

# Mumuksha.Pant.HW1

September 23, 2024

## 1 PART I

### 1.1 1 ) Basic Sequence Validation: (10%)

• Write a function called “is\_valid\_rna” to validate if a given string is a valid RNA sequence (contains only A, C, G, U). The function should return True for valid sequences and False for invalid ones.

Example: For a given sequence “AUGCAUGCAUGC” is\_valid\_rna: True

For a given sequence “AUGTXAGCAUGC” is\_valid\_rna: False

```
[192]: import re
def is_valid_rna(rna):
    pattern_to_match= r'^[ACGU]+$'
    result= re.search(pattern_to_match, rna, re.IGNORECASE)
    if result:
        return True

    else:
        return False
```

```
[193]: #Test cases
print(is_valid_rna("AUGCAUGCAUGC")) # true

print(is_valid_rna("AUGTXAGCAUGC")) #false

print(is_valid_rna("XXYYZ")) #false
print(is_valid_rna("auauau")) #true
```

True  
False  
False  
True

[ ]:

[ ]:

## 1.2 2 )Nucleotide Count: (10%)

- Create a function called 'nucleotide\_count' to count the occurrence of each nucleotide (A, C, G, U) in a given RNA sequence.

The function should return a dictionary with nucleotides as keys and their counts as values.

Example:

For a given sequence "AUGCAUGCAUGC"

Nucleotide count: {'A': 3, 'C': 3, 'G': 3, 'U': 3}

```
[194]: def nucleotide_count(neocleotide) :  
        neocleotide = neocleotide.upper() # Converting all RNA to upper case  
        counts = {'A': 0, 'C': 0, 'G': 0, 'U': 0}  
        valid_neocleotides=set(counts.keys())  
        for i in neocleotide :  
            if i not in valid_neocleotides:  
                raise ValueError("Invalid RNA sequence")  
            counts[i] += 1  
        return counts
```

```
[195]: # test cases  
try:  
    print(nucleotide_count("AUGCAUGCAUGC")) # valid sequence, upper case  
    print(nucleotide_count("auauau")) # valid sequence , lower case  
    print(nucleotide_count("XXYY")) # invalid sequence  
  
except ValueError as e:  
    print(e)
```

{'A': 3, 'C': 3, 'G': 3, 'U': 3}

{'A': 3, 'C': 0, 'G': 0, 'U': 3}

Invalid RNA sequence

[ ]:

[ ]:

[ ]:

## 1.3 3) Finding Motifs: (10%)

- Write a function called 'find\_motifs' to identify and return all occurrences of a given motif (subsequence) within the RNA sequence.

An example of a sequence with Repeated Motifs AUGCUGCAUGCAUGCUGCAUGCAUGCUAG .

The function should handle motifs of varying lengths.

Example: For a given sequence “AUGCAUGCAUGC” Motif ‘AUG’ found at positions: [0, 4,8 ]

```
[196]: def find_motifs(rna, motif):  
  
        position=[] # list to store the positions of the motifs  
  
        for match in re.finditer(motif, rna, re.IGNORECASE):  
            position.append(match.start()) # Add the starting position of each  
            ↪match  
  
        return position
```

```
[197]: #Test case 1  
find_motifs("AUGCAUGCAUGC", "aug") #valid, lowercase motif
```

```
[197]: [0, 4, 8]
```

```
[198]: #Test case 2  
find_motifs("augcaugCAUGCUGCAUGCAUGCUG", "AUG") #valid, lowercase RNA
```

```
[198]: [0, 4, 8, 15, 19]
```

```
[199]: #test case 3  
find_motifs("AUGAUGAUGAUG", "AUGAUG") #overlapping sequence
```

```
[199]: [0, 6]
```

```
[200]: #test case 4  
find_motifs("XXYY" , "aug") #motif does not exist in the sequence
```

```
[200]: []
```

#### 1.4 4) Sequence Complementarity: (10%)

- In RNA, A pairs with U and C pairs with G.

Create a function called ‘complementary\_sequence’ to generate the complementary sequence of a given RNA sequence by swapping pairs.

Example:

For a given sequence “AUGCAUGCAUGC”

Complementary sequence: UACGUACGUACG

```
[ ]:
```

```
[220]: def complementary_sequence(rna):
    # pairing rules
    complements = {'A': 'U', 'U': 'A', 'C': 'G', 'G': 'C'}

    # Generate the complementary sequence, swapping pairs
    complementary_seq = ''.join(complements.get(base, base) for base in rna)

    return complementary_seq

#test cases
print(complementary_sequence("AUGCAUGCAUGC"))
print(complementary_sequence("AUGCAUGCAUGC"))    #expected : AUGAUGAUGAUG
print(complementary_sequence("AUGCRY"))           #expected : UACGYR
```

UACGUACGUACG  
UACGUACGUACG  
UACGRY

[ ]:

## 1.5 5 ) GC Content Calculation: (10%)

- Write a function called 'gc\_content' to calculate the GC content (percentage of nucleotides G and C) in the RNA sequence, which is significant in determining the stability of the molecule. Hint: GC content = GC counts / length of the sequence

Example:For a given sequence "AUGCAUGCAUGC" GC content: 50.0 %

```
[204]: #This is the normal code I had written previously, without using the regex.
# def gc_content(rna):
#     count_g= {'G':0}
#     count_c= {'C':0}

#     for i in rna:
#         if i=='G':
#             count_g[i]+=1
#         if i=='C':
#             count_c[i]+=1

#     GCcontent= ((count_g['G']+count_c['C'])/len(rna))*100
#     return round(GCcontent, 2)

#Code using regular expression
import re

def gc_content(rna):
    count_g = len(re.findall('G', rna))
```

```
count_c = len(re.findall('C', rna))

GCcontent = ((count_g + count_c) / len(rna)) * 100
return round(GCcontent, 2)
```

```
[205]: #test case
print(gc_content("AUGCAUGCAUGC")) #50.0
print(gc_content("AAUUAAC"))      #14.29
print(gc_content("XXYY"))          #0.0
print(gc_content("CGCGCG"))        #100.0
```

```
50.0
14.29
0.0
100.0
```

```
[ ]:
```

## 2 PART II

### 2.1 1) Advanced Sequence Validation: (10%)

- Create a modified version of the 'is\_valid\_rna' function to also check for commonly used ambiguity codes in RNA sequences (e.g., N for any nucleotide, R for A or G) and validate accordingly.

Example:

valid\_sequence\_with\_ambiguity = "AUGCRYSWKMBDHAVN"

invalid\_sequence = "AUGTXZGCAUGC"

AGCTU

```
[206]: import re
def is_valid_rna_modified(rna):
    pattern_to_match= r'^[AGCURYSWKMBDHAVN]+$'

    result= re.search(pattern_to_match, rna, re.IGNORECASE)
    if result:
        return True
    else:
        return False
```

```
[207]: #test case
is_valid_rna_modified("AUGCRYSWKMBDHAVN")
```

```
[207]: True
```

```
[208]: #test case
is_valid_rna_modified("AUGTXZGCAUGC")
```

[208]: False

```
[209]: #test case
is_valid_rna_modified("AUGCRY")
```

[209]: True

```
[ ]:
```

## 2.2 2) Regex-based Motif Search with Ambiguities: (20%)

- Adapt the 'find\_motifs' function to accept motifs with ambiguity codes and identify potential matches in the sequence.

Example:

sequence = "AUGCRYSN"

find\_motifs(sequence, "RY")

output: "Motif 'RY' found at positions: [0, 2]"

```
[229]: # Mapping ambiguity codes
ambiguity_codes = {
    'R': '[AG]', # A or G
    'Y': '[CTU]', # C, T or U
    'S': '[CG]', # C or G
    'W': '[ATU]', # A, T or U
    'K': '[GTU]', # G, T or U
    'M': '[AC]', # A or C
    'B': '[CGTU]', # C, G, T or U
    'D': '[AGTU]', # A, G, T or U
    'H': '[ACTU]', # A, C, T or U
    'V': '[ACG]', # A, C, G
    'N': '[ACGTU]', # A, C, G, T or U
}

def find_motifs_modified(sequence, motif):

    res = []

    for char in motif:
        if char in ambiguity_codes:
            res.append(ambiguity_codes[char])
        else:
            res.append(char)
```

```

motif_regex = ''.join(res)

# finding all overlapping match in sequence
matches = [match.start() for match in re.finditer(f'(?=({motif_regex}))',
↪sequence)]

return f"Motif '{motif}' found at positions: {matches}"

```

```

[230]: # Test case 1
sequence = "AUGCRYSN"
motif = "A"
print(find_motifs_modified(sequence, motif))

```

Motif 'A' found at positions: [0]

```

[231]: # Test case 2
sequence = "AUGCRYSN"
motif = "RY"
print(find_motifs_modified(sequence, motif))

```

Motif 'RY' found at positions: [0, 2]

[ ]:

## 2.3 3 ) Sequence Fragmentation and Analysis: (20%)

- Create a function called 'fragment\_and\_analyze' that fragments the RNA sequence into smaller segments of a specified length and performs a detailed analysis on each fragment including 'is\_valid\_rna', 'gc\_content' and 'complementary\_sequence'

Example: sequence = "AUGCRYNAUGCRYXNAUGCRYSN", fragment\_length = 6

```

[215]: def gc_content_modified(rna):
        # Define the GC bases and their contributions for ambiguity codes
        gc_bases = {'G', 'C'}
        ambiguity_codes = {
            'S': 1.0,    # C or G contributes 100%
        }

        gc_count = 0

        for base in rna:
            if base in gc_bases:
                gc_count += 1
            elif base in ambiguity_codes:
                gc_count += ambiguity_codes[base]    # Add partial GC content for
↪ambiguity codes

```

```

# Avoid division by zero
sequence_length = len(rna)
if sequence_length == 0:
    return 0.0

gc_content_percentage = (gc_count / sequence_length) * 100
return round(gc_content_percentage, 2)

```

```

[216]: #modifying existing complementary sequence code
def complementary_sequence_modified(rna):
    complementary_sequence_list = [] # result list to store the complementary
    ↪sequence

    complement = {
        'A': 'U',
        'U': 'A',
        'C': 'G',
        'G': 'C',
        'S': 'S', # S = [C or G] so complement remains S
        'N': 'N', # N can be any base, so complement remains N
        'R': 'Y', # R = [A or G] so complements to Y
        'Y': 'R'  # Y = [U or C] so complements to R
    }

    return ''.join([complement.get(char, char) for char in rna])

# Test cases
print(complementary_sequence_modified("AUGCAUGCAUGC")) # Expected: UACGUACGUACG
print(complementary_sequence_modified("AUGCRY"))       # Expected: UACGYR
print(complementary_sequence_modified("GCRYSN"))       # Expected: CGYRNS

```

```

UACGUACGUACG
UACGYR
CGYRNS

```

```

[217]: def fragment_and_analyze(sequence, fragment_length):
    fragments = [] #to store results

    i = 0
    while i < len(sequence):
        fragment = sequence[i:i + fragment_length]

        #checking valid RNA ( take in account ambiguity codes )
        is_valid = is_valid_rna_modified(fragment)

```



```

        #checking gc content only if valid RNA ( take in account ambiguity
↳codes )
        gc = gc_content_modified(fragment) if is_valid else 'N/A'

        #checking complementary sequence only if valid RNA ( take in account
↳ambiguity codes )
        comp_seq = complementary_sequence_modified(fragment) if is_valid else
↳'N/A'

        #add all the results to fragments.
        fragments.append({
            'fragment': fragment,
            'is_valid_rna': is_valid,
            'gc_content': gc,
            'complementary_sequence': comp_seq
        })

        i += fragment_length #move to next

    return fragments

```

```

[218]: #test case
fragment_and_analyze("AUGCRYSNAUGCRYXNAUGCRYSN", 6)

```

```

[218]: [{'fragment': 'AUGCRY',
        'is_valid_rna': True,
        'gc_content': 33.33,
        'complementary_sequence': 'UACGYR'},
        {'fragment': 'SNAUGC',
        'is_valid_rna': True,
        'gc_content': 50.0,
        'complementary_sequence': 'SNUACG'},
        {'fragment': 'RYXNAU',
        'is_valid_rna': False,
        'gc_content': 'N/A',
        'complementary_sequence': 'N/A'},
        {'fragment': 'GCRYSN',
        'is_valid_rna': True,
        'gc_content': 50.0,
        'complementary_sequence': 'CGYRSN'}]

```

```

[219]: #test case
fragment_and_analyze("AUGCRY",2)

```

```

[219]: [{'fragment': 'AU',
        'is_valid_rna': True,

```

```
'gc_content': 0.0,  
'complementary_sequence': 'UA'},  
{ 'fragment': 'GC',  
  'is_valid_rna': True,  
  'gc_content': 100.0,  
  'complementary_sequence': 'CG'},  
{ 'fragment': 'RY',  
  'is_valid_rna': True,  
  'gc_content': 0.0,  
  'complementary_sequence': 'YR'}]
```

[ ]: