STRUCTURAL BIOINFORMATICS ASSIGNMENT 3

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THEORITICAL EXERCISES

Q1. Using the simple Markov Model shown in Figure 1.1, write the transition probability matrix and calculate the probability that the weather for the next five days will be Rainy, Rainy, Cloudy, Sunny, Sunny, given that today is Sunny. (2 points) You can use numpy or other tools to do actual calculations (in this case you still need to provide a transition matrix and describe steps to solve this task).

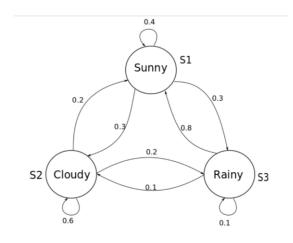


Figure 1.1: Simple Markov Model

Calculating initial/ stationary state

S R C

Since the present day is 'Sunny' so we are supposing $\pi = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}$

Solving the equation $\pi A = \pi$

$$\begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0.4 & 0.3 & 0.3 \\ 0.8 & 0.1 & 0.1 \\ 0.2 & 0.2 & 0.6 \end{bmatrix} = \begin{bmatrix} 0.4 & 0.3 & 0.3 \\ 0.8 & 0.1 & 0.1 \\ 0.2 & 0.2 & 0.6 \end{bmatrix} = \begin{bmatrix} 0.46 & 0.21 & 0.33 \end{bmatrix}$$

$$\begin{bmatrix} 0.4 & 0.3 & 0.3 \\ 0.8 & 0.1 & 0.1 \\ 0.2 & 0.2 & 0.6 \end{bmatrix} = \begin{bmatrix} 0.418 & 0.225 & 0.357 \end{bmatrix}$$

$$\begin{bmatrix} 0.418 & 0.225 & 0.357 \end{bmatrix} \begin{bmatrix} 0.4 & 0.3 & 0.3 \\ 0.8 & 0.1 & 0.1 \\ 0.2 & 0.2 & 0.6 \end{bmatrix} = \begin{bmatrix} 0.4186 & 0.2193 & 0.3621 \end{bmatrix}$$

$$\begin{bmatrix} 0.4186 & 0.2193 & 0.3621 \end{bmatrix} \begin{bmatrix} 0.4 & 0.3 & 0.3 \\ 0.8 & 0.1 & 0.1 \\ 0.2 & 0.2 & 0.6 \end{bmatrix} = \begin{bmatrix} 0.4153 & 0.21993 & 0.36477 \end{bmatrix}$$

$$\begin{bmatrix} 0.4153 & 0.21993 & 0.36477 \end{bmatrix} \begin{bmatrix} 0.4 & 0.3 & 0.3 \\ 0.8 & 0.1 & 0.1 \\ 0.2 & 0.2 & 0.6 \end{bmatrix} = \begin{bmatrix} 0.415 & 0.219 & 0.365 \end{bmatrix}$$

$$\begin{bmatrix} 0.4153 & 0.21993 & 0.36477 \end{bmatrix} \begin{bmatrix} 0.4 & 0.3 & 0.3 \\ 0.8 & 0.1 & 0.1 \\ 0.2 & 0.2 & 0.6 \end{bmatrix} = \begin{bmatrix} 0.415 & 0.219 & 0.365 \end{bmatrix}$$

Since,
$$\pi A = \pi$$

Therefore, $\pi = \begin{bmatrix} 0.415 & 0.219 & 0.365 \end{bmatrix}$

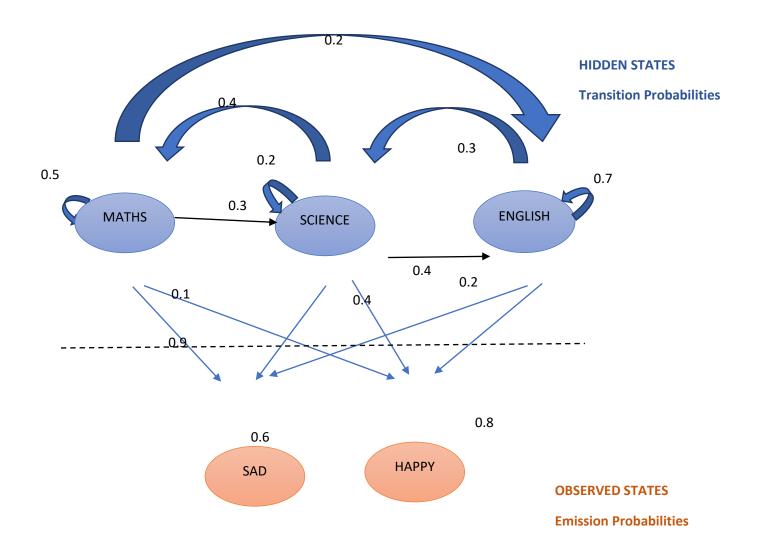
"To find the probability of the given sequence "Rainy, Rainy, Cloudy, Sunny, Sunny" given that today is Sunny,

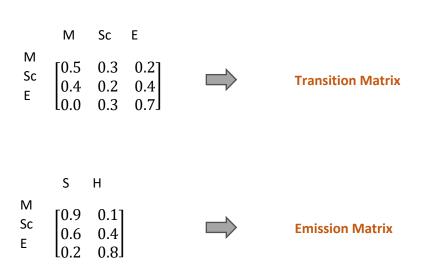
$$\Rightarrow$$
 P(S) x [P(R) | S] x [P(R) | R] x [P(C) | R] x [P(S) | C] x [P(S) | S]

- \Rightarrow 0.415 x 0.3 x 0.1 x 0.1 x 0.2 x 0.4
- ⇒ 0.0000996

Therefore, the probability of the sequence given is **0.0000996**

Q2. Explain Hidden Markov Models (HMM) architecture with a sample diagram (don't use the one from the lecture). Make sure to mark all of the components in the diagram along with their probabilities and write down the total number of parameters.





PARAMETERS: -

X = Hidden States = Maths (M), Science (Sc), English (E)

Y = Observed States = Happy (H). Sad (S)

A = Transition probability, which is:

$$\begin{array}{ccccc} & \mathsf{M} & \mathsf{Sc} & \mathsf{E} \\ \\ \mathsf{M} & \\ \mathsf{Sc} & \begin{bmatrix} 0.5 & 0.3 & 0.2 \\ 0.4 & 0.2 & 0.4 \\ 0.0 & 0.3 & 0.7 \end{bmatrix} \end{array}$$

B = Output/ Emission probability, which is:

$$\begin{array}{c} & \text{S} & \text{H} \\ \text{M} \\ \text{S} \\ \text{E} & \begin{bmatrix} 0.9 & 0.1 \\ 0.6 & 0.4 \\ 0.2 & 0.8 \end{bmatrix} \end{array}$$

Let's consider the example below for better explanation:-

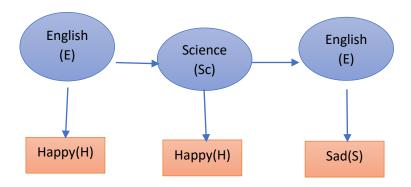


Figure 2

Finding the probability of the above sequence.

For reference:

Step 1: We have to find Initial/stationary state first.

M Sc E

Since today the student is studying English (E), so we are supposing that $\pi = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}$

Solving the equation $\pi A = \pi$

$$\begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{1} \end{bmatrix} \begin{bmatrix} 0.5 & 0.3 & 0.2 \\ 0.4 & 0.2 & 0.4 \\ 0.0 & 0.3 & 0.7 \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \mathbf{0}.\mathbf{3} & \mathbf{0}.\mathbf{7} \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{0} & \mathbf{0}.\mathbf{3} & \mathbf{0}.\mathbf{7} \end{bmatrix} \begin{bmatrix} 0.5 & 0.3 & 0.2 \\ 0.4 & 0.2 & 0.4 \\ 0.0 & 0.3 & 0.7 \end{bmatrix} = \begin{bmatrix} \mathbf{0}.\mathbf{12} & \mathbf{0}.\mathbf{27} & \mathbf{0}.\mathbf{61} \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{0.12} & \mathbf{0.27} & \mathbf{0.61} \end{bmatrix} \begin{bmatrix} 0.5 & 0.3 & 0.2 \\ 0.4 & 0.2 & 0.4 \\ 0.0 & 0.3 & 0.7 \end{bmatrix} = \begin{bmatrix} \mathbf{0.168} & \mathbf{0.273} & \mathbf{0.559} \end{bmatrix}$$

$$\begin{bmatrix} \textbf{0.168} & \textbf{0.273} & \textbf{0.559} \end{bmatrix} \begin{bmatrix} 0.5 & 0.3 & 0.2 \\ 0.4 & 0.2 & 0.4 \\ 0.0 & 0.3 & 0.7 \end{bmatrix} = \begin{bmatrix} \textbf{0.1932} & \textbf{0.2727} & \textbf{0.5341} \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{0.1932} & \mathbf{0.2727} & \mathbf{0.5341} \end{bmatrix} \begin{bmatrix} 0.5 & 0.3 & 0.2 \\ 0.4 & 0.2 & 0.4 \\ 0.0 & 0.3 & 0.7 \end{bmatrix} = \begin{bmatrix} \mathbf{0.20568} & \mathbf{0.27273} & \mathbf{0.52159} \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{0.20568} & \mathbf{0.27273} & \mathbf{0.52159} \end{bmatrix} \begin{bmatrix} 0.5 & 0.3 & 0.2 \\ 0.4 & 0.2 & 0.4 \\ 0.0 & 0.3 & 0.7 \end{bmatrix} =$$

 $[0.211932 \quad 0.272727 \quad 0.51534]$

$$\begin{bmatrix} \textbf{0.211932} & \textbf{0.272727} & \textbf{0.51534} \end{bmatrix} \begin{bmatrix} 0.5 & 0.3 & 0.2 \\ 0.4 & 0.2 & 0.4 \\ 0.0 & 0.3 & 0.7 \end{bmatrix} = \begin{bmatrix} \textbf{0.218} & \textbf{0.273} & \textbf{0.51} \end{bmatrix}$$

Since, $\pi A = \pi$

Therefore, $\pi = [0.218 \quad 0.273 \quad 0.51]$

P(Y = H, H, S; X = E, Sc, E)

$$P(X_1 = E) \times P(Y_1 = H \mid X_1 = E) \times P(Y_2 = H \mid X_2 = Sc) \times P(Y_3 = S \mid X_3 = E) \times P(X_2 = Sc \mid X_1 = E) \times P(X_3 = E \mid X_2 = Sc)$$

- \Rightarrow 0.51× 0.8 x 0.4 x 0.2 x 0.3 x 0.4
- ⇒ 0.00391

Therefore, probability for the above sequence is **0.00391**

Q3. Explain sequence logos and compare them to sequence profiles. Where can they be used? (1 point)

Sequence logos are representation of conserved sequence along a series of multiple sequence alignment of genetically similar sequences in a single graphical form. It is created by a consensus sequence of all the given sequences. The higher the frequency of occurrence of a certain base pair in a given sequence alignment of DNA, RNA or protein, higher it will be the height of that particular base in the graphical representation. This way we can easily see which bases or amino acids are more common compared to others in an alignment.

On the other hand, sequence profiles give much more information about consensus sequences. This is due to information coming from occurrences. In addition to consensus sequence, sequence profiles also calculate the occurrence of amino acids or nucleotides for each of the position as exact numbers. This gives an estimate prediction of probability of which amino acid or nucleotide can occur on that position.

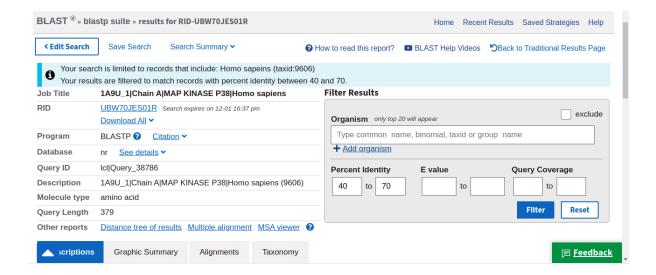
Both methods can be used any of the multiple sequence alignments. They both can make it easier for users to detect the abundance of gene or amino acids on particular positions.

Q4. What are the differences between the traditional artificial neural networks and deep learning? (1 point)

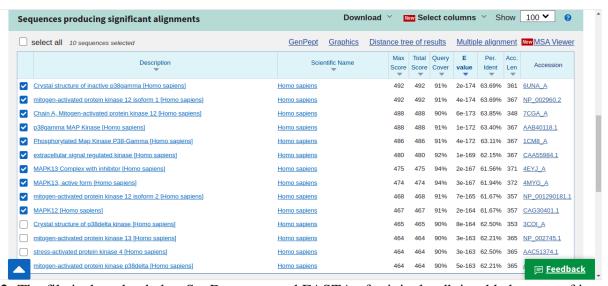
	Traditional Artificial neural network	Deep learning
1.	An artificial neural network imitates the	Deep learning imitates the data processing
	actual human brain neurons and trains	techniques of human brain just like ANN but
	itself to give best possible output	it is rather trained based on representation of
	according to the real world trained	data which is unstructured unlike ANN.
	based on assorted sets of algorithms	
	designed to mimic how neurons	
	perceive and react to sensory data	
2.	A neural network basically consists of 3	A Deep learning system can be referred to as
	layers usually with 1 hidden layer along	an ANN with more than 3 layers including1
	with 1 input layer and 1 output layer.	input layer and 1 output layer
3.	Traditional artificial neural networks are	Deep learning is a subset of the field of
	a subset of the field of Machine	Artificial neural networks in the area of
	learning.	Machine learning.
4.	It is applicable to detect objects and	It can be in speech and textual recognition
	facial character recognition.	and categorization and for generation of HD
	Identification and classification of text	videos depending om the observations on
	recognition according to the relevant	low quality image and footages which can
	certain categories.	further be used for development of high-
		quality images of historic data. It can also be
		sued for digital marketing by showing
		advertisements based on the surfer's
		previous search history.

PROGRAMMING EXERCISES

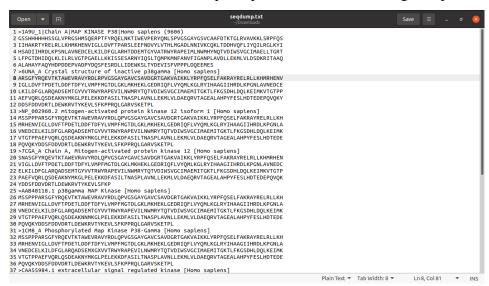
1- 1A9U.pdb is used for this assignment.



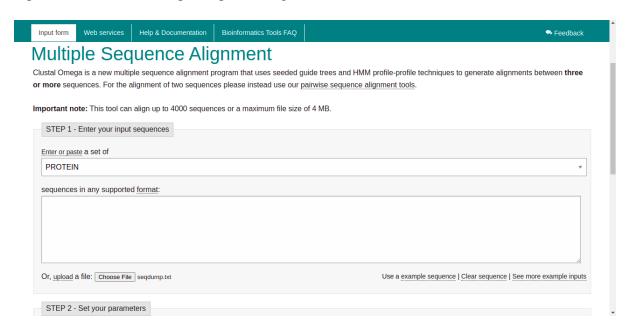
10 proteins with 40 to 70 percent identity is chosen for multiple alignment.



2- The file is downloaded as SeqDump.txt and FASTA of original .pdb is added on top of it.



Input is selected for multiple sequence alignment.



Result of alignment.

3-

```
# Panda is called for DataFrame
import pandas as pd
# Bio and Bio.Align is specifically used for consensus calculations
from Bio import AlignIO as al
from Bio.Align import AlignInfo as alI

# Alignment is called with the format "clustal"
alignment = al.read("clustalo-E20211130-094437-0140-87358764-
p2m.clustal_num", "clustal")
```

```
# Summary info is assigned
align = alI.SummaryInfo(alignment)
# Dumb_consensus function of the AlignInfo module is used to generate
consensus
consensus = align.dumb_consensus()
print("Consensus of the clustal is:" + "\n" + consensus)
```

Gives the output as:

Consensus of the clustal is:

MGSSHHHHHHSSGLVPRGXSXXXXXRSGFYRQEVTKTAWEVRAVYRDLXPVGSGA YGAVCSAVDGRTGAKVAIKKLYRPFQSELFAKRAYRELRLLKHMRHENVIGLLDVF TPDETLDDFXDFYLVMPFMGTDLGKLMKHEKLGEDRIQFLVYQMLKGLRYIHXAGI IHRDLKPGNLAVNEDCELKILDFGLARQADSEMTGYVVTRWYRAPEVILNWMXYT QTVDIWSVGCIMAEMITGKTLFKGSDHLDQLKEIMKVTGTPPAEFVQRLQSDEAKN YMKGLPELEKKDFASILTNASPLAVNLLEKMLVLDAXXRXTAGEALAHPYFESLHD TEDEPQAVQKYDDSFDXXDRTLDEWKRVTYKEVLSFKPPRQLGARVSKETPL