INPUT:

Protein Sequence = ATWGRTG

$$\ell = 7$$

$$k = 3$$

Example of using software (CMD line)

python DebruijnExtend.py gfp.fasta 4 gfp.ss3

STEP 0 – Hash Table (Training)

For each k-mer in a training database, find every possible secondary structure and its probability.

RTG
$$\longrightarrow$$
 EEE, 0.5 EEC, 0.4 CCC, 0.1

ATW \longrightarrow CCE, 0.3 ECC, 0.2 HHH, 0.5

GRT \longrightarrow EEE, 1

TWG \longrightarrow CEE, 0.9 CCH, 0.1

WGR \longrightarrow CHE, 0.1 EEE, 0.9

<u>DebruijnExtend</u>

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STEP 1 – K-mer Mapping

Look up the corresponding set of secondary structures for each k-mer using the precomputed hash table.

STEP 2 - Stitch-Extend

Use BFS to traverse the Debruijn graph to find the highest weighted path. This is implemented using a dynamic programming method where the subproblem is matching the contracted nodes to the nodes of the next layer.

OUTPUT (most probable):

CCEEEEE Prob: 0.1215

 $TC: O(3^{\ell+1} * (\ell - k + 1))$

