, 7]	[16, 6, 8]	[26, 6, 9]

```
In [10]: arrow2 = []
         letter1 = []
         letter2 = []

print("Maximum element in matrix, it's coordinates in the table, coordinates of where
is pointing from this position, index of max element in the array ="
      ,max([(v,i) for i,v in enumerate(maxf)]))

# Setting initial conditions, starting from the last element of the table
r =5
c =9
nextr = 4
nextc = 8
arrow2.append(df3.iloc[5,9][0])
# Same as:
# Backward pass
if((c==nextc) and (r==nextr)):
    letter2.append('-')
    letter1.append(df3.index[r])
elif((c!=nextc) and (r==nextr)):
    letter1.append('-')
    letter2.append(df3.columns[c])
elif((c!=nextc) and (r!=nextr)):
    letter1.append(df3.index[r])
    letter2.append(df3.columns[c])

# Looping through the table to find the backward pass elements and their corrisponding
for r in range(7, 1,-1):
    for c in range(10,-1,-1):
        if r == nextr and c == nextc: # Similar implementation as in Backward pass, t
                                         # direction has been stored in an array direcnt
                                         # in a separate list
            arrow2.append(df3.iloc[r,c][0])
            nextr = df3.iloc[r,c][1]
            nextc = df3.iloc[r,c][2]
            if c == 9 and r==5: # Handling starting condition
                letter.append(df3.columns[c])
                letter1.append(df3.index[r-1])
            if c != 9 and r!=5:
                if((c==nextc) and (r==nextr)):
                    letter2.append('-')
                    letter1.append(df3.index[r])
                elif((c!=nextc) and (r==nextr)):
                    letter1.append('-')
```

```

        letter2.append(df3.columns[c])
    else:
        letter1.append(df3.index[r])
        letter2.append(df3.columns[c])

arrow2.append(0)
arrow2 = np.asarray(arrow2)
print(letter2[::-1])
print(letter1[::-1])
print(arrow2)

```

Maximum element in matrix, it's coordinates in the table, coordinates of where the arrow is pointing

```

['A', 'W', 'G', 'H', 'E']
['A', 'W', '-', 'H', 'E']
[28 22 12 20  5  0]

```

Find the best local match between:

MQNSHSGVNQLGGVFVNGRPLPDSTRQKIVELAHSGARPCDISRILQVSNGCVSKILGRY
and TDDECHSGVNQLGGVFVGGRPLPDSTRQKIVELAHSGARPCDISRI

In [11]: # Creating a table to Match the protein sequence SALPQPTTPVSSFTSGSMLGRTDTALTNTYSAL with

```

m = 61
n = 47

# adding ' ' and , automatically to string
# import re
# st = 'T D D E C H S G V N Q L G G V F V G G R P L P D S T R Q K I V E L A H S G A R P C D I S R I L Q V S N G C V S K I L G R Y'
# print(re.findall(r"[\w']+", st))

# adding column and row headers
h = [' ', 'M', 'Q', 'N', 'S', 'H', 'S', 'G', 'V', 'N', 'Q', 'L', 'G', 'G', 'V', 'F', 'V', 'G', 'G', 'R', 'P', 'L', 'P', 'D', 'S', 'T', 'R', 'Q', 'K', 'I', 'V', 'E', 'L', 'A', 'H', 'S', 'G', 'A', 'R', 'P', 'C', 'D', 'I', 'S', 'R', 'I', 'L', 'Q', 'V', 'S', 'N', 'G', 'C', 'V', 'S', 'K', 'I', 'L', 'G', 'R', 'Y']
header2 = [' ', 'T', 'D', 'D', 'E', 'C', 'H', 'S', 'G', 'V', 'N', 'Q', 'L', 'G', 'G', 'V', 'F', 'V', 'G', 'G', 'R', 'P', 'L', 'P', 'D', 'S', 'T', 'R', 'Q', 'K', 'I', 'V', 'E', 'L', 'A', 'H', 'S', 'G', 'A', 'R', 'P', 'C', 'D', 'I', 'S', 'R', 'I', 'L', 'Q', 'V', 'S', 'N', 'G', 'C', 'V', 'S', 'K', 'I', 'L', 'G', 'R', 'Y']
df4 = pd.DataFrame(data=[np.zeros(1)]*m]*n)
df4.rename(index = dict(zip(range(len(header2)),header2)),inplace =True)
df4.rename(columns=dict(zip(range(len(h)),h)), inplace = True)

df4

```

```

Out[11]:
      M      Q      N      S      H      S      G      V      N  \
[0.0] [0.0] [0.0] [0.0] [0.0] [0.0] [0.0] [0.0] [0.0] [0.0]
T [0.0] [0.0] [0.0] [0.0] [0.0] [0.0] [0.0] [0.0] [0.0] [0.0]

```

[illegible]

[illegible]

```

In [12]: # Filling the Global Alignment Table (array in row-column pair)
         #Forward Pass

cost = -8 # Cost of insertion or delition

# Calculating price of substitution when arrows moves diagonally
def blos(r, c):
    cname = df4.columns[c]
    rname = df4.index[r]
    if r == 0 or c == 0:
        return np.nan # Handling nan error when filling first row/column
    else:
        return int(df[rname][cname]) + int(df4.iloc[r-1,c-1][0])

arrow = []
maxf = []

# Loop to fill the table, deciding between if the upelement, leftelement or the diagelement
for r in range(0,47):
    for c in range(0,61):
        zero = 0
        upelement = int(df4.iloc[r-1,c][0]) + cost if r >= 1 else np.nan # Handling nan error
        leftelement = int(df4.iloc[r,c-1][0]) + cost if c >= 1 else np.nan # Handling nan error
        diagelement = blos(r, c)
        if r == 0 and c == 0:
            upelement = 0
        list1 = np.array([zero, diagelement, upelement, leftelement])
        re = np.nanargmax(list1)
        # Storing the location of the selected max element to find arrow direction during backtracking
        if list1[re] == zero: # Added condition of 0 with priority 1 between the options
            vec = [0,0] # Added vec2 to find the index of the max element in the table
            vec2 = [r,c]
            arrow.extend([0,0, r,c])
        elif list1[re] == diagelement:
            vec = [r-1,c-1]
            vec2 = [r,c]
            arrow.extend([r-1,c-1, r,c])
        elif list1[re] == upelement:
            vec = [r-1,c]
            vec2 = [r,c]
            arrow.extend([r-1,c, r,c])
        elif list1[re] == leftelement:
            vec = [r,c-1]
            arrow.extend([r,c-1, r,c])
        # Storing value, row and column coordinates in an array for each row-column pair
        df4.iloc[r,c] = np.array([list1[re], vec[0], vec[1]])
        maxf.append([list1[re],vec[0], vec[1], vec2[0], vec2[1]]) # Array for later filling the
                                                                    # table

```

df4

Out[12]:

		M	Q	N \
	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
T	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
D	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[2, 1, 2]
D	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[2, 2, 2]
E	[0.0, 0.0, 0.0]	[0, 0, 0]	[2, 3, 1]	[0, 0, 0]
C	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
H	[0.0, 0.0, 0.0]	[0, 0, 0]	[1, 5, 1]	[1, 5, 2]
S	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[2, 6, 2]
G	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
V	[0.0, 0.0, 0.0]	[1, 8, 0]	[0, 0, 0]	[0, 0, 0]
N	[0.0, 0.0, 0.0]	[0, 0, 0]	[1, 9, 1]	[7, 9, 2]
Q	[0.0, 0.0, 0.0]	[0, 0, 0]	[7, 10, 1]	[1, 10, 2]
L	[0.0, 0.0, 0.0]	[3, 11, 0]	[0, 0, 0]	[3, 11, 2]
G	[0.0, 0.0, 0.0]	[0, 0, 0]	[1, 12, 1]	[0, 0, 0]
G	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[1, 13, 2]
V	[0.0, 0.0, 0.0]	[1, 14, 0]	[0, 0, 0]	[0, 0, 0]
F	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
V	[0.0, 0.0, 0.0]	[1, 16, 0]	[0, 0, 0]	[0, 0, 0]
G	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
G	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
R	[0.0, 0.0, 0.0]	[0, 0, 0]	[1, 19, 1]	[0, 0, 0]
P	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
L	[0.0, 0.0, 0.0]	[3, 21, 0]	[0, 0, 0]	[0, 0, 0]
P	[0.0, 0.0, 0.0]	[0, 0, 0]	[2, 22, 1]	[0, 0, 0]
D	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[4, 23, 2]
S	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[1, 24, 2]
T	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
R	[0.0, 0.0, 0.0]	[0, 0, 0]	[1, 26, 1]	[0, 0, 0]
Q	[0.0, 0.0, 0.0]	[0, 0, 0]	[7, 27, 1]	[1, 27, 2]
K	[0.0, 0.0, 0.0]	[0, 0, 0]	[2, 28, 1]	[7, 28, 2]
I	[0.0, 0.0, 0.0]	[2, 29, 0]	[0, 0, 0]	[0, 0, 0]
V	[0.0, 0.0, 0.0]	[1, 30, 0]	[0, 0, 0]	[0, 0, 0]
E	[0.0, 0.0, 0.0]	[0, 0, 0]	[3, 31, 1]	[0, 0, 0]
L	[0.0, 0.0, 0.0]	[3, 32, 0]	[0, 0, 0]	[0, 0, 0]
A	[0.0, 0.0, 0.0]	[0, 0, 0]	[2, 33, 1]	[0, 0, 0]
H	[0.0, 0.0, 0.0]	[0, 0, 0]	[1, 34, 1]	[3, 34, 2]
S	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[2, 35, 2]
G	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
A	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
R	[0.0, 0.0, 0.0]	[0, 0, 0]	[1, 38, 1]	[0, 0, 0]
P	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
C	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
D	[0.0, 0.0, 0.0]	[0, 0, 0]	[0, 0, 0]	[2, 41, 2]
I	[0.0, 0.0, 0.0]	[2, 42, 0]	[0, 0, 0]	[0, 0, 0]

S	[0.0, 0.0, 0.0]	[0, 0, 0]	[2, 43, 1]	[1, 43, 2]
R	[0.0, 0.0, 0.0]	[0, 0, 0]	[1, 44, 1]	[1, 44, 2]
I	[0.0, 0.0, 0.0]	[2, 45, 0]	[0, 0, 0]	[0, 0, 0]

	S	H	S	G \
	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
T	[2, 0, 3]	[0, 0, 0]	[2, 0, 5]	[0, 0, 0]
D	[0, 0, 0]	[1, 1, 4]	[0, 0, 0]	[1, 1, 6]
D	[2, 2, 3]	[0, 0, 0]	[1, 2, 5]	[0, 0, 0]
E	[1, 3, 3]	[2, 3, 4]	[0, 0, 0]	[0, 0, 0]
C	[0, 0, 0]	[0, 0, 0]	[1, 4, 5]	[0, 0, 0]
H	[0, 0, 0]	[10, 5, 4]	[2, 6, 5]	[0, 0, 0]
S	[6, 6, 3]	[2, 6, 5]	[15, 6, 5]	[7, 7, 6]
G	[2, 7, 3]	[4, 7, 4]	[7, 7, 6]	[23, 7, 6]
V	[0, 0, 0]	[0, 0, 0]	[2, 8, 5]	[15, 8, 7]
N	[1, 9, 3]	[1, 9, 4]	[1, 9, 5]	[7, 9, 7]
Q	[7, 10, 3]	[2, 10, 4]	[1, 10, 5]	[0, 0, 0]
L	[0, 0, 0]	[4, 11, 4]	[0, 0, 0]	[0, 0, 0]
G	[3, 12, 3]	[0, 0, 0]	[4, 12, 5]	[8, 12, 6]
G	[0, 0, 0]	[1, 13, 4]	[0, 0, 0]	[12, 13, 6]
V	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[4, 14, 7]
F	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
V	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
G	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[8, 17, 6]
G	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[8, 18, 6]
R	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
P	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
L	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
P	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
D	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
S	[9, 24, 3]	[1, 25, 4]	[5, 24, 5]	[0, 0, 0]
T	[3, 25, 3]	[7, 25, 4]	[3, 25, 5]	[3, 25, 6]
R	[0, 0, 0]	[3, 26, 4]	[6, 26, 5]	[0, 0, 0]
Q	[0, 0, 0]	[1, 27, 4]	[3, 27, 5]	[4, 27, 6]
K	[1, 28, 3]	[0, 0, 0]	[1, 28, 5]	[1, 28, 6]
I	[4, 29, 3]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
V	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
E	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
L	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
A	[1, 33, 3]	[0, 0, 0]	[1, 33, 5]	[0, 0, 0]
H	[0, 0, 0]	[11, 34, 4]	[3, 35, 5]	[0, 0, 0]
S	[8, 35, 3]	[3, 35, 5]	[16, 35, 5]	[8, 36, 6]
G	[2, 36, 3]	[6, 36, 4]	[8, 36, 6]	[24, 36, 6]
A	[1, 37, 3]	[0, 0, 0]	[7, 37, 5]	[16, 37, 7]
R	[0, 0, 0]	[1, 38, 4]	[0, 0, 0]	[8, 38, 7]
P	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
C	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
D	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]

I	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
S	[5, 43, 3]	[0, 0, 0]	[5, 43, 5]	[0, 0, 0]
R	[0, 0, 0]	[5, 44, 4]	[0, 0, 0]	[2, 44, 6]
I	[0, 0, 0]	[0, 0, 0]	[2, 45, 5]	[0, 0, 0]

