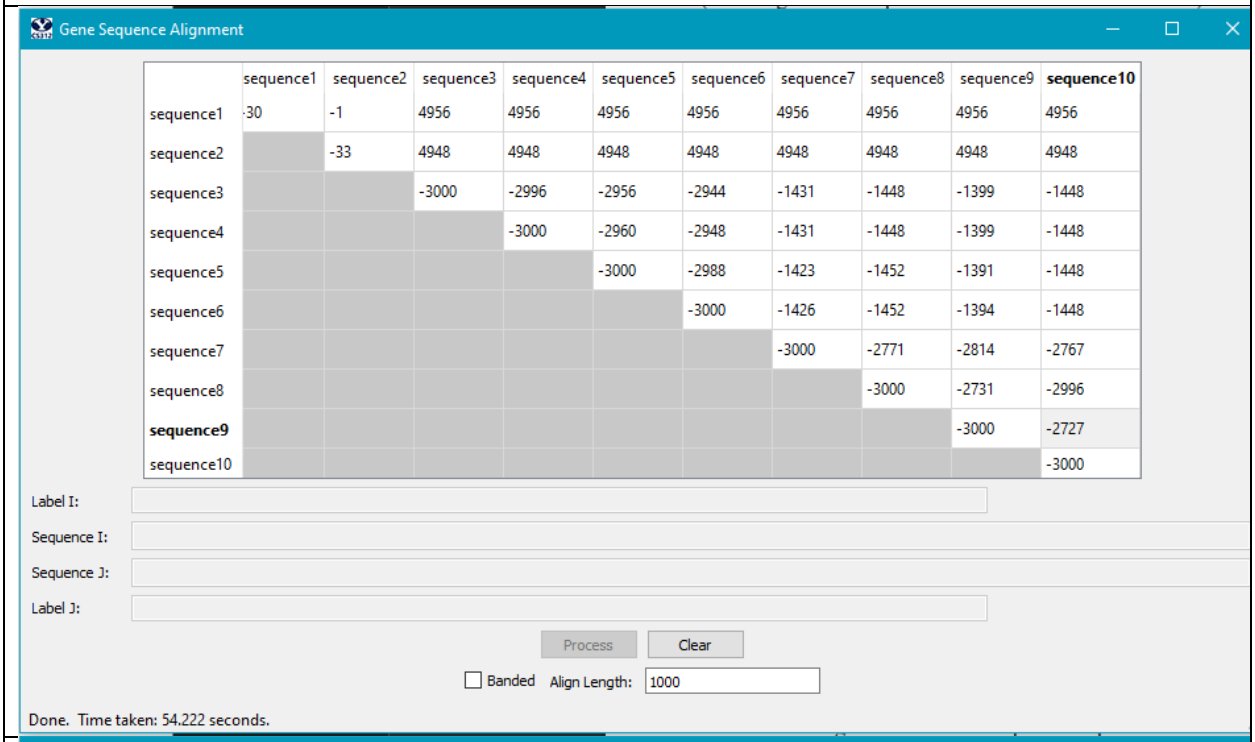
Trevor Ashby

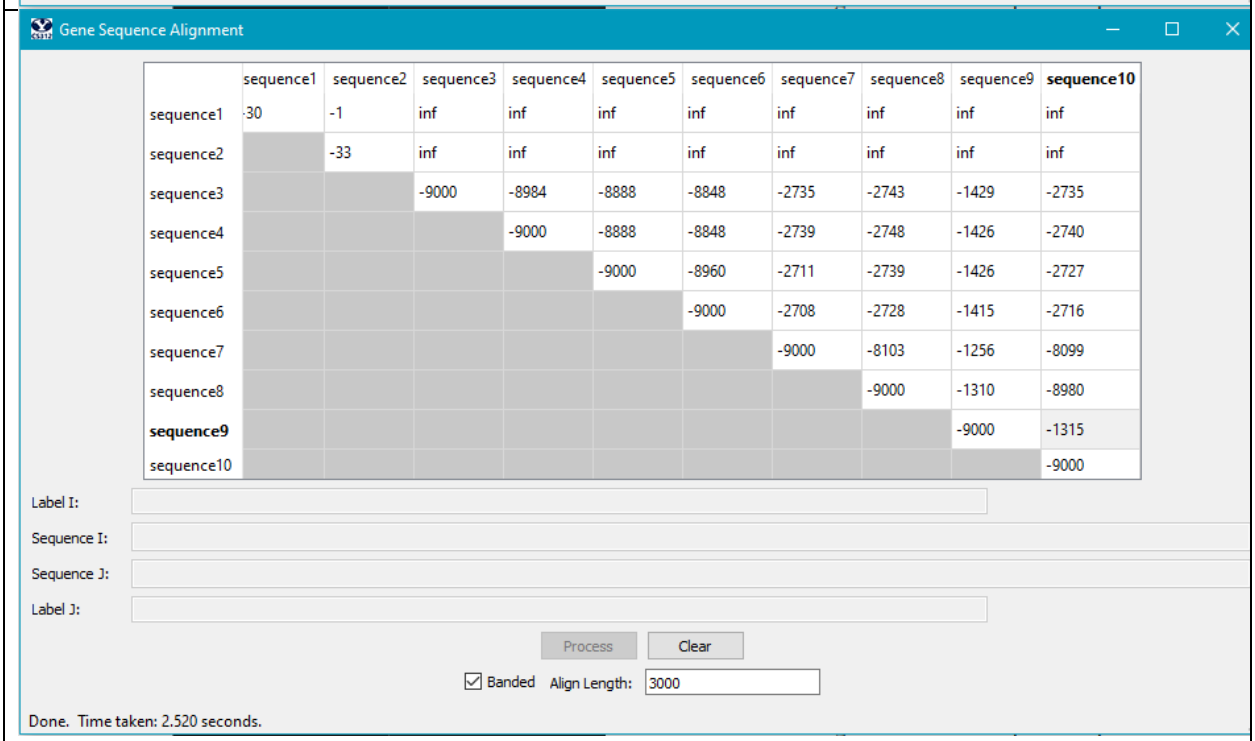
Gene Sequencing

1. Time and Space Complexity	
Unrestricted	Banded
<u>Space & Time O(n*m)</u> initialize array **->O(n*m)** for I in len(seq1) **->O(n)** set axis for I in len(seq2) **->O(m)** set axis for I in len(seq1) **-> (O(n*m))** for j in len(seq2) set array[j][i] = min(left cell, top cell, diag cell) go through back pointers **->O(n)** build alignment string based on pointers reverse alignments **-> O(n) O(m)**	<u>Space & Time: O(n*k)</u> Initialize array w/ shortest seq **->O(n*k)** For I in len(k) **->O(k)** Set axis For I in len(n) **->O(n)** Set axis For I in len(n) **->O(n*k)** For j in len(k) If I or j out of range, set to inf Set array[n][k] = min(left cell, top cell, diag cell) Go through back pointers **->O(n)** Build alignment string based on pointers Reverse alignments **-> O(n) O(m)**

2. Alignment Extraction
To extract the alignment, I inserted tuples into my matrix that had the edit distance value, as well as a character that determined what kind of transition the value was taken