1. **Time and Space Complexities**

TIME	**unrestrictedAlignment /bandedAlignment**	**generateAlignment /generateBandedAlignment**	**findMin**	**checkBoundaries**	sum	**Align (calls others)**
Unrestricted	O(nm)	O(n + m)	O(1)	O(1)	O(nm + n + m + 1 + 1)	O(nm)
Banded	O(kn)	O(n)	O(1)	O(1)	O(kn + n + 1 + 1)	O(kn)

SPACE	**unrestrictedAlignment /bandedAlignment**	**generateAlignment /generateBandedAlignment**	**findMin**	**checkBoundaries**	**sum**	**Align (calls others)**
Unrestricted	O(nm)	O(n + m)	O(1)	O(1)	O(nm + n + m + 1 + 1)	O(nm)
Banded	O(kn)	O(n)	O(1)	O(1)	O(kn + n + 1 + 1)	O(kn)

- **unrestrictedAlignment:**
  Time:
  O(nm) it will repeat at max n*m times as there are m cols and n rows max
  the cols and rows are the min of lengths of the strings and align_length
  In most cases the align_length < the length of the strings so in most cases it
  would be O(a^2) where a is the align_length
  Space:
  O(nm) the two arrays used for storage are cols = m and rows = n
  and so the storage needed is 2*m*n (2 arrays)
  In most cases the align_length < the length of the strings so in most cases it
  would be O(a^2) where a is the align_length
- **bandedAlignment**

  Time:
  O(kn) it will repeat at max k times as the cols are set to be 2*MAXINDELS + 1 *
  n which is how many rows there are.
  In most cases the align_length < the length of the strings so in most cases it
  would be O(ka) where a is the align_length
  Space:
  O(kn) the two arrays used for storage are cols = k and rows = n
  and so the storage needed is 2*k*n (2 arrays)
  In most cases the align_length < the length of the strings so in most cases it
  would be O(ka) where a is the align_length
- **generateAlignment**

  Time:
  O(n + m) as the max legnth of the alignment which would be the max repeats.
  This would be the case if it were all indels the length of one string and
  then the entire other string and vice versa. Because align_length is normally
  less than the legnths the O(a) where a is the align_length in most cases
  Space:
  O(n + m) as the max legnth of the alignment.
  This would be the case if it were all indels the length of one string and
  then the entire other string and vice versa. Because align_length is normally
  less than the legnths the O(a) where a is the align_length in most cases

- **generateBandedAlignment**

  Time:
  O(n) as the max legnth of the alignment which would be the max repeats.
  This would be because the legnth is bound by the legnth of the smaller string

+ some indels which are restricted by the banding algorithm so it would be
O(n + i) (i is number of indels) i << n --> O(n)
align_legnth is normally less than the legnths so it can be simplified to
O(a) where a is the align_length in most cases

Space:
O(n) as the max legnth of the alignment.
This would be because the legnth is bound by the legnth of the smaller string
+ some indels which are restricted by the banding algorithm so it would be
O(n + i) (i is number of indels) i << n --> O(n)
align_legnth is normally less than the legnths so it can be simplified to
O(a) where a is the align_length in most cases

