CS F364 Assignment 2

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Problem Statement

The aim of the problem is to obtain a secondary structure of maximum energy (The energy of a secondary structure is proportional to the number of base pairs in it) from a given RNA sequence while following the given rules.

Rules

- An RNA molecule is a string $B = b_1 b_2 \ldots b_n;; b_i \in A, C, G, U; \forall; 1 \leq i \leq n$
- The pairing of bases are as follows
  - **A**denine always matches with **U**racil.
  - **C**ytosine always matches with **G**uanine.
- Every base pairs with atmost one other base
- (No sharp turns) The ends of each pair are separated by at least 4 intervening bases i.e. if $b_i b_j$ is a pairing, then $i < j - 4$
- (No knots) If $b_i b_j$ and $b_k b_l$ are two pairings, then we cannot have $i < k < j < l$

Dynamic Programming Approach

Using the Dynamic Programming Approach, we consider the entire problem made up of smaller sub-problems that can be recursively solved. Here, a subproblem is defined as finding the maximum number of base pairings for a particular subsequence.

$OPT(i, j)$ is the maximum number of base pairs in a secondary structure for $b_i b_{i+1} \ldots b_j$. Hence, the solution for the problem is $OPT(1, n)$, where n is the length of the RNA sequence.

If $i > j - 4$, then $OPT(i, j) = 0$.

In the optimal secondary structure on $b_i b_{i+1} \ldots b_j$,

- If j is not a member of any pair in the subsequence, use $OPT(i, j - 1)$

- If j pairs with some $t < j-4$, the knot condition yields two independent sub-problems; $OPT(i, t-1)$ and $OPT(t+1, j-1)$.

From this, we arrive at the recurrence relation

$$OPT(i,j) = \max\{\ OPT(i, j-1),\ \max_t(1 + OPT(i, t-1) + OPT(t+1, j-1))$$

From the above recurrence relation, it can be seen that there are $O(n^2)$ subproblems.

Note that computing $OPT(i,j)$ involves sub-problems $OPT(l,m)$ where $m - l < j - i$. Hence, the way to solve this recurrence relation is to first solve all subproblems of size $s-1$ before moving on to subproblems of size s. This is described in the psuedocode mentioned below.

Initialize $OPT(i,j) = 0$ whenever $i \geq j-4$
For $k = 5, 6, \ldots n-1$
  For $i = 1, 2, \ldots n-k$
    Set $j = i + k$
    Compute $OPT(i,j)$ using the recurrence relation
  Endfor
Endfor
Return $OPT(1,n)$

Implementation Details

Since the recurrence relation has two dimensions, a double-dimensional array `maxMatchings` is used for storing the values of OPT. Three `for` loops are used to iterate over the double-dimensional array to compute the answer every possible sub-problem.

A structure `Match` is used to store the indices of the matching base pair.

The array `matches` is used for storing all the base pairs obtained as per the dynamic programming logic.

Time Complexity Analysis

In the function `calculateMaxMatchings()`, the outermost loop runs from $s = 6; to; n$.

The middle loop runs from $i = 0; to; n+s-1$.

The innermost loop runs from $t = i; to; j$, where $j = i + s - 1$.

Since there are no `break` statements inside any of the loops, the maximum number of times the statements in the innermost loop can be found by

$\sum_{s=6}^{n} \sum_{i=0}^{n+s-1} \sum_{t=i}^{i+s-1} O(1)$

$= \sum_{s=6}^{n} \sum_{i=0}^{n+s-1} (i+s-1-i+1) \cdot O(1)$

$= \sum_{s=6}^{n} \sum_{i=0}^{n+s-1} s \cdot O(1)$

$= \sum_{s=6}^{n} s(n+s-1-0+1) \cdot O(1)$

$= \sum_{s=6}^{n} s(n+s) \cdot O(1)$

$= \sum_{s=6}^{n} (s^2+ns) \cdot O(1)$

$= O(1) \cdot \sum_{s=6}^{n} (s^2+ns)$

$= O(1) \cdot (\sum_{s=6}^{n} s^2 + \sum_{s=0}^{n} ns)$

$= O(1) \cdot (\sum_{s=6}^{n} s^2 + n\sum_{s=0}^{n} s)$

$= O(1) \cdot ((\sum_{s=0}^{n} s^2 - \sum_{s=0}^{6} s^2) + n(\sum_{s=0}^{n} s - \sum_{s=6}^{n} s))$

$$= O(1) \cdot ((\frac{n(n+1)(2n+1)}{6} - \frac{6(6+1)(2(6)+1)}{6}) + n(\frac{n(n+1)}{2} - \frac{6(6+1)}{2}))$$

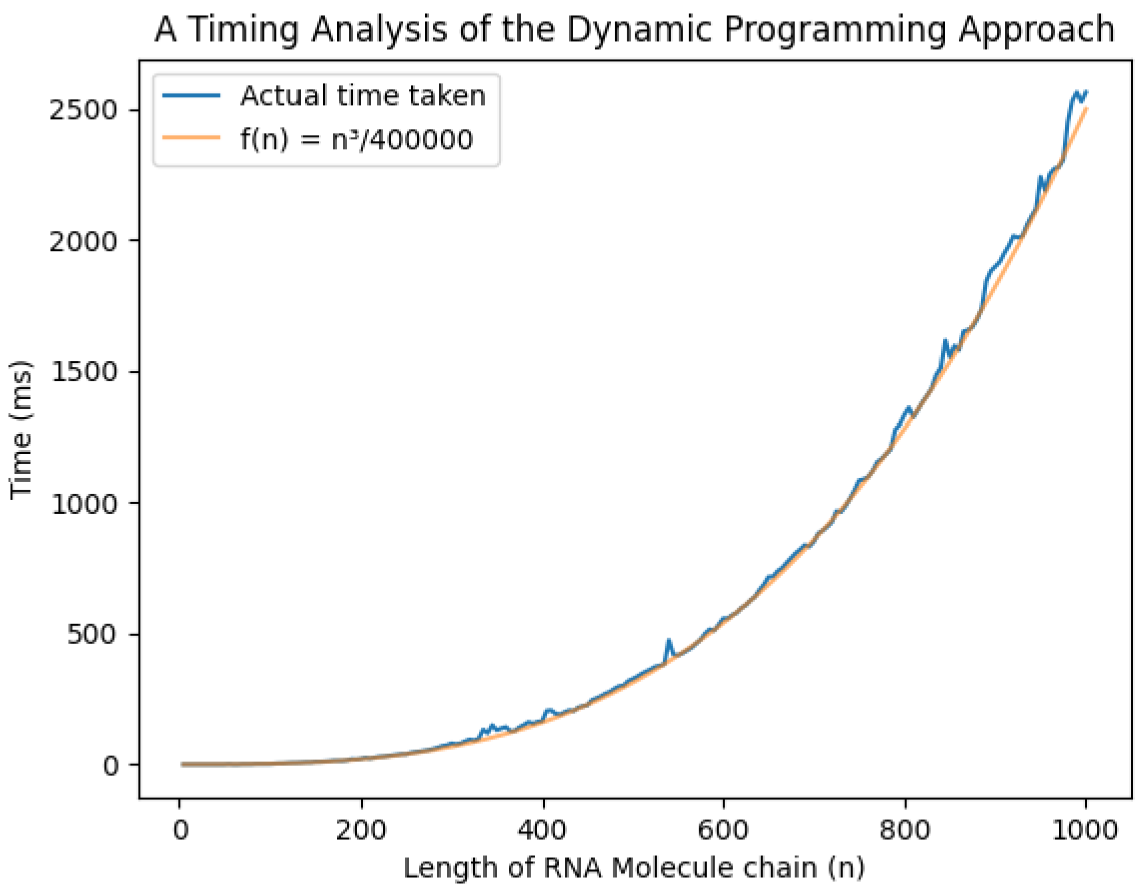
$$= O(1) \cdot ((\frac{n^3}{3} + \frac{n^2}{2} + \frac{n}{6} - 91) + n(\frac{n^2}{2} + \frac{n}{2} - 21))$$

$$= O(1) \cdot (\frac{n^3}{3} + \frac{n^2}{2} + \frac{n}{6} - 91 + \frac{n^3}{2} + \frac{n^2}{2} - 21n)$$

$$= O(1) \cdot (\frac{2n^3}{3} + n^2 - \frac{125n}{6} - 91)$$

$= O(n^3)$

Timing Analysis



From the above plot, it can be seen that the actual time taken t can be approximated by the curve $t = \frac{n^3}{400000}$, which is indeed $O(n^3)$.

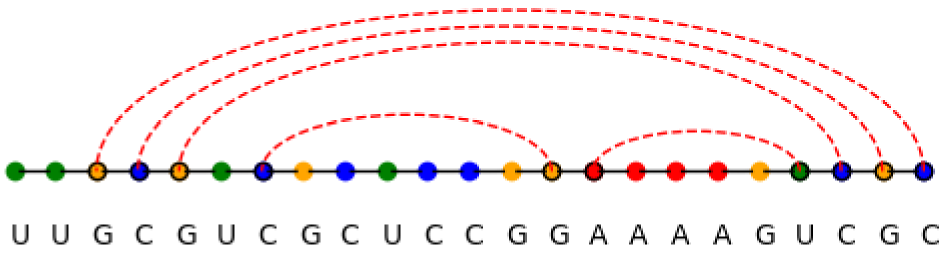
Space Complexity Analysis

As shown in the the recurrence relation, since there are $O(n^2)$ sub-problems, and each sub-problem requires $O(1)$ space to store its value, the space complexity of the Dynamic Programming Approach is $O(n^2)$.

Test Cases

The code was tested with the Nucleic Acid Database (NDB) by Rutgers University that has 12016 structures as of April 13th, 2022.

Taking an example from the database; $UUGCGUCGCUCCGGAAAAGUCGC$, the base pairings determined by the algorithm are as shown below.



Conclusion

We see that using the recurrence relation, the complexity of the algorithm is exponential, however, when we use memoization to store the results of previously computed sub-problems, we see that the time complexity is reduced to polynomial time ($O(n^3)$), at the cost of $O(n^2)$ space.