from. For example, ‘s’ represented that the characters in the strings were the same and that the value that was paired with it was obtained by subtracting 3 from the diagonal (Non-banded) or above (banded) value. Later, I back tracked from the optimal value, following the trail of character pointers that were left, and depending on the character, I would append either a character from the strings, or a ‘-‘ depending on the value of the pointer.

3. Results


Gene Sequence Alignment
sequence1 sequence2 sequence3 sequence4 sequence5 sequence6 sequence7 sequence8 sequence9 sequence10
sequence1 -30 -1 4956 4956 4956 4956 4956 4956 4956 4956
sequence2 -33 4948 4948 4948 4948 4948 4948 4948 4948
sequence3 -3000 -2996 -2956 -2944 -1431 -1448 -1399 -1448
sequence4 -3000 -2960 -2948 -1431 -1448 -1399 -1448
sequence5 -3000 -2988 -1423 -1452 -1391 -1448
sequence6 -3000 -1426 -1452 -1394 -1448
sequence7 -3000 -2771 -2814 -2767
sequence8 -3000 -2731 -2996
sequence9 -3000 -2727
sequence10 -3000
Label I:
Sequence I:
Sequence J:
Label J:
Process
Clear
Banded
Align Length: 1000
Done. Time taken: 54.222 seconds.


Gene Sequence Alignment
sequence1 sequence2 sequence3 sequence4 sequence5 sequence6 sequence7 sequence8 sequence9 sequence10
sequence1 -30 -1 inf inf inf inf inf inf inf inf
sequence2 -33 inf inf inf inf inf inf inf inf
sequence3 -9000 -8984 -8888 -8848 -2735 -2743 -1429 -2735
sequence4 -9000 -8888 -8848 -2739 -2748 -1426 -2740
sequence5 -9000 -8960 -2711 -2739 -1426 -2727
sequence6 -9000 -2708 -2728 -1415 -2716
sequence7 -9000 -8103 -1256 -8099
sequence8 -9000 -1310 -8980
sequence9 -9000 -1315
sequence10 -9000
Label I:
Sequence I:
Sequence J:
Label J:
Process
Clear
Banded
Align Length: 3000
Done. Time taken: 2.520 seconds.

4. Results 2: Extracted Alignments

Un-Banded

Sequence 3:	attgcgagcgatttgcgtgcgtgcatcccgcttc-actg--at-ctcttgttagatcttttcataatctaaacttttataaaaacatccactccctgta-g
Sequence 10:	ataa-gagtgattggcgtccgtacgtacccttttctactctcaaactcttgttagtttaaatc-taatctaaacttttataaa--cggc-acttcctgtgtg

Banded

Sequence 3:	attgcgagcgatttgcgtgcgtgcatcccgcttc-actg--at-ctcttgttagatcttttcataatctaaacttttataaaaacatccactccctgta-g
Sequence 10:	ataa-gagtgattggcgtccgtacgtacccttttctactctcaaactcttgttagtttaaatc-taatctaaacttttataaa--cggc-acttcctgtgtg