	V	N	...	G \
	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	...	[0.0, 0.0, 0.0]
T	[0, 0, 0]	[0, 0, 0]	...	[0, 0, 0]
D	[0, 0, 0]	[2, 1, 8]	...	[0, 0, 0]
D	[0, 0, 0]	[2, 2, 8]	...	[3, 2, 50]
E	[0, 0, 0]	[0, 0, 0]	...	[0, 0, 0]
C	[0, 0, 0]	[0, 0, 0]	...	[0, 0, 0]
H	[0, 0, 0]	[1, 5, 8]	...	[0, 0, 0]
S	[0, 0, 0]	[1, 6, 8]	...	[1, 6, 50]
G	[15, 8, 7]	[7, 8, 8]	...	[9, 7, 50]
V	[28, 8, 7]	[20, 9, 8]	...	[1, 8, 50]
N	[20, 9, 8]	[35, 9, 8]	...	[0, 0, 0]
Q	[12, 10, 8]	[27, 10, 9]	...	[5, 10, 50]
L	[4, 11, 8]	[19, 11, 9]	...	[2, 11, 50]
G	[0, 0, 0]	[11, 12, 9]	...	[8, 12, 50]
G	[4, 13, 7]	[3, 13, 9]	...	[14, 13, 50]
V	[17, 14, 7]	[9, 15, 8]	...	[10, 14, 50]
F	[9, 15, 8]	[13, 15, 8]	...	[2, 15, 50]
V	[5, 16, 7]	[6, 16, 8]	...	[0, 0, 0]
G	[0, 0, 0]	[5, 17, 8]	...	[9, 17, 50]
G	[4, 18, 7]	[0, 0, 0]	...	[8, 18, 50]
R	[5, 19, 7]	[3, 19, 8]	...	[4, 19, 50]
P	[0, 0, 0]	[3, 20, 8]	...	[0, 0, 0]
L	[1, 21, 7]	[0, 0, 0]	...	[0, 0, 0]
P	[0, 0, 0]	[0, 0, 0]	...	[0, 0, 0]
D	[0, 0, 0]	[2, 23, 8]	...	[0, 0, 0]
S	[0, 0, 0]	[1, 24, 8]	...	[2, 24, 50]
T	[0, 0, 0]	[0, 0, 0]	...	[1, 26, 50]
R	[0, 0, 0]	[0, 0, 0]	...	[6, 26, 50]
Q	[0, 0, 0]	[0, 0, 0]	...	[0, 0, 0]
K	[1, 28, 7]	[0, 0, 0]	...	[0, 0, 0]
I	[5, 29, 7]	[0, 0, 0]	...	[1, 30, 50]
V	[5, 30, 7]	[2, 30, 8]	...	[7, 31, 50]
E	[0, 0, 0]	[5, 31, 8]	...	[15, 32, 50]
L	[1, 32, 7]	[0, 0, 0]	...	[28, 33, 50]
A	[0, 0, 0]	[0, 0, 0]	...	[41, 34, 50]
H	[0, 0, 0]	[1, 34, 8]	...	[59, 35, 50]
S	[0, 0, 0]	[1, 35, 8]	...	[72, 36, 50]
G	[16, 37, 7]	[8, 37, 8]	...	[88, 36, 50]
A	[24, 37, 7]	[16, 38, 8]	...	[101, 38, 50]
R	[16, 38, 8]	[23, 38, 8]	...	[116, 39, 50]
P	[8, 39, 8]	[15, 39, 9]	...	[134, 40, 50]
C	[0, 0, 0]	[7, 40, 9]	...	[155, 41, 50]

D	[0, 0, 0]	[2, 41, 8]	...	[171, 42, 50]
I	[4, 42, 7]	[0, 0, 0]	...	[184, 43, 50]
S	[0, 0, 0]	[5, 43, 8]	...	[197, 44, 50]
R	[0, 0, 0]	[0, 0, 0]	...	[212, 45, 50]
I	[6, 45, 7]	[0, 0, 0]	...	[225, 46, 50]

