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Date:

CSX4176: *Bioinformatics*

L-T-P-Cr: 2-0-2-3

Pre-requisites: Fundamental knowledge of algorithms, prior completion of “Machine Learning” course is preferred.

Objectives:

- To understand common biology concepts in Bioinformatics.
- To learn common approaches for sequence analysis.
- To learn common techniques in phylogenetic analysis.
- To learn common approaches for analysing protein interaction data.

Course Outcomes

By the end of this course, students will be able to:

Sl. No.	Course Outcome (CO)	Program Outcome (PO)
1	Explain the fundamental concepts of molecular biology relevant to bioinformatics, including the central dogma and the structure and function of DNA, RNA, and proteins.	PO1, PO2
2	Analyze biological data formats like FASTA and PDB and apply sequence alignment techniques (local and global) using algorithms like Smith-Waterman and Needleman-Wunsch. Additionally, utilize tools like BLAST for sequence similarity searches.	PO1, PO2, PO5
3	Apply multiple sequence alignment methods and interpret the results to identify conserved motifs and domains within protein sequences.	PO2, PO4
4	Implement feature-based approaches like Bag-of-Words and Tf-Idf for analyzing biological sequences and utilize these techniques for tasks like protein function prediction.	PO2, PO3, PO5
5	Construct phylogenetic trees using distance matrix and character-based methods (UPGMA, NJ, Parsimony) and evaluate the robustness of these trees using bootstrapping and jackknifing techniques.	PO2, PO4, PO5
6	Analyze protein-protein interaction networks and apply computational methods for predicting protein interactions and protein-protein interaction sites using machine learning techniques like decision trees and support vector machines (SVMs).	PO2, PO3, PO5

7	Integrate knowledge from various bioinformatics techniques (sequence analysis, phylogenetics, protein interaction networks) to address biological problems.	PO2, PO3, PO11
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UNIT I: Biology in Bioinformatics

Lectures: 08

Importance of Bioinformatics; Central Dogma of Molecular Biology; DNA, Transcription, RNA, Translation, Protein; Coding and non-coding portions of gene: Exons and Introns. Biological data types, some important biological databases: NCBI, GenBank, DDBJ, EMBL, Swiss-Prot, RCSB-PDB.

UNIT II: Sequence analysis

Lectures: 16

- A) Representing sequences in Computer: Sequence file formats: FASTA and PDB formats.
- B) Sequence alignment methods, local and global alignment, Dynamic programming based approaches: Smith-Waterman algorithm, Needleman-Wunsch Algorithm, Details of BLAST, Multiple Sequence Alignment: methods, tools, and techniques.
- C) Motifs/Domain Analysis: Introduction. Subsequence Analysis Algorithms: Gibbs Algorithm, Expectation Maximization Algorithm, Kernel Methods.
- D) Feature Based Approaches: Bag-of-words model, Tf-Idf.
- E) Case Study: Protein function prediction based on protein sequences

UNIT III: Computational Phylogenetics

Lectures:14

- A) Concept of trees- Computer representation of phylogenetic trees, Popular tree formats.
- B) Deriving trees: Distance matrix methods, Character based methods. Solving UPGMA, NJ and small parsimony problems.
- C) Evaluating phylogenetic Analysis methods: Boot-Strapping, jack-knifing. Phylogenetic consensus methods: MRT, Strict consensus.

UNIT IV: Protein Interaction Network

Lectures: 10

- A) Introduction: Importance of Protein Interaction Networks, Existing approaches for predicting protein function from protein interaction network: Neighbourhood- based Approach, Global Optimization Based Approaches, Clustering-Based Approach, Association Analysis Based Approach.
- B) Computational Methods for Prediction of protein-protein interaction site: Machine learning based techniques using – Decision trees, Support Vector Machines (SVM)

Text/Reference Books

1. Bioinformatics: A Primer - P. Narayanan
2. Bioinformatics: Sequence and Genome Analysis - D. W. Mount
3. An introduction to bioinformatics algorithms - Neil C. Jones, Pavel A. Pevzner
4. Protein-Protein Interactions: Computational and Experimental Tools - Weibo Cai & Hao Hong
5. Molecular Biology of the Gene – J. D. Watson
6. Bioinformatics: The Machine Learning Approach – Pierre Baldi
7. Pandey, Gaurav, Vipin Kumar, and Michael Steinbach. "Computational approaches for protein function prediction: A survey." Twin Cities: Department of Computer Science and Engineering, University of Minnesota (2006).
8. Immunological Bioinformatics: Ole Lund, Morten Nielsen, Soren Brunak, Claus Lundegaard, Can Kesmir, MIT Press, 2005