5. Code

```
#!/usr/bin/python3

from which_pyqt import PYQT_VER
if PYQT_VER == 'PYQT5':
   from PyQt5.QtCore import QLineF, QPointF
elif PYQT_VER == 'PYQT4':
   from PyQt4.QtCore import QLineF, QPointF
else:
   raise Exception('Unsupported Version of PyQt: {}'.format(PYQT_VER))

import math
import time
import random

# Used to compute the bandwidth for banded version
MAXINDELS = 3

# Used to implement Needleman-Wunsch scoring
MATCH = -3
INDEL = 5
SUB = 1

class GeneSequencing:

   def __init__( self ):
      pass
# This is the method called by the GUI.  _seq1_ and _seq2_ are two sequences to be aligned, _banded_ is a boolean that tells
# you whether you should compute a banded alignment or full alignment, and _align_length_ tells you
# how many base pairs to use in computing the alignment

   def align( self, seq1, seq2, banded, align_length):
      t0 = time.clock()
      self.banded = banded
      self.MaxCharactersToAlign = align_length

      # First, determine if the full length of the string can be used, or if it has to be
      # shortened based on the align_length parameter
      if len(seq1) > align_length:
         seq1 = seq1[:align_length]
      if len(seq2) > align_length:
         seq2 = seq2[:align_length]

      cnt = 0
      # if a banded check is to be ran
      ##########################
      # Time Complexity: O(k*n)
      # Space Complexity: O(k*n)
      ##########################
      if (self.banded):
         bandwidth = 7
         distance = 3
         width = 0
         seq1Used = True

         # if the strings that are being compared are too different in length, return not possible
         if (abs(len(seq1) - len(seq2)) > bandwidth):
            return {'align_cost': float('inf'), 'seqi_first100': "No Alignment Possible", 'seqj_first100': "No Alignment
Possible"}
         myArray = []

         # initialize array based on shortest sequence
         if len(seq1) < len(seq2):
            myArray = [[(-1, 'n') for x in range(bandwidth)] for y in range(len(seq1)+1)]
            width = len(seq1)+1
            seq1Used = True
         elif len(seq2) < len(seq1):
            myArray = [[(-1, 'n') for x in range(bandwidth)] for y in range(len(seq2)+1)]
            width = len(seq2)+1
            seq1Used = False
         else:
            myArray = [[(-1, 'n') for x in range(bandwidth)] for y in range(len(seq1)+1)]
            width = len(seq1)+1
            seq1Used = True
```

```
        #initialize top row of array with axis values
        temp = 0
        for col in range(bandwidth):
           if col < 3:
              myArray[0][col] = (float('inf'), 'x')
           else:
              myArray[0][col] = (temp, 'b')
              temp += 5

        # initialize diagonal of array with axis values
        temp = 15
        row = 3
        for col in range(distance):
           myArray[row][col] = (temp, 'b')
           temp -= 5
           row -= 1

        # initialize 1,1
        myArray[1][1] = (float('inf'), 'x')

        # initialize 1,0
        myArray[1][0] = (float('inf'), 'x')

        # initialize 2,0
        myArray[2][0] = (float('inf'), 'x')

        distance = 3
        end = bandwidth
        begin = distance

        # run through each value in the matrix starting at 0,0
        for row in range(0, width):
           for col in range(0, bandwidth):

              # if the row and col fits within the region available to edit, change the value
              if (row + col - 3 - (abs(len(seq1) - len(seq2)))) >= width:
                 myArray[row][col] = (float('inf'), 'x')

              # if the value at the desired location is infinity or set to 'b' for base, do not edit matrix cell
              elif myArray[row][col][0] == float('inf') or myArray[row][col][1] == 'b':
                 continue
              else:

                 wereSame = False
                 optimalSame = (myArray[row-1][col][0] + MATCH, 's')

                 # if seq1 is the shorter sequence, use the following for string comparison
                 if seq1Used:
                    adj = col - 3
                    if (seq1[row-1] == seq2[row+adj-1]):
                       wereSame = True
                 # if not, use this instead
                 else:
                    adj = col - 3
                    if (seq1[row+adj-1] == seq2[row-1]):
                       wereSame = True

                 # check left cell
                 if col-1 < 0:
                    optimalLeft = (float('inf'), 'x')
                 else:
                    optimalLeft = (myArray[row][col-1][0] + INDEL, 'l')

                 # check top cell
                 if col+1 >= bandwidth:
                    optimalTop = (float('inf'), 'x')
                 else:
                    optimalTop = (myArray[row-1][col+1][0] + INDEL, 'd')

                 # check diag cell
                 if row-1 < 0:
                    optimalDiag = (float('inf'), 'x')
                 else:
                    optimalDiag = (myArray[row-1][col][0] + SUB, 't')

                 # if the values are the same, consider the optimalSame value, if not, ignore
                 if wereSame:
                    lowest = min(optimalSame[0], optimalTop[0], optimalDiag[0], optimalLeft[0])
                 else:
                    lowest = min(optimalTop[0], optimalDiag[0], optimalLeft[0])

                 # if same is lowest
                 if lowest == optimalSame[0] and wereSame:
                    myArray[row][col] = optimalSame
                 # if left is lowest
                 if lowest == optimalLeft[0]:
                    myArray[row][col] = optimalLeft
                 # if diag is lowest
                 elif lowest == optimalTop[0]:
                    myArray[row][col] = optimalTop
                 # if top is lowest
                 elif lowest == optimalDiag[0]:
                    myArray[row][col] = optimalDiag
                 end -= 1
           if begin > 0:
```

```
            begin -= 1
        # iterate through the last row until the value of infinity is hit. Set the previous value before that
        # to the optimal score
        start_row, start_col = 0, 0
        for col in range(bandwidth):
            if myArray[width-1][col][0] == float('inf'):
                score = myArray[width-1][col-1][0]
                start_row = width-1
                start_col = col-1
                break

        alignment1 = ""
        alignment2 = ""
        # loop through the previous pointer paths from the optimal value
        # until a 'b' base value is hit
        while(1):
            tuple = myArray[start_row][start_col]
            adj = start_col - 3
            if tuple[1] == 'b':
                #alignment1 += seq1[start_row-1]
                #alignment2 += seq2[0]
                break
            if tuple[1] == 's':
                alignment1 += seq1[start_row-1]
                alignment2 += seq2[start_row+adj-1]
                start_row -= 1
            elif tuple[1] == 'l':
                alignment1 += '-'
                alignment2 += seq2[start_row+adj-1] # may need minus 1 here
                start_col -= 1
            elif tuple[1] == 't':
                alignment1 += seq1[start_row-1]
                alignment2 += seq2[start_row+adj-1] # may need minus 1 here
                start_row -= 1

            elif tuple[1] == 'd':
                alignment1 += seq1[start_row-1]
                alignment2 += '-'
                start_row -= 1
                start_col += 1
    # if un-banded calculation is desired
    ##########################
    # Time Complexity: O(n*m)
    # Space Complexity: O(n*m)
    ##########################
    else:
        # initialize array
        myArray = [[(-1, 'b') for x in range(len(seq1) + 1)] for y in range(len(seq2) + 1)]

        # initialize top row with axis
        temp = 0
        for i in range(len(seq1)+1):
            myArray[0][i] = (temp, 'b')
            temp += 5

        # initialize left col with axis
        temp = 5
        for i in range(1, len(seq2)+1):
            myArray[i][0] = (temp, 'b')
            temp += 5

        # begin Needleman/Wunsch
        for i in range(1, len(seq1)+1):
            for j in range(1, len(seq2)+1):

                # check if the same character
                wereSame = False
                optimalSame = (myArray[j - 1][i - 1][0] + MATCH, 's')
                if (seq1[i - 1] == seq2[j - 1]):
                    wereSame = True

                # check top cell
                optimalTop = (myArray[j - 1][i][0] + INDEL, 't')

                # check top left cell
                optimalDiag = (myArray[j - 1][i - 1][0] + SUB, 'd')

                # check left cell
                optimalLeft = (myArray[j][i - 1][0] + INDEL, 'l')

                # if the characters in the strings are the same, consider the optimalSame value. If not, igore it
                if wereSame:
                    lowest = min(optimalSame[0], optimalTop[0], optimalDiag[0], optimalLeft[0])
                else:
                    lowest = min(optimalTop[0], optimalDiag[0], optimalLeft[0])

                # if same is lowest
                if lowest == optimalSame[0] and wereSame:
                    myArray[j][i] = optimalSame
                # if left is lowest
                if lowest == optimalLeft[0]:
                    myArray[j][i] = optimalLeft
                # if top is lowest
                elif lowest == optimalTop[0]:
                    myArray[j][i] = optimalTop
```

```
            # if diag is lowest
            elif lowest == optimalDiag[0]:
               myArray[j][i] = optimalDiag

      score = myArray[len(seq2)][len(seq1)][0]
      alignment1 = ""
      alignment2 = ""
      row = len(seq2)
      col = len(seq1)
      # loop through the previous pointer paths from the optimal value
      # until row and col = 0
      while(row > 0 and col > 0):
         tuple = myArray[row][col]
         if tuple[1] == 'b':
            alignment1 += seq1[col-1]
            alignment2 += seq2[row-1]
         if tuple[1] == 's':
            alignment1 += seq1[col-1]
            alignment2 += seq2[row-1]
            row -= 1
            col -= 1
         elif tuple[1] == 'l':
            alignment1 += seq1[col-1]
            alignment2 += '-'
            col -= 1
         elif tuple[1] == 't':
            alignment1 += '-'
            alignment2 += seq2[row-1]
            row -= 1
         elif tuple[1] == 'd':
            alignment1 += seq1[col-1]
            alignment2 += seq2[row-1]
            row -= 1
            col -= 1
   alignment1 = alignment1[::-1]
   alignment2 = alignment2[::-1]

   t1 = time.clock() - t0
   return {'align_cost':score, 'seqi_first100':alignment1[0:100], 'seqj_first100':alignment2[0:100]}
```