	C	V	S	K \
	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
T	[0, 0, 0]	[0, 0, 0]	[2, 0, 53]	[0, 0, 0]
D	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[1, 1, 54]
D	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
E	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[1, 3, 54]
C	[13, 4, 51]	[5, 5, 52]	[0, 0, 0]	[0, 0, 0]
H	[5, 5, 52]	[9, 5, 52]	[4, 5, 53]	[0, 0, 0]
S	[0, 0, 0]	[3, 6, 52]	[14, 6, 53]	[6, 7, 54]
G	[1, 8, 51]	[0, 0, 0]	[6, 7, 54]	[12, 7, 54]
V	[8, 8, 51]	[6, 8, 52]	[0, 0, 0]	[4, 8, 55]
N	[0, 0, 0]	[5, 9, 52]	[7, 9, 53]	[0, 0, 0]
Q	[0, 0, 0]	[0, 0, 0]	[5, 10, 53]	[9, 10, 54]
L	[3, 11, 51]	[1, 11, 52]	[0, 0, 0]	[2, 11, 54]
G	[0, 0, 0]	[0, 0, 0]	[1, 12, 53]	[0, 0, 0]
G	[6, 14, 51]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
V	[13, 14, 51]	[11, 14, 52]	[3, 15, 53]	[0, 0, 0]
F	[8, 15, 51]	[12, 15, 52]	[8, 15, 53]	[0, 0, 0]
V	[1, 16, 51]	[13, 16, 52]	[10, 16, 53]	[5, 16, 54]
G	[1, 18, 51]	[5, 17, 53]	[13, 17, 53]	[8, 17, 54]
G	[6, 18, 51]	[0, 0, 0]	[5, 18, 53]	[11, 18, 54]
R	[4, 19, 51]	[3, 19, 52]	[0, 0, 0]	[8, 19, 54]
P	[0, 0, 0]	[1, 20, 52]	[2, 20, 53]	[0, 0, 0]
L	[0, 0, 0]	[1, 21, 52]	[0, 0, 0]	[0, 0, 0]
P	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
D	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
S	[0, 0, 0]	[0, 0, 0]	[5, 24, 53]	[0, 0, 0]
T	[1, 25, 51]	[0, 0, 0]	[2, 25, 53]	[4, 25, 54]
R	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[5, 26, 54]
Q	[3, 27, 51]	[0, 0, 0]	[0, 0, 0]	[2, 27, 54]
K	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[6, 28, 54]
I	[0, 0, 0]	[4, 29, 52]	[0, 0, 0]	[0, 0, 0]
V	[0, 0, 0]	[5, 30, 52]	[2, 30, 53]	[0, 0, 0]
E	[7, 32, 51]	[0, 0, 0]	[4, 31, 53]	[3, 31, 54]
L	[20, 33, 51]	[12, 33, 52]	[4, 33, 53]	[1, 32, 54]
A	[33, 34, 51]	[25, 34, 52]	[17, 34, 53]	[9, 34, 54]
H	[51, 35, 51]	[43, 35, 52]	[35, 35, 53]	[27, 35, 54]
S	[64, 36, 51]	[56, 36, 52]	[48, 35, 53]	[40, 36, 54]
G	[80, 37, 51]	[72, 37, 52]	[64, 37, 53]	[56, 37, 54]
A	[93, 38, 51]	[85, 38, 52]	[77, 38, 53]	[69, 38, 54]
R	[108, 39, 51]	[100, 39, 52]	[92, 39, 53]	[84, 39, 54]
P	[126, 40, 51]	[118, 40, 52]	[110, 40, 53]	[102, 40, 54]

C	[147, 40, 51]	[139, 41, 52]	[131, 41, 53]	[123, 41, 54]
D	[163, 42, 51]	[155, 42, 52]	[147, 42, 53]	[139, 42, 54]
I	[176, 43, 51]	[168, 43, 52]	[160, 43, 53]	[152, 43, 54]
S	[189, 44, 51]	[181, 44, 52]	[173, 43, 53]	[165, 44, 54]
R	[204, 45, 51]	[196, 45, 52]	[188, 45, 53]	[180, 45, 54]
I	[217, 46, 51]	[209, 46, 52]	[201, 46, 53]	[193, 46, 54]

	I	L	G	R \
	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]	[0.0, 0.0, 0.0]
T	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
D	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
D	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
E	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
C	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
H	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
S	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
G	[4, 8, 55]	[0, 0, 0]	[8, 7, 57]	[0, 0, 0]
V	[16, 8, 55]	[8, 9, 56]	[0, 0, 0]	[5, 8, 58]
N	[8, 9, 56]	[12, 9, 56]	[8, 9, 57]	[0, 0, 0]
Q	[1, 11, 55]	[6, 10, 56]	[10, 10, 57]	[9, 10, 58]
L	[11, 11, 55]	[6, 11, 56]	[2, 11, 57]	[7, 11, 58]
G	[3, 12, 56]	[7, 12, 56]	[14, 12, 57]	[6, 13, 58]
G	[0, 0, 0]	[0, 0, 0]	[15, 13, 57]	[11, 13, 58]
V	[4, 14, 55]	[1, 14, 56]	[7, 14, 58]	[12, 14, 58]
F	[0, 0, 0]	[5, 15, 56]	[0, 0, 0]	[4, 15, 58]
V	[4, 16, 55]	[1, 16, 56]	[1, 16, 57]	[0, 0, 0]
G	[1, 17, 55]	[0, 0, 0]	[9, 17, 57]	[1, 18, 58]
G	[4, 18, 55]	[0, 0, 0]	[8, 18, 57]	[6, 18, 58]
R	[7, 19, 55]	[1, 19, 56]	[0, 0, 0]	[15, 19, 58]
P	[5, 20, 55]	[3, 20, 56]	[0, 0, 0]	[7, 20, 59]
L	[2, 21, 55]	[10, 21, 56]	[2, 22, 57]	[0, 0, 0]
P	[0, 0, 0]	[2, 22, 57]	[8, 22, 57]	[0, 0, 0]
D	[0, 0, 0]	[0, 0, 0]	[1, 23, 57]	[6, 23, 58]
S	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
T	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]
R	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[7, 26, 58]
Q	[2, 27, 55]	[0, 0, 0]	[0, 0, 0]	[1, 27, 58]
K	[0, 0, 0]	[0, 0, 0]	[0, 0, 0]	[3, 28, 58]
I	[11, 29, 55]	[3, 30, 56]	[0, 0, 0]	[0, 0, 0]
V	[4, 30, 55]	[12, 30, 56]	[4, 31, 57]	[0, 0, 0]
E	[0, 0, 0]	[4, 31, 57]	[9, 31, 57]	[4, 31, 58]
L	[5, 32, 55]	[5, 32, 56]	[1, 32, 58]	[6, 32, 58]
A	[1, 34, 55]	[3, 33, 56]	[5, 33, 57]	[0, 0, 0]
H	[19, 35, 55]	[11, 35, 56]	[3, 35, 57]	[5, 34, 58]
S	[32, 36, 55]	[24, 36, 56]	[16, 36, 57]	[8, 36, 58]
G	[48, 37, 55]	[40, 37, 56]	[32, 36, 57]	[24, 37, 58]
A	[61, 38, 55]	[53, 38, 56]	[45, 38, 57]	[37, 38, 58]
R	[76, 39, 55]	[68, 39, 56]	[60, 39, 57]	[52, 38, 58]

P	[94, 40, 55]	[86, 40, 56]	[78, 40, 57]	[70, 40, 58]
C	[115, 41, 55]	[107, 41, 56]	[99, 41, 57]	[91, 41, 58]
D	[131, 42, 55]	[123, 42, 56]	[115, 42, 57]	[107, 42, 58]
I	[144, 42, 55]	[136, 43, 56]	[128, 43, 57]	[120, 43, 58]
S	[157, 44, 55]	[149, 44, 56]	[141, 44, 57]	[133, 44, 58]
R	[172, 45, 55]	[164, 45, 56]	[156, 45, 57]	[148, 44, 58]
I	[185, 45, 55]	[177, 46, 56]	[169, 46, 57]	[161, 46, 58]

	Y
	[0.0, 0.0, 0.0]
T	[0, 0, 0]
D	[0, 0, 0]
D	[0, 0, 0]
E	[0, 0, 0]
C	[0, 0, 0]
H	[2, 5, 59]
S	[0, 0, 0]
G	[0, 0, 0]
V	[0, 0, 0]
N	[3, 9, 59]
Q	[1, 11, 59]
L	[8, 11, 59]
G	[4, 12, 59]
G	[3, 13, 59]
V	[10, 14, 59]
F	[16, 15, 59]
V	[8, 16, 60]
G	[0, 0, 0]
G	[0, 0, 0]
R	[7, 20, 59]
P	[12, 20, 59]
L	[6, 21, 59]
P	[0, 0, 0]
D	[0, 0, 0]
S	[4, 24, 59]
T	[0, 0, 0]
R	[0, 0, 0]
Q	[6, 27, 59]
K	[0, 0, 0]
I	[2, 29, 59]
V	[0, 0, 0]
E	[0, 0, 0]
L	[3, 32, 59]
A	[4, 33, 59]
H	[2, 34, 59]
S	[3, 35, 59]
G	[16, 37, 59]
A	[29, 38, 59]

```

R      [44, 39, 59]
P      [62, 40, 59]
C      [83, 41, 59]
D      [99, 42, 59]
I      [112, 43, 59]
S      [125, 44, 59]
R      [140, 45, 59]
I      [153, 46, 59]

```

```
[47 rows x 61 columns]
```

```

In [13]: arrow2 = []
         letter1 = []
         letter2 = []

```

```

print("Maximum element in matrix, it's coordinates in the table, coordinates of where
is pointing from this position, index of max element in the array ="
      ,max([(v,i) for i,v in enumerate(maxf)]))

```

```
# Setting initial conditions, starting from the last element of the table
```

```
r =46
```

```
c =45
```

```
nextc = 45
```

```
nextc = 44
```

```
#arrow2.append(df4.iloc[r,c][0])
```

```
# Same as:
```

```
# Backward pass
```

```
if((c==nextc) and (r==nextc)):
```

```
    letter2.append('-')
```

```
    letter1.append(df4.index[r])
```

```
elif((c!=nextc) and (r==nextc)):
```

```
    letter1.append('-')
```

```
    letter2.append(df4.columns[c])
```

```
elif((c!=nextc) and (r!=nextc)):
```

```
    letter1.append(df4.index[r])
```

```
    letter2.append(df4.columns[c])
```

```
# Looping through the table to find the backward pass elements and their corresponding
```

```
for r in range(46, 0,-1):
```

```
    for c in range(60,4,-1): # Skipping the first 4 elements because we already analyzed
```

```
        if r == nextc and c == nextc: # Similar implementation as in Backward pass, the
            # direction has been stored in an array directly
            # in a separate list
```

```
            arrow2.append(df4.iloc[r,c][0])
```

```
            nextc = df4.iloc[r,c][1]
```

```
            nextc = df4.iloc[r,c][2]
```

```
            if c == 45 and r==46: # Handling starting condition
```

```
                letter.append(df4.columns[c])
```

```

        letter1.append(df4.index[r-1])
    if c != 45 and r!=46:
        if((c==nextc) and (r==nextr))or (nextr==-1 and nextc==0):
            letter2.append('-')
            letter1.append(df4.index[r])
        elif((c!=nextc) and (r==nextr)):
            letter1.append('-')
            letter2.append(df4.columns[c])
        else:
            letter1.append(df4.index[r])
            letter2.append(df4.columns[c])

    arrow2.append(0)
    arrow2 = np.asarray(arrow2)
    print(letter2[::-1])
    print(letter1[::-1])
    print(arrow2)
    # HSGVNLGGVVFVNGRPLPDSTRQKIVELAHSGARPCDISRI
    # HSGVNLGGVVFVNGRPLPDSTRQKIVELAHSGARPCDISRI

```

Maximum element in matrix, it's coordinates in the table, coordinates of where the arrow is pointing

['H', 'S', 'G', 'V', 'N', 'Q', 'L', 'G', 'G', 'V', 'F', 'V', 'N', 'G', 'R', 'P', 'L', 'P', 'D']
['H', 'S', 'G', 'V', 'N', 'Q', 'L', 'G', 'G', 'V', 'F', 'V', 'G', 'G', 'R', 'P', 'L', 'P', 'D']
[268 261 256 251 243 230 220 213 208 200 195 185 180 175 169 164 159 153
146 139 134 129 121 111 106 96 89 81 81 76 68 63 55 47 42 35
28 23 15 10 0]

1.1.3 3) BLAST algorithm test

In [11]: *#Pax6 protein for the mouse*

```

# MQNSHSGVNLGGVVFVNGRPLPDSTRQKIVELAHSGARPCDISRILQVSNGCVSKILGRY
# YETGSIRPRAIGGSKPRVATPEVVSKIAQYKRECPSIFAWIIRDRLLEGGVCTNDNIPSV
# SSINRVLRNLASEKQMGADGMYDKLRMLNGQTGSWGTRPGWYPGTSVPGQPTQDGCQQQ
# EGGGENTNSISSNGEDSDEAQMRLQLKRKLQRNRTSFTQEIEALEKEFERTHYPDFAR
# ERLAAKIDLPEARIQVWFSNRRAKWRREEKLRNQRQASNTPSHIPISSEFSTSVYQPI
# QPTTPVSSFTSGSMLGRDALTNTYSALPPMPSFTMANNLPMQPPVPSQTSSYSCLPT
# SPSVNGRSYDTPPHMQTHMNSQPMGTSGTTSTGLISPGVSVPVQVPGSEPDMQYWPR
# LQ

```

eyeless protein for the fruit fly

```

# NVIAMRNLPLGTAGGSGGGIAGKPSPTMEAVEASTASHPHSTSSYFATYYHLTDDEC
# HSGVNLGGVVFVNGRPLPDSTRQKIVELAHSGARPCDISRI

```

Comparison result: <https://blast.ncbi.nlm.nih.gov/Blast.cgi>

```
df5=pd.read_csv('6P13GW4F114-Alignment-HitTable.csv')
df5.head()
```

```
Out[11]:
```

	Query_124327	Query_124329	97.561	41	1	0	5	45	61	101	1.72e-26	\
0	Query_124327	Query_124329	26.667	30	22	0	300	329	26	55	2.1	
1	Query_124327	Query_124329	40.000	20	11	1	279	297	35	54	2.7	
2	Query_124327	Query_124329	31.250	16	11	0	361	376	27	42	5.2	

	88.2	97.56
0	13.9	36.67
1	13.5	65.00
2	12.7	50.00

```
In [12]: f = open('6P13GW4F114-Alignment.txt', 'r')
file_contents = f.read()
print (file_contents)
f.close()
```

BLASTP 2.8.1+

Reference: Stephen F. Altschul, Thomas L. Madden, Alejandro A. Schaffer, Jinghui Zhang, Zheng Zhang, Webb Miller, and David J. Lipman (1997), "Gapped BLAST and PSI-BLAST: a new generation of protein database search programs", Nucleic Acids Res. 25:3389-3402.

