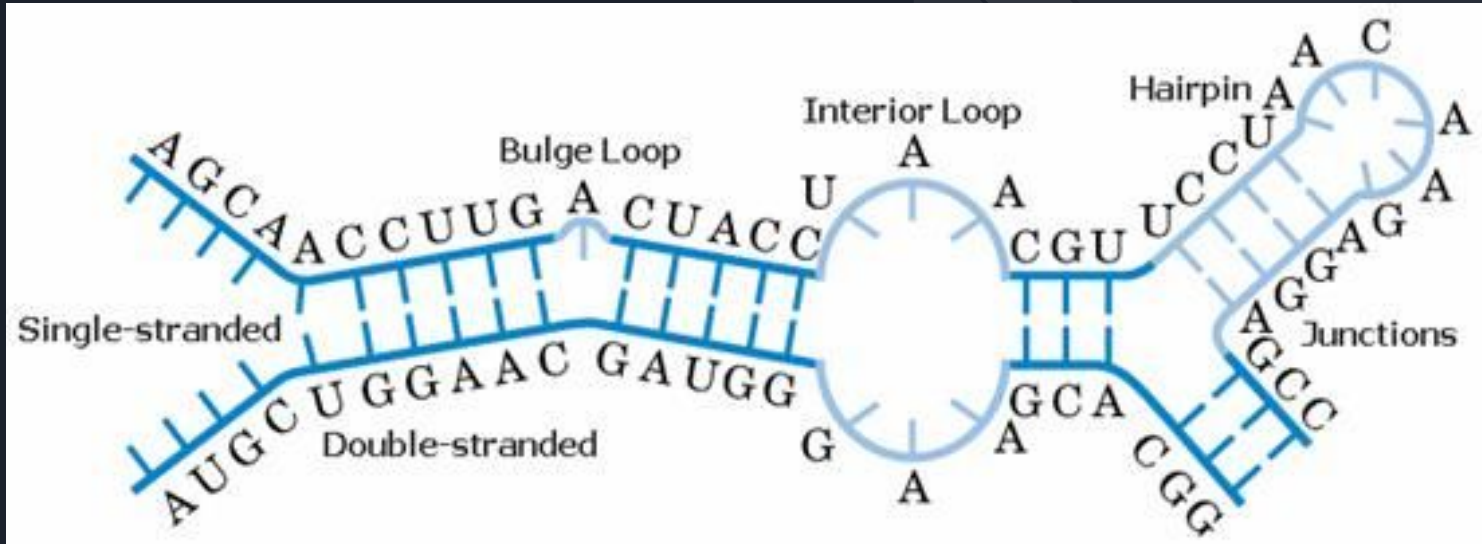# RNA Folding

Tamara Fleet,  Spring 2018
CSCI 582 Bioinformatics

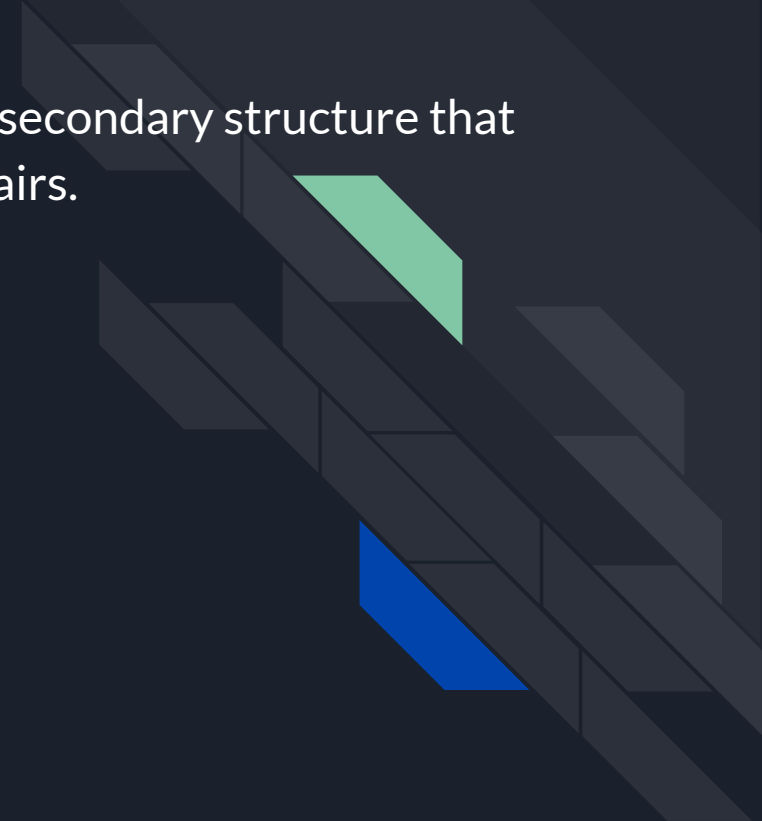# RNA Secondary Structure
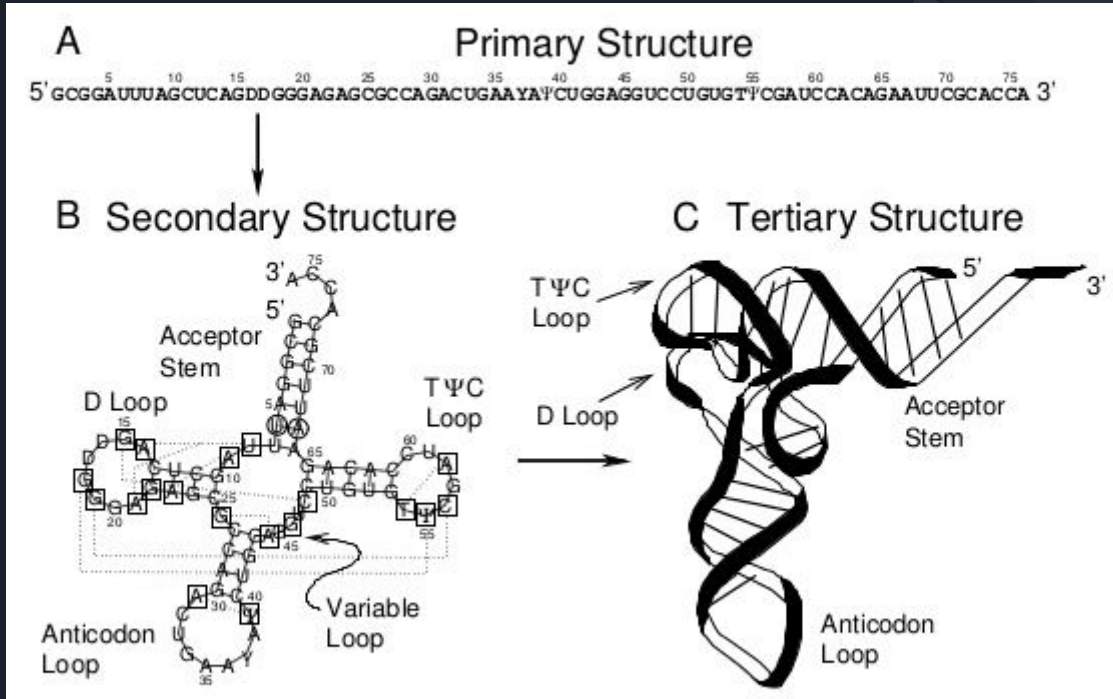
# Secondary Structural Elements

# RNA Secondary Structure Prediction

Given a string over {A, U, C, G}, find the optimal set of base pairs i, j such that

1. There must be at least 4 positions between i and j (i < j – 4)
2. Only A can pair with U and only C can pair with G
3. A position is in at most one pairing
4. If (i, j) and (i', j') are paired, then i < i' < j < j' is not permitted (no pseudoknots)

# Base Pair Maximization using Nussinov Algorithm

Problem: Given a RNA sequence, find the secondary structure that maximizes the number of matched base pairs.
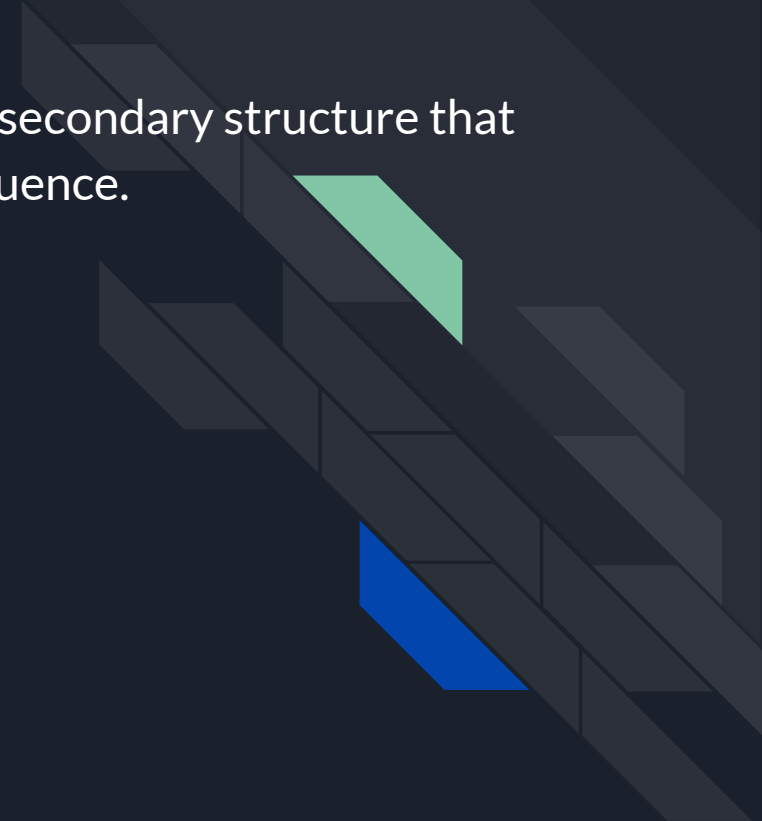
# Nussinov Algorithm

Recursion: (for $1 \leq i < j \leq n$)

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{\substack{i \leq k < j \\ S_k, S_j \, complementary}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

# Free Energy Minimization using Zuker's Algorithm

Problem: Given a RNA sequence, find the secondary structure that minimizes the total free energy of the sequence.

# Code Demo

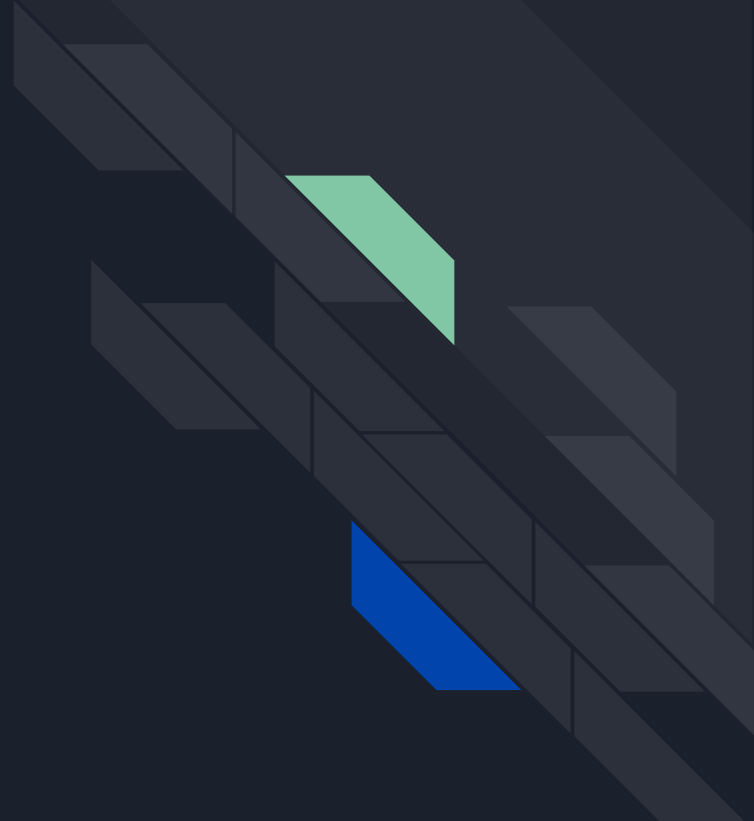CGCUUCAUAUAAUCCUAAUGAUAUGGUUUGGGAGUUUCUACCAAGAGCCUUAAACUCUUGAUUAUGAAGUG

**MY RESULTS:**
(.((((((((((.((.((..........)))) (((((.................))))))))).))..)))))).)

**RNA FOLD RESULTS (using MFE):**
...((((((((..(((((.........))))))......).(((((........))))))..))))))...

# Visual Representation of Secondary Structure

# References

[1] Nussinov, R. & Jacobson, A. B. (1980). Fast algorithm for predicting the secondary structure of single stranded RNA. Proc. Natl Acad. Sci. USA, 77, 6309–6313.

[2] Zuker, M., & Stiegler, P. (1981). Optimal computer folding of large RNA sequences using thermodynamics and auxiliary information. Nucleic Acids Research, 9(1), 133–148.

[3] Intro to the RNA folding problem and recurrences, UC Davis: https://youtu.be/bzJNFhBWNTg