- **findMin**

Time:
O(1) just 3 steps max

Space:
O(1) doesn't store anything

- **checkBoundaries**

Time:
O(1) just 3 steps max

Space:
O(1) doesn't store anything

2. Explanation of Algorithm

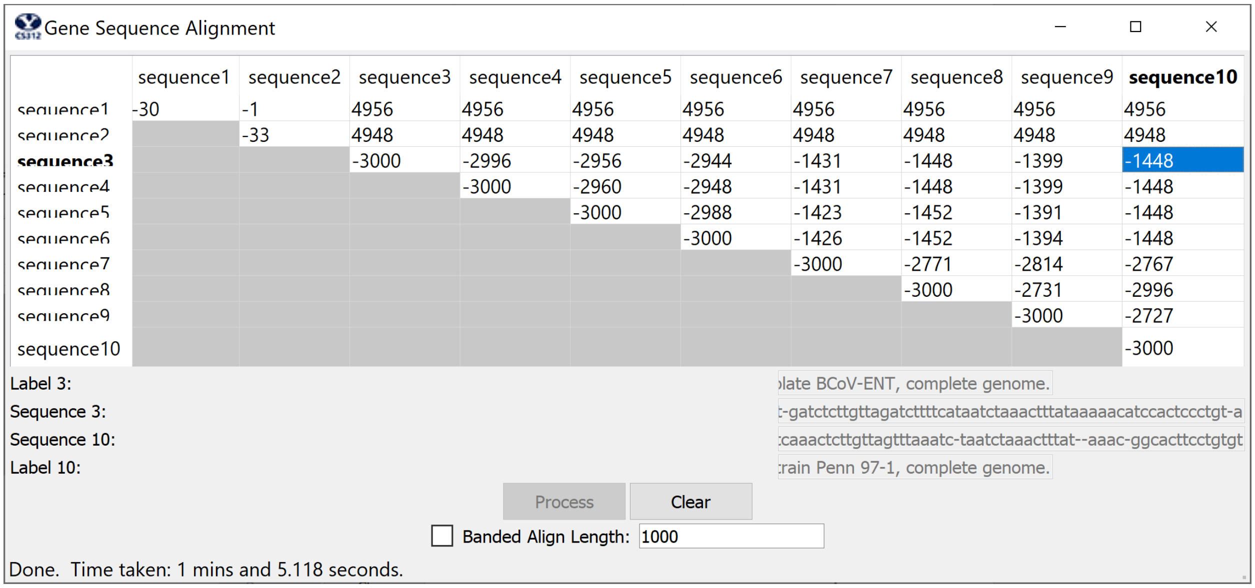
This algorithm works by going through the strings and seeing how they best align in a dynamic way. At each step it will determine what is the best step at this point (going right, down, or diagonal). It will then store the best result in two arrays, cost and fromArray (fromArray is for backtracking later). The cost stored in the cost array is the sum of the previous solution plus the cost to get to the new solution. The algorithm is continued till we have analyzed the entire alignment length.

The algorithm determines the best solution at each step by taking the value in the cells above, to the left, and diagonal and adding 5 if its from the left or above (insertion or deletions), 1 if the letters are different when traveling diagonal and -3 if they match. It then finds the min and adds this value to the cost array and the direction to the fromArray. The solution to the entire problem is in the bottom right corner in the unrestricted algorithm and the last cell in the last row with a solution in it. This is read and returned to the GUI to show the cost.

The Backtracking is done by getting the index of the final solution in the fromArrray and then going backwards through the array. This is where the string of the alignment is calculated. If it was from above, one letter from the vertical string is added and a '-' for an insertion or deletion is added for the horizontal string. The opposite is done if it was from the left ad a letter from each string is added from diagonal. The indexes are then adjusted to go to the cell that is being pointed to by the current cell. In unrestricted this is literally above, to the left, or diagonal, but with banded it is different as diagonal is above, above is diagonal to the right and left is still to the left. This is how the banding algorithm fits everything into a smaller array.

3. Results:

n =1000 Unrestricted



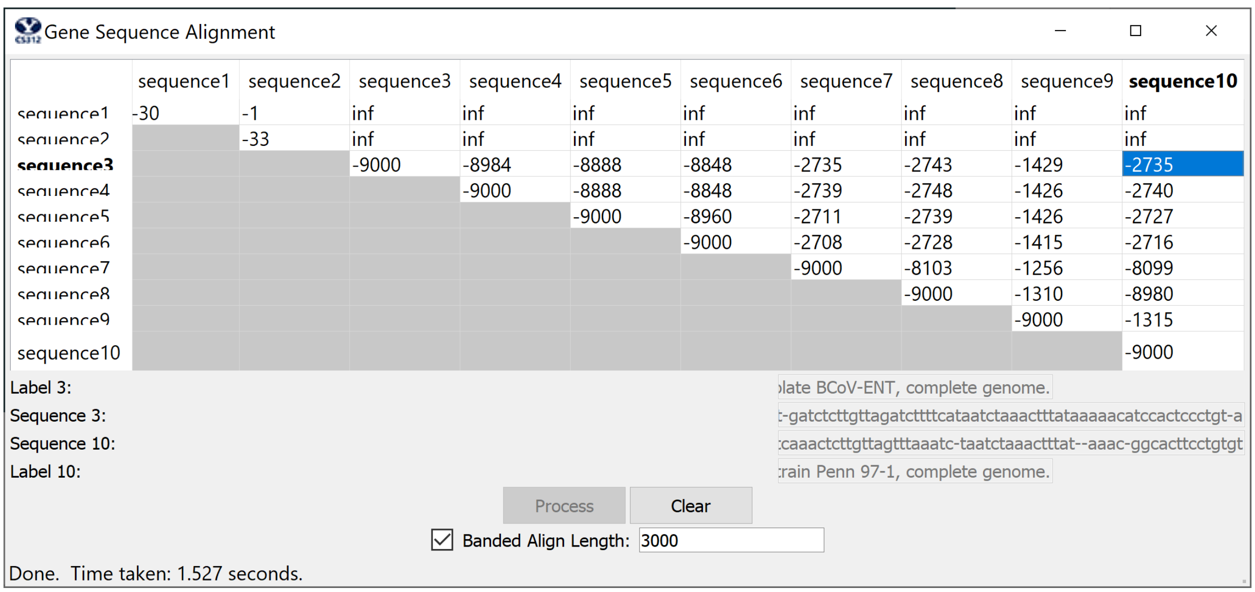
Gene Sequence Alignment

	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 3: late BCoV-ENT, complete genome.
Sequence 3: t-gatctcttgttagatcttttcataatctaaactttataaaaacatccactccctgt-a
Sequence 10: caaactcttgttagtttaaatc-taatctaaactttat--aaac-ggcacttcctgtgt
Label 10: rain Penn 97-1, complete genome.
Process Clear
Banded Align Length: 1000
Done. Time taken: 1 mins and 5.118 seconds.

Alignments:

n =3000 Banded d=3



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 3: late BCoV-ENT, complete genome.
Sequence 3: t-gatctcttgttagatcttttcataatctaaactttataaaaacatccactccctgt-a
Sequence 10: caaactcttgttagtttaaatc-taatctaaactttat--aaac-ggcacttcctgtgt
Label 10: rain Penn 97-1, complete genome.
Process Clear
Banded Align Length: 3000
Done. Time taken: 1.527 seconds.

4. Alignments:

n =1000 Unrestricted

```
3  gattgcgagcgatttgcgtgcgtgcat-ccc--gcttcact-gatctcttgttagatcttttcataatctaaactttataaaaacatccactccctgt-a
10 -a-taagagtgattggcgtccgtacgtaccctttctactctcaaactcttgttagtttaaatc-taatctaaactttat--aaac-ggcacttcctgtgt
```

n =3000 Banded d=3

```
3 gattgcgagcgatttgcgtgcgtgcat-ccc--gcttcact-gatctcttgttagatcttttcataatctaaactttataaaaacatccactccctgt-a
10 -a-taagagtgattggcgtccgtacgtaccctttctactctcaaactcttgttagtttaaatc-taatctaaactttat--aaac-ggcacttcctgtgt
```

5. Code:

```
#!/usr/bin/python3
```

```
# from PyQt5.QtCore import QLineF, QPointF


import math
import time

# 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
    '''
        Checks the boundaries and returns True or False
        Time:
            O(1) just 3 steps max
        Space:
            O(1) doesn't store anything
    '''

    def checkBoundaries(self, i, j, rows, cols):
        if i < 0 or j < 0:
            return False
        if i >= rows or j >= cols:
            return False
        else:
            return True
    '''
        Find min and returns string of that is the min
        Time:
            O(1) just 3 steps max
        Space:
            O(1) doesn't store anything
    '''

    def findMin(self, leftCost, aboveCost, diagonalCost):
        if diagonalCost <= leftCost and diagonalCost <= aboveCost:
```

```
            return "diagonal"
        elif aboveCost <= leftCost and aboveCost <= diagonalCost:
            return "above"
        elif leftCost <= diagonalCost and leftCost <= aboveCost:
            return "left"
    '''
        Generates the Alignment String
        n the length of the smaller string
        Time:
            O(n) as the max legnth of the alignment which would be the max repeats.
            This would be because the legnth is bound by the legnth of the smaller string
            + some indels which are restricted by the banding algorithm so it would be
            O(n + i) (i is number of indels) i << n  --> O(n)
            align_legnth is normally less than the legnths so it can be simplified to
            O(a) where a is the align_length in most cases
        Space:
            O(n) as the max legnth of the alignment.
            This would be because the legnth is bound by the legnth of the smaller string
            + some indels which are restricted by the banding algorithm so it would be
            O(n + i) (i is number of indels) i << n  --> O(n)
            align_legnth is normally less than the legnths so it can be simplified to
            O(a) where a is the align_length in most cases
    '''

    def generateBandedAlignment(self, horizontalSeq, verticalSeq, fromArray, align_length,
                                retJ):
        horizontalAlignment = []
        verticalAlignment = []
        v = len(fromArray) - 1
        h = retJ - 1  # 7 in our case
        while fromArray[v][h] != "START":
            adjustH = v + h - MAXINDELS
            if fromArray[v][h] == "LEFT":
                verticalAlignment.append("-")
                horizontalAlignment.append(horizontalSeq[adjustH-1])
                h -= 1
            elif fromArray[v][h] == "ABOVE":
                verticalAlignment.append(verticalSeq[v-1])
                horizontalAlignment.append("-")
                v -= 1
                h += 1
            elif fromArray[v][h] == "DIAGONAL":
                verticalAlignment.append(verticalSeq[v-1])
                v -= 1
                horizontalAlignment.append(horizontalSeq[adjustH - 1])
```

```
        else:
            print(fromArray[v][h])
            raise ValueError("UNKNOWN VALUE")
    return "".join(horizontalAlignment[::-1]), "".join(verticalAlignment[::-1])
'''
    Generates the Alignment String
    n and m are the lengths of the strings
    Time:
        O(n + m) as the max legnth of the alignment which would be the max repeats.
        This would be the case if it were all indels the length of one string and
        then the entire other string and vice versa. Because align_length is normally
        less than the legnths the O(a) where a is the align_length in most cases
    Space:
        O(n + m) as the max legnth of the alignment.
        This would be the case if it were all indels the length of one string and
        then the entire other string and vice versa. Because align_length is normally
        less than the legnths the O(a) where a is the align_length in most cases
'''

def generateAlignment(self, horizontalSeq, verticalSeq, fromArray, align_length):
    horizontalAlignment = []
    verticalAlignment = []
    v = len(fromArray) - 1
    h = len(fromArray[0]) - 1
    while fromArray[v][h] != "START":
        if fromArray[v][h] == "LEFT":
            verticalAlignment.append("-")
            horizontalAlignment.append(horizontalSeq[h-1])
            h -= 1
        elif fromArray[v][h] == "ABOVE":
            verticalAlignment.append(verticalSeq[v-1])
            horizontalAlignment.append("-")
            v -= 1
        elif fromArray[v][h] == "DIAGONAL":
            verticalAlignment.append(verticalSeq[v-1])
            v -= 1
            horizontalAlignment.append(horizontalSeq[h-1])
            h -= 1
        else:
            print(fromArray[v][h])
            raise ValueError("UNKNOWN VALUE")
    return "".join(horizontalAlignment[::-1]), "".join(verticalAlignment[::-1])
'''
    Generates the Alignment String
    k is the bandwidth and n is the length of the smaller string
```

```
    nested for loop dominates so the other function calls and the generateAlignment
    does not make an impact on big Oh
    Time:
        O(kn) it will repeat at max k times as the cols are set to be 2*MAXINDELS + 1 *
        n which is how many rows there are.
        In most cases the align_length < the length of the strings so in most cases it
        would be O(ka) where a is the align_length
    Space:
        O(kn) the two arrays used for storage are cols = k and rows = n
        and so the storage needed is 2*k*n (2 arrays)
        In most cases the align_length < the length of the strings so in most cases it
        would be O(ka) where a is the align_length
'''

def bandedAlignment(self, horizontalSeq, verticalSeq, align_length):
    maxJ = min(align_length, len(horizontalSeq))
    cols = min((align_length + 1), len(horizontalSeq) + 1)
    # n is legnth of smaller string which is always the 2nd argument
    rows = min((align_length + 1), len(verticalSeq) + 1)
    if cols - rows > MAXINDELS:
        return float('inf'), "No Alignment Possible", "No Alignment Possible"
    cols = 2*MAXINDELS + 1  # 2*MAXINDELS + 1 == k
    cost = [[float('inf')]*(cols) for _ in range(rows)]
    fromArray = [["NONE"]*(cols) for _ in range(rows)]
    cost[0][MAXINDELS] = 0
    fromArray[0][MAXINDELS] = "START"
    retJ = 0
    for i in range(rows):
        for j in range(cols):
            if i == 0 and j <= MAXINDELS:
                continue
            adjustJ = j + i - MAXINDELS
            if adjustJ > maxJ or adjustJ < 0:
                continue
            if i == rows - 1:
                retJ += 1
            # print(jEnd, adjustJ, i, j, len(horizontalSeq))
            if horizontalSeq[adjustJ - 1] == verticalSeq[i-1]:
                diagonalCost = (
                    cost[i - 1][j] + MATCH) if self.checkBoundaries(i - 1, j, rows, cols)
                                            else float('inf')
            else:
                diagonalCost = (
                    cost[i-1][j] + SUB) if self.checkBoundaries(i-1, j, rows, cols)
                                        else float('inf')
```

```
            aboveCost = (
                cost[i-1][j + 1] + INDEL) if self.checkBoundaries(i-1, j + 1, rows, cols)
                                          else float('inf')
            leftCost = (
                cost[i][j - 1] + INDEL) if self.checkBoundaries(i, j - 1, rows, cols)
                                        else float('inf')
            minCost = self.findMin(
                leftCost, aboveCost, diagonalCost)
            if minCost == "left":
                cost[i][j] = leftCost
                fromArray[i][j] = "LEFT"
            elif minCost == "above":
                cost[i][j] = aboveCost
                fromArray[i][j] = "ABOVE"
            elif minCost == "diagonal":
                cost[i][j] = diagonalCost
                fromArray[i][j] = "DIAGONAL"
    assert(cost[0][MAXINDELS] == 0)
    alignment1, alignment2 = self.generateBandedAlignment(
        horizontalSeq, verticalSeq, fromArray, align_length, retJ)
    return cost[rows-1][retJ - 1], alignment1, alignment2
'''
    Generates the Alignment String
    n and m are the lengths of the strings
    Time:
        O(nm) it will repeat at max n*m times as there are m cols and n rows max
        the cols and rows are the min of lengths of the strings and align_length
        In most cases the align_length < the length of the strings so in most cases it
        would be O(a^2) where a is the align_length
    Space:
        O(nm) the two arrays used for storage are cols = m and rows = n
        and so the storage needed is 2*m*n (2 arrays)
        In most cases the align_length < the length of the strings so in most cases it
        would be O(a^2) where a is the align_length
'''

def unrestrictedAlignment(self, horizontalSeq, verticalSeq, align_length):
    cols = min((align_length + 1), len(horizontalSeq) + 1)  # m
    rows = min((align_length + 1), len(verticalSeq) + 1)  # n
    cost = [[float('inf')]*cols for _ in range(rows)]
    fromArray = [["NONE"]*cols for _ in range(rows)]
    cost[0][0] = 0
    fromArray[0][0] = "START"
    for i in range(rows):
        for j in range(cols):
```

```
            # left
            if i != 0 or j != 0:
                if horizontalSeq[j-1] == verticalSeq[i-1]:
                    diagonalCost = (
                        cost[i - 1][j - 1] + MATCH) if self.checkBoundaries(i - 1, j - 1,
                                                        rows, cols) else float('inf')
                else:
                    diagonalCost = (
                        cost[i-1][j-1] + SUB) if self.checkBoundaries(i-1, j-
                                                  1, rows, cols) else float('inf')
                aboveCost = (
                    cost[i-1][j] + INDEL) if self.checkBoundaries(i-
                                              1, j, rows, cols) else float('inf')
                leftCost = (
                    cost[i][j-1] + INDEL) if self.checkBoundaries(i, j-
                                              1, rows, cols) else float('inf')
                minCost = self.findMin(leftCost, aboveCost, diagonalCost)
                if minCost == "left":
                    cost[i][j] = leftCost
                    fromArray[i][j] = "LEFT"
                elif minCost == "above":
                    cost[i][j] = aboveCost
                    fromArray[i][j] = "ABOVE"
                elif minCost == "diagonal":
                    cost[i][j] = diagonalCost
                    fromArray[i][j] = "DIAGONAL"
        alignment1, alignment2 = self.generateAlignment(
            horizontalSeq, verticalSeq, fromArray, align_length)
        # print(alignment1, alignment2)
        return cost[rows-1][cols-1], alignment1, alignment2

# This is the method called by the GUI.  _sequences_ is h list of the ten sequences, _table_ i
s h
# handle to the GUI so it can be updated as you find results, _banded_ is h boolean that tells
# you whether you should compute h banded alignment or full alignment, and _align_length_ tell
s you
# how many base pairs to use in computing the alignment
    '''
        calls either bandedAlignment or unrestrictedAlignment
        k is bandwidth
        n and m are lengths of the strings
        a is align_length
        time and space:
            if banded:
                O(kn) --> avg large n's O(ka)
```

```
        else:
            O(nm) --> avg large n and m O(a^2)
    see other functions for explanation
'''

def align(self, sequences, table, banded, align_length):
    self.banded = banded
    self.MaxCharactersToAlign = align_length
    results = []

    for i in range(len(sequences)):
        jresults = []
        for j in range(len(sequences)):
            if j < i:
                s = {}
            else:
                if i == j:
                    legnth = min((align_length + 1),
                                 len(sequences[i]) + 1)
                    score, alignment1, alignment2 = MATCH * \
                        (legnth-1), sequences[i], sequences[j]
                elif banded:
                    if len(alignment1) > len(alignment2):
                        score, alignment1, alignment2 = self.bandedAlignment(
                            sequences[i], sequences[j], align_length)
                    else:
                        score, alignment2, alignment1 = self.bandedAlignment(
                            sequences[j], sequences[i], align_length)
                else:
                    score, alignment1, alignment2 = self.unrestrictedAlignment(
                        sequences[i], sequences[j], align_length)
                # if i == 2 and j == 9:
                #     print("3", alignment1[:100])
                #     print("10", alignment2[:100])
                s = {'align_cost': score, 'seqi_first100': alignment1[:100],
                     'seqj_first100': alignment2[:100]}
                table.item(i, j).setText('{}'.format(
                    int(score) if score != math.inf else score))
                table.repaint()
            jresults.append(s)
        results.append(jresults)
    return results
```