Reference for compositional score matrix adjustment: Stephen F. Altschul, John C. Wootton, E. Michael Gertz, Richa Agarwala, Aleksandr Morgulis, Alejandro A. Schaffer, and Yi-Kuo Yu (2005) "Protein database searches using compositionally adjusted substitution matrices", FEBS J. 272:5101-5109.

RID: 6P13GW4F114

Query=
Length=422

Sequences producing significant alignments:	Score (Bits)	E Value	Max ident
Query_124329 unnamed protein product	88.2	2e-26	98%

ALIGNMENTS

>Query_124329 unnamed protein product

Length=101

Score = 88.2 bits (217), Expect = 2e-26, Method: Compositional matrix adjust.
Identities = 40/41 (98%), Positives = 40/41 (98%), Gaps = 0/41 (0%)

```
Query   5   HSGVNLGGVVFVNGRPLPDSTRQKIVELAHSGARPCDISRI   45
          HSGVNLGGVVFV GRPLPDSTRQKIVELAHSGARPCDISRI
Sbjct  61   HSGVNLGGVVFVGRPLPDSTRQKIVELAHSGARPCDISRI  101
```

Score = 13.9 bits (24), Expect = 2.1, Method: Compositional matrix adjust.
Identities = 8/30 (27%), Positives = 11/30 (37%), Gaps = 0/30 (0%)

```
Query  300 PQPTTPVSSFTSGSMLGRTDTALTNTYSAL  329
          P PT      ++ S      T +      TY L
Sbjct  26   PSPTMEAVEASTASHPHSTSSYFATTYYHL  55
```

Score = 13.5 bits (23), Expect = 2.7, Method: Compositional matrix adjust.
Identities = 8/20 (40%), Positives = 13/20 (65%), Gaps = 1/20 (5%)

```
Query  279 SNTPSHIPISSS-FSTSVYQ  297
          ++T SH   +SS F+T+ Y
Sbjct  35   ASTASHPHSTSSYFATTYYH  54
```

Score = 12.7 bits (21), Expect = 5.2, Method: Compositional matrix adjust.
Identities = 5/16 (31%), Positives = 8/16 (50%), Gaps = 0/16 (0%)

```
Query  361 SPSVNGRSYDTYTPPH  376
          SP++      T + PH
Sbjct  27   SPTMEAVEASTASHPH  42
```

1.1.4 4) HMM for detecting CG regions

```
In [167]: import random
```

```
def roll(sides, bias_list):
    assert len(bias_list) == sides
    number = random.uniform(0, sum(bias_list))
    current = 0
    for i, bias in enumerate(bias_list):
```



```

        current += bias
        if number <= current:
            return i + 1

prob1 = [0.2698, 0.3237, 0.2080, 0.1985]
stayleave1 = [0.9998, 0.0002]
# stayleave1 = [0.7, 0.3]
prob2 = [0.2459, 0.2079, 0.2478, 0.2984]
stayleave2 = [0.9997, 0.0003]
# stayleave2 = [0.4, 6]

initialstate = [0.5,0.5]

selectstate = roll(2, initialstate)
if selectstate == 1:
    print('Starting in state 1 \n')
    state1=1
    state2=0
else:
    print("Starting in state 2 \n")
    state1=0
    state2=1

numlist = []
letlist = []

for i in range(0,500):
    if state1==1:
        numlist.append(roll(4, prob1))
        letlist.append('AT')
        switchstate = roll(2, stayleave1)
        if switchstate == 1:
            state1=1
            state2=0
        else:
            print("Switching to state 2 \n")
            state1=0
            state2=1
    if state2==1:
        numlist.append(roll(4, prob2))
        letlist.append('CG')
        switchstate = roll(2, stayleave2)
        if switchstate == 1:
            state1=0
            state2=1
        else:
            print("Switching to state 1 \n")
            state1=1

```

```
state2=0
# print(len(probl))

letlist = ''.join(letlist)
numlist = int(''.join(str(i) for i in numlist))

print(letlist)
print(numlist)
```

Starting in state 2

Switching to state 1

Switching to state 2

[illegible]