



Birla Institute of Technology and Science, Pilani

Hyderabad Campus

FIRST SEMESTER 2020-2021

Course Handout (Part II)

Date: 28.10.2020

In addition to part I (General Handout for all courses appended to the timetable) this portion gives further specific details regarding the course.

Course No.: BIO G532
Course Title: Biostatistics and Biomodelling
Instructor-in-Charge: NAGA MOHAN
Co-Instructors: Debashree Bandyopadhyay
Purbali Chakraborty

1. Course Description:

Probability analysis variables in biology; standard deviation and standard errors; correlation and correlation coefficient; regression analysis; significance test; chi-square and goodness of fit; applications of computers in statistics; handling of software on enzyme kinetics and protein sequence analysis; computer analysis of nucleic acid structure..

Scope and Objectives of the Course: The student would learn how to collect data suitable for statistical analyses, understand the general features of the data collected, making statistical inferences and likelihood of occurrence of an event using probability calculations and tests of significance. The course is designed to provide students the first hand experience of potential utility of biomolecular modeling especially in structure-function elucidation, and in cellular and structural biology. It describes the functionality, advantages, and limitations of standard computing strategies for the simulation of biomolecules. Provide a working knowledge of freely available software to carry out independent research projects in biomolecular modeling. Explore the possibilities of modeling to complement 3D structure determination, analysis, evaluation and data retrieval in a research or industry based laboratory.

2.

3. Textbooks:

1. Introduction to Biostatistics and Research Methods. P.S.S. Sundar Rao and J. Richard, Fifth edition, PHI Learning Private Limited. 2018.
2. Biostatistics: A foundation for Analysis in the Health Sciences. Wayne Daniel, Seventh Edition, Wiley-India Edition, 2005.
3. "Molecular modeling: Principles and Applications" By Andrew R Leach, 2nd Edition, 2001, Pearson Education Lim.

Reference Books:

1. Principles of Biostatistics, M. Pagano and K. Gauvereau, Thomson Learning Publ., Indian Ed., 2007.
2. "Molecular Modeling and Simulation - An Interdisciplinary Guide" By Tamar Schlick, Springer, New York, 2002.
3. "Principles of protein structure" By Schulz, G.E. and Schirmer, R.H., NewYork, Springer-Verlag, 1979.



4. Lecture Plan:

Lecture No.	Learning Objectives	Topics to be covered	Book (Sec/Chap)
1-2	Introduction	What is modeling? Scope and application of modeling in modern biology	R-1 (1-2)
3	System Biology and modeling of organs	Brief overview of system biology and organ modeling	Class notes
4-5	Protein structure and conformation	Protein structural hierarchy, Structural motifs, classification	R-1 (3-4)
6	Molecular graphics, Visualization and modeling packages	Introduction to graphic representation, Representation of molecular structure: macromolecules Database of macromolecular structures, Usages of freely available visualization packages like VMD, Rasmol, Pymol, SpdbViewer , Chimera, Cn3D	R-3 (4), Class-notes/websites
7-8	Protein sequence analysis	Description and usage of protein sequence analysis	Class notes
9-10	Protein structure prediction	First principle methods for predicting protein structure, comparative modeling, threading, CASP	T(10) R-4 (8-9)
10-11	Advanced homology modelling	Refined structure modeling by incorporation of experimentally derived spatial restraints	User guide to MODELLE R
12-13	Nucleic Acid Structure and analysis	Nucleic acid structure description and software used to analyze the structures	Class notes
14-17	Quantum chemical approaches to solve biological problems	Basic quantum mechanics, H-F approximation, Basis set, application of quantum chemistry in Biological systems	T(2-3)
18-19	Forcefield and Molecular Mechanics	Forcefields in understanding protein structures (salt bridge, long range interactions etc.)	T (4)
20-21	Molecular dynamics	Basic and Advanced MD simulation techniques, simulated annealing, parallel tempering	T (6-7), class notes
22-24	Introduction to statistical analyses in biology	How statistical analyses are used in different facets of biology?	TB1 (1-3)
25-28	Descriptive statistics: Understanding the general features of the data collected for a study	Variables, Collection of data (sampling) and representation of variables, Measures of Central Tendency and Location, Measures of Dispersion	TB1 (4-7)
29-32	Probability: Estimating the likelihood of occurrence of an event	Understanding probability of occurrence of an event, Probability distributions.	TB1 (8-9)
33-34	Statistical Inference – I: Understanding the basis	Type I and Type II errors, Tests of Significance and Estimation	TB1 (11)



	that the observed results are not real		
35-38	Statistical Inference – II: Estimating whether the obtained results conform to the null hypothesis	Chi-Square test, Analysis of Variance, Non-parametric or Distribution-free statistical tests	TB1 (12-16)
39-42	Understanding Excel's statistical capabilities	Statistical analysis of descriptive data, drawing conclusions from data, modeling distributions, writing Macros for performing statistical tests	

5. Experiments:

1. Solving problems in statistics.
2. Computer experiments for Biomolecular Modeling

6. Evaluation Scheme:

Component	Duration	Marks	%	Date and Time	Venue	Remarks
Mid-Sem	90 min	60	30	31/12 9.00 - 10.30AM 31/12 9.00 - 10.30AM	TBA	OB
Laboratory Evaluation	-	40	20	Announced	-	OB
Take home	-	40	20	Announced	-	OB
Comprehensive exam	120 min	60	30	24/02 FN	TBA	OB
Total		200	100			

7. Attendance Policy:

It is expected that the student attends every laboratory session and theory class. Individual students may be assigned specific tasks to be done before or during the lab hours, the completion of which may be required for the entire class group. If failure to complete the task due to absence is anticipated, it is the student's responsibility to inform the instructor.

8. Grading Policy:

Award of grades would be guided in general by the histogram of marks. Decision for borderline cases would be based on the individual's sincerity, attendance in classes and the instructor's assessment of the student's capability.

9. Office Consultation Hour: To be Announced

10. Make-up Policy:

Clause 4.07 of BITS *Academic Regulations* booklet should be consulted. Make-up can be requested only on health grounds and emergency reasons.

11. Notices:

All course announcements shall be displayed in CMS only.



12. Academic Honesty and Integrity Policy:

Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

INSTRUCTOR-IN-CHARGE
BIO G532

