Birla Institute of Technology and Science, Pilani
Hyderabad Campus

SECOND SEMESTER -2021-2022

Course Handout (Part II)

Date: 11.01.2022

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:	Ramakrishna Vadrevu
Co-Instructors:	Sridev Mohapatra
	I.Shivkumar, Nikhil P.T, Vartika Singh

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.

   Biomodelling describes the functionality, advantages, and limitations of standard computing strategies for the simulation of biomolecules. Biomolecular Conformation, Protein folding, Forecefield, simulation, Conformational analysis, abinitio structure, prediction, comparative modeling, lattice models, usage of modelling packages. Biostatistics describes how statistics is used to analyze biological data and answer questions in quantitative biology. Topics include Probability analysis, Variables in biology, Standard deviation and standard errors; correlation and correlation coefficient; regression analysis; significance test; chisquare and goodness of fit.

2. **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.

3. **Textbooks:**

   1. Molecular modeling: Principