

CMSC423

Chapter 4 – Leaderboard searching

Implementation details

Simple...but complex

- Need multiple helper functions:
 - map from letters to masses
 - linear spectrum from amino-acid string
 - circular spectrum from amino-acid string
 - is linear spectrum contained in theoretical spectrum?
 - is circular spectrum equal to theoretical spectrum?
 - how well does linear/circular spectrum match theoretical spectrum?
 - leaderboard management: delete incompatible peptides
 - leaderboard management: add a letter to all peptides
 - leaderboard management: trim to size
- Test each separately using made-up data!!!

Small tricks save time

```
for i in [0..len(peptide)]  
  for j in [i .. len(peptide)]  
    mass = 0  
    for x in [i..j]  
      mass += mass(peptide[x])  
    spectrum.append(mass)
```

$O(N^3)$

versus:

```
prefix[0] = mass(peptide[0])  
for i in [1..len(peptide)]  
  prefix[i] = prefix[i - 1] + mass(peptide[i])  
for i in [0..len(peptide)]  
  for j in [i..len(peptide)]  
    spectrum.append(prefix[j] - prefix[i])
```

$O(N^2)$