



Lahore University of Management Sciences
BIO 331/CS 330 – Computational Biology II
Fall 2023

Instructor	Dr. Safee Ullah Chaudhary
Room No.	9-314
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Secretary/TA	Maham Hamid and Zainab Nasir
TA Office Hours	TBA
Course URL (if any)	

Course Basics				
Credit Hours	3			
Lecture(s)	Nbr of Lec(s) Per Week	2	Duration	1 hr 15 mins
Recitation (per week)	Nbr of Rec (s) Per Week		Duration	
Lab (if any) per week	Nbr of Session(s) Per Week		Duration	
Tutorial (per week)	Nbr of Tut(s) Per Week	1	Duration	1 hr 15 mins

Course Distribution	
Core	Yes
Elective	
Open for Student Category	Any
Closed for Student Category	

COURSE DESCRIPTION	
<p>The primary focus of the course is to understand theoretical foundation of some of the most widely used computational biology techniques. The principles and methods for pair-wise and multiple sequence analysis using hidden Markov models, phylogenetic analysis, protein sequence analysis and structure prediction are extensively covered. In addition, systems biology is introduced at a glance with a significant amount of time spent on network analysis. The tutorials will provide hands-on training of programming in MATLAB with the aim of developing problem-solving skills in computational biology research using scripting languages.</p>	

COURSE PREREQUISITE(S)	
<ul style="list-style-type: none">••	BIO 231 or CS 232 MATH 230

COURSE OBJECTIVES	
<ul style="list-style-type: none">•••	To understand theory behind of some of the most widely used computational biology techniques. To provide in depth knowledge of sequence and evolutionary analyses. To provide hands-on training of programming in MATLAB for computational biology.

Learning Outcomes	
<ul style="list-style-type: none">•••	After the course, the student should: Understand the inner working of some of the most widely used computational biology techniques. Be able to apply the techniques to biological data. Be able to solve moderate complexity problems related to bioinformatics using MATLAB and R.



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Grading Breakup and Policy

Assignment(s): 20% (4 in total)
 Quiz(s): 16% (4 in total)
 Attendance: 4%
 Midterm Examination: 30%
 Final Examination: 30%

Examination Detail

Midterm Exam	Yes/No: Yes Combine Separate: Combine Duration: 2-3 hrs Preferred Date: Exam Specifications:
Final Exam	Yes/No: Yes Combine Separate: Combine Duration: 2-3 hrs Exam Specifications:

COURSE OVERVIEW

No.	Topic	Key Dates	Objectives/ Application
1	Introduction to Course, Introduction to Sequence Proteomics		
2	Protein Sequence Analysis		
3	Techniques for Sequencing Protein		
4	Protein Sequence Search Engines	A1(out)	
5	Scoring Schemes for Protein Searching		
6	Protein and PTM Databases		
7	a. Protein Search Engines b. SPECTRUM/PERCEPTOR Demo	Q1	
8	a. Introduction to Structural Proteomics b. Protein Secondary Structure Prediction	A1(in), A2(out)	
9	X-ray Crystallography & NMR		
10	Homology Modeling I		
11	Homology Modeling II		
12	Threading (Fold Recognition)		
13	Ab initio Structure Prediction	Q1, A2(in)	
14	Advanced Techniques		

Mid Term

Module 3: Advanced Sequence Analysis, Alignment & Phylogenetics

15	Markov Chains - Calculating Sequence Probabilities	A3(out)	
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16	Introduction to Hidden Markov Models		
17	Calculating Sequence Probabilities - Forward Algorithm		
18	Identifying the Most Probable State Path - Backward Algorithm		
19	Generating complicated sequences using HMM		
20	Global Alignment using Pair HMM		
21	Optimal Alignment and Alignment Probabilities for Pair HMMs		
22	Local Alignments and Sub-optimal Alignments Profile HMMs for Sequence Families		
23	Models of Sequence Evolution - JC69 & K2P Estimating the Number of Substitutions between DNA Sequences	Q3, A3(in)	
Network Biology			
24	Biomolecular Networks		
25	Boolean Modeling		
26	Boolean Modeling		
27	Dynamical Analysis		
28	Interpreting Outcomes	Q4, A4(in)	
Final			

Textbook(s)/Supplementary Readings
<ul style="list-style-type: none"> • Computational Methods for Mass Spectrometry Proteomics by Ingvar Eidhammer • Bioinformatics Sequence Analysis by David Mount • Bioinformatics and Functional Genomics by Pevzner • Biological Sequence Analysis. Probabilistic Models of Proteins and Nucleic Acids, Richard Durbin, Sean R. Eddy, Anders Krogh, Graeme Mitchison. Cambridge University Press, 1998. • Inferring Phylogenies, 2nd Edition, Joseph Felsenstein. Sinauer Associates, 2003. • Introduction to Computational Biology. An Evolutionary Approach. Bernhard Haubold, Thomas Wiehe. Birkhauser, Verlag 2006. • Handouts