Gregory Knapp

CS 312

Dr. Grimsman

11/4/2021

Project 4 Gene Alignment Project Report

Time Complexity Analysis of Project 4

The time complexity for each part of the code is pulled from the source code comments, with any additional notes added here for things that aren't explained within the code.

Summary of unrestricted algorithm time/space complexity.

Analysis of Unrestricted Algorithm Time/Space Complexity

GeneSequencing.py Lines 441-446. Space complexity when initializing array.

```
# Initialize 2d matrix for calculating edit distance of sequences
# Time of np.zeros - O(nm) where n is length of align_length_seq1 and m is
length of align_length_seq2
# Time is O(nm) because each value is iterated over in order to initialize
it.
#
# Space is O(nm) because the 2d array has values equal to n * m or the length
of the two sequences after
# taking the align length variable into account.
```

Genesequencing.py Lines 457-468. Time complexity of while loop in unrestricted algorithm.

```
# Solve for remaining values in matrix starting from second row/column to end
of table.
# Time O((n-1)(m-1)) which is equal to O(nm).
#
# Time complexity is O(nm) because the two nested for loops iterate over each
value in the sequences.
# The way the code is set up, all of the actual genetic sequences are longer
than the expected values of
# 1000 or 3000 for align_length that we were supposed to test for, so in most
of the test cases, n and m
# are equal, so the time could be written as O(n^2). However, the algorithm
does not force the two
# sequences to be the same length. The test examples using polynomial or
exponential against one of the
# gene sequences have vastly different lengths, resulting in significant
differences between n and m.
```

```
# On top of that, the value for align length is subjective, meaning that
while our test cases did not
# cause it to happen, it is very possible that with higher values of
align_length more cases would have
# different values for n and m, so time complexity is best stated as O(nm)
instead of O(n^2) or O(m^2)
```

GeneSequencing.py Lines 26-43. Time/space complexity of traceback function for unrestricted algorithm.

```
# Function that takes in the matrix solved by the unrestricted algorithm and returns an array containing the two
# alignments for the sequences. The backtrace alignment is found by starting at the cell containing the score and
# traversing the O(nm) matrix backwards. The next cell is found by doing the same checks used to calculate the edit
# distance (left insert, top insert, diagonal sub/match) in the same order to ensure the correct alignment is
# produced.
# The time complexity of this algorithm has a worst case of O(nm) which would happen if every single backtrace was
# an insert, from the score cell to the very left of the matrix then up to the top left cell. This is an extremely
# unlikely, if impossible case, so it isn't a good time analysis of the function.
# # In reality, the average case is approximately O(n) where n is the length of the longer sequence. In our cases,
# since we limit the sequences with the align_length parameter to our program, so in most cases, the two
# sequences have the same sliced length. In cases where it doesn't, the algorithm will need at least as many
# iterations as there are characters in the longer sequence so the complete alignment can be found for both. If only
# subs/matches are made, then we get the best case O(n), where n = align_length/longest sequences. Realistically,
# there are almost always inserts made, which add 1 extra loop to the algorithm. These additional loops are,
# except in the worst of cases, insignificant to the overall complexity of the function, so the average case
# should still be O(n) when n = align length/len of the longest sequence.
```

Summary of Unrestricted algorithm

Time Complexity = O(nm)

Space Complexity = O(nm)

Time complexity of Traceback O(n) n = length of longer sequence

As described in the above comments, the time and space complexity of the unrestricted algorithm are both O(nm). The space complexity is straightforward. The array is initialized with the parameters of the

length of the two sequences for rows and columns, giving us a clear array of size O(nm). No other arrays are initialized in this function, so there is no other space complexity to consider here.

Time complexity is dictated by the way the function progresses. Since it is the standard edit distance function, it loops through every value in the array and calculates the edit distance in the array, unlike the banded algorithm. Since we know the space complexity of the array is O(nm), and the algorithm loops through each value to calculate it, we know the time complexity is also O(nm), the same as the size of the array. The time is not greater than this, thanks to the dynamic programming approach of using min and checking previous values in the array. That way, instead of constantly repeating the same problems and having a time of O(nm^2) or something worse, we only perform each calculation once, giving us the time that is the same as the array space.

Of note, the time complexity is not changed by the traceback function, because the traceback is only of O(n) time, which does not impact the overall time performance. The reasons for this time are detailed in the comment, but generally speaking, the average case loops through just a few times more than the length of the longer string, depending on the number of inserts, but its not enough to make the complexity get higher than O(n), except in the very worst cases.

Analysis of Banded Algorithm Time/Space Complexity

GeneSequencing.py Lines 492-508. Time complexity summary of Banded algorithm.

```
# Use banded approach to solve edit distance of two sequences. Bandwidth is caluclated from globally defined
# variable MAXINDELS, which for testing purposes is defaulted to 3. A matrix separate from the one used in the
# unrestricted algorithm is created and used. This array of size O(kn), where k is 2 *MAXINDELS + 1 and n is
# the length of the shorter string, is used for storing and calculating score values.
# # The algorithm works by initializing the first band of values since there are no previous values to reference,
# so to avoid out of bounds errors, the first 7 values are done separately. Then inside of the main while loop,
# the value diagonal to the first value is calculated. From there, values for 3 inserts/deletes both down and
# right of that value are calculate, referencing values previously calculated in the matrix. This gives us the
# 2d+1 (k) size band that makes up the array, resulting in the space complexity of the algorithm being O(kn),
# since only those 2d+1 values are stored in the initialized array.
# Time complexity of the algorithm is straightforward. The while loop iterates until j = length of the shorter
# sequence. For each iteration of j, 2d+1 (in our cases since MAXINDELS = 3, 2d+1 = 7) values, which are stored
# in the array. If the two strings have very different lengths, less values than k may be calculated on a
# single iteration, but this is not significant enough to change that the
```

```
time complexity of this algorithm is \# also O(kn), where k = 2d + 1 and n = length of the shorter sequence.
```

Genesequencing.py Line 513. Space complexity of initializing array O(kn)

```
# Initialize O(kn) size matrix - Time O(kn) (each value initialized to 0) and Space - O(kn)
```

Genesequencing.py Lines 95-119. Time/Space complexity of traceback function for banded algorithm.

Summary of Banded algorithm

Time Complexity = O(kn)

Space Complexity = O(kn)

Time complexity of Traceback O(n), n = length of longer sequence

The analysis of the banded algorithm is very similar to that of the unrestricted one, just with different values. The space complexity is clearly O(kn), since I initialize the matrix array with the value k calculated from 2*d+1. I know this for sure also because I originally implemented this with time O(kn) but space O(nm) by using the full array, since I was unaware of the requirement, so I had to learn the hard way what the difference was.

Like the unrestricted algorithm, the function then calculates a distance for each value in the array (with the exception of a few cells at the end when there is a difference in sequence length, but those are not enough to change the time complexity). Since we are using dynamic programming and only iterating over each value one time, we have the time complexity O(kn), instead of something worse.

Again, the traceback function does not change the time complexity since it does not dominate the main time complexity of the main algorithm. The function for the banded one works the same as the unrestricted one, just with a different pattern for tracing back through the array since the set up is completely different.

Explanation of Extraction Algorithms

The extraction algorithms work by starting from the "score" cell (the cell containing the final score of the ideal alignments) and working backwards until it reaches the first cell of the array. The functions start with two blank strings and an iterator for each string that each start at the final index of the string. Next, the function starts from the final square and essentially does what the alignment function does in reverse order; it checks the previous array values and sees if one of them equals the current value with either the indel penalty, substitution penalty, or match reward values added. Importantly, it searches for these in the same left, top, diagonal tie breaking order so that the alignments are the correct ones that the code originally solved for. When it finds the previous value, it updates the alignment strings. If a substitution was made, the current letter the sequence index points to is appended. If an insert/deletion is made, the string keeps the value gets the letter and the iterator is decremented. The other string adds a "-" to it and does not decrement the counter. This pattern continues until both string iterators reach 0, and all the characters from the sequence are appended to the strings. The result is packaged into an array which main extracts, checks if there is a valid alignment and then slices down to the 100 characters displayed on the screen.

I made two functions, one for the unrestricted algorithm and one for the banded one, since the different array sizes and order the variables are stored in made it hard to write one that worked for either one. (If

I had used the array of pointers or indices/tuples approach, it probably would have been possible to do). However, there are no core differences between the two functions, except for the pattern which previous values are checked for. The O(kn) array has some special cases since sometimes values that are used to calculate the score are not part of the banded array, so considerations for those sorts of cases are made in there. Otherwise, the pattern is the same, start from the bottom and work up to the first cell while appending letters to either or both strings depending on the result found.

Results

1. 10x10 matrix using unrestricted algorithm with align length n = 1000

	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
				Proce	ess C	lear				

Time taken: 1 minute and 6.764 seconds. 66.6764 < 120 seconds, passes performance requirement.

2.10x10 matrix using banded algorithm with align length n = 3000.



Time taken: 1.986 seconds. 1.986 < 10, passes performance requirement.

3.Extracted alignment for first 100 characters of sequences #3 and #10 for both unrestricted and banded algorithms.

Unrestricted sequences for #3 and #10 (#3 is top, #10 is below)

ataa-gagtgattggcgtccgtaccgtaccctttctactctcaaactcttgttagtttaaatc-taatctaaactttataaa--cggc-acttcctgtgtg attgcgagcgatttgcgtgcgtgcatcccgcttc-actg--at-ctcttgttagatcttttcataatctaaactttataaaaacatccactccctgta-g

Banded sequences for #3 and #10 (#3 is top, #10 is below)

ataa-gagtgattggcgtccgtaccgtaccctttctactctcaaactcttgttagtttaaatc-taatctaaactttataaa--cggc-acttcctgtgtg attgcgagcgatttgcgtgcgtgcatcccgcttc-actg--at-ctcttgttagatcttttcataatctaaactttataaaaacatccactccctgta-g

Source Code Files

GeneSequencing.py

```
from which pygt import PYQT VER
Lf PYOT VER == 'PYOT5':
   from PyQt5.QtCore import QLineF, QPointF
   raise Exception ('Unsupported Version of PyQt: {}'.format(PYQT VER))
MAXINDELS = 3
```

```
tracebackj - 1] + indel penalty: # If statement evaluation -
```

```
alignment1 = ""
        alignment2 = ""
indel penalty == \
                    alignment1 = "-" + alignment1
MAXINDELS] + indel penalty == \
```

```
alignment1
indel penalty == \
                    alignment1 = "-" + alignment1
indel penalty == matrix[startingj][
                    alignment1 = align length seq1[tracebacki - 1] +
```

```
if tracebacki > 0 and matrix[starting]][startingk - 1] +
alignment1
```

```
elif startingk == MAXINDELS + 1: # If statement evaluation -
                if tracebackj > 0 and matrix[startingj][0] + indel penalty ==
matrix[startingj][startingk]:
                    alignment1 = "-" + alignment1
```

```
alignment2
indel penalty == matrix[startingj][
                    alignment1 = "-" + alignment1
```

```
indel penalty == matrix[startingj][
                    alignment1 = "-" + alignment1
alignment1
```

```
matrix[0][j] = j * indel penalty # Assign variable with
```

```
indel penalty), (matrix[i - 1][j]) + indel penalty,
indel penalty), (matrix[i - 1][j]) + indel penalty,
sub penalty)
```

```
k = 2 * MAXINDELS + 1
                   matrix[0][j + 3] = j * indel penalty
1][iterator k + 1 + MAXINDELS] + indel penalty,
```

```
1][iterator k + 1 + MAXINDELS] + indel penalty,
                    elif iterator k < MAXINDELS: # If statement evaluation -</pre>
align length seq2[
1][iterator k] + sub penalty)
                    elif iterator k == MAXINDELS: # If statement evaluation
```

```
matrix[j -
offset = iterator k
offset = 1
```

```
1 [iterator k + 1] + indel penalty,
                   elif iterator k == 2*MAXINDELS: # If statement
                                                       matrix[j -
```

```
matrix[j -
if diff > k: # Evaluate if statement - Time O(1)
   alignment1 = alignments[0] # Extract value from array - Time
```

```
return {'align_cost': score, 'seqi_first100': alignment1,
'seqj_first100': alignment2}
```

Proj4GUI.py

```
from which pyqt import PYQT VER
if PYQT VER == 'PYQT5':
  from PyQt5.QtWidgets import *
   from PyQt5.QtGui import *
  from PyQt5.QtCore import *
   from PyQt4.QtGui import *
  from PyQt4.QtCore import *
  raise Exception ('Unsupported Version of PyQt: {}'.format(PYQT VER))
     super(Proj4GUI, self). init ()
     self.seqs = self.loadSequencesFromFile()
      self.solver = GeneSequencing()
  def processClicked(self):
     start = time.time()
```

```
jresults.append(s)
  ns = end-start
   nm = math.floor(ns/60.)
def clearClicked(self):
```

```
def cellClicked(self, i, j):
   print('Cell {},{} clicked!'.format(i,j))
def loadSequencesFromFile( self ):
       line = liner.strip()
def getTableDims( self ):
```

```
vbox = QVBoxLayout()
self.table.setRowCount(NSEQ)
self.table.setColumnCount(NSEQ)
self.table.setHorizontalHeaderLabels(headers)
self.table.setVerticalHeaderLabels(headers)
self.table.setHorizontalScrollBarPolicy(Qt.ScrollBarAlwaysOff)
self.table.setVerticalScrollBarPolicy(Qt.ScrollBarAlwaysOff)
     qitem.setFlags( Qt.ItemIsSelectable | Qt.ItemIsEnabled )
         qitem.setBackground(QColor(200,200,200))
  self.table.resizeColumnToContents(i)
self.table.setFixedWidth(w)
self.table.setFixedHeight(h)
self.clearButton = QPushButton('Clear')
                = QCheckBox('Banded')
font = QFont()
font.setFamily("Courier")
```

```
h.addStretch(1)
h.addStretch(1)
vleft = QVBoxLayout()
vright = QVBoxLayout()
h.addLayout(vleft)
h.addStretch(1)
h.addStretch(1)
```

```
app = QApplication(sys.argv)
w = Proj4GUI()
sys.exit(app.exec())
```

PYQT_VER = 'PYQT5'