INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR

End-Spring Semester 2022-23

Date of Examination: ---04-2023 Session: AN Duration: 3 hrs Full Marks: 80
Subject No: CS61060 Subject: Computational Biophysics: Algorithms to Applications
Department/Center/School: Department of Computer Science and Engineering
Specific charts, graph paper, log book etc., required: None
Special Instructions (if any): *(1) Answer all the questions. (2) In case of reasonable doubt, make practical assumptions and write that on your answer script. (3) The parts of each question must answered be together.*

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1. Define and elaborate on the following topics. Add necessary diagram/algorithm/software whenever is required.

(a) Role of phi (Φ) and psi (Ψ) angles in protein backbone
(b) SCOP class
(c) Protein design problem
(d) Bound and unbound docking

Marks: 4+4+4+3=15

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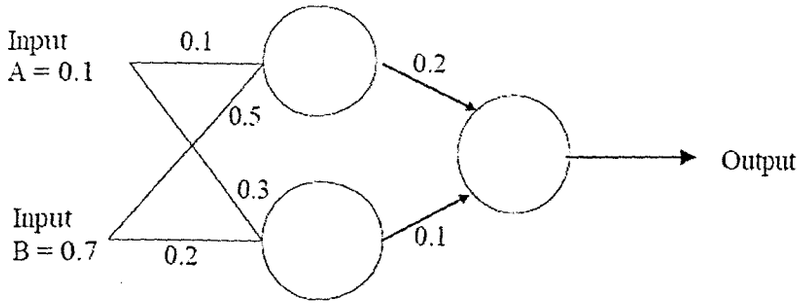
2. Assume that the neurons have a Sigmoid activation function

(a) Perform a forward pass on the network
(b) Perform a reverse pass (training) once (target=1, Learning rate=1)



Marks: 6+9=15

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3. (a) How do you measure the goodness of a protein folding problem when the target/native structure is known to you? Write down the steps.

(b) Modify your above-mentioned steps to measure the goodness of a protein docking program when the complex structure is known.

Marks: 5+5=10

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4. (a) Define the surface and interface of a protein by rolling probe method
   (b) Compare rolling probe based method and grid-based method in connection with computing protein contact region.
   (c) Write down the algorithm/pseudo code of a fast Fourier transform based protein docking method that utilizes grid-based protein contact area computation as a score function. What will be the computational complexity of this method?

Marks: (3+3)+4+(8+2)=20

5. (a) State the Monte-Carlo (MC) algorithm in connection with protein folding.

   (b) Illustrate the lacuna with the help of protein energy landscape. Draw the energy landscape and explain.

   (c) Suggest all kinds of modifications (in pseudo-code format) to overcome the above-mentioned lacuna and suitably modify your MC algorithm.

Marks: 8+4+(4+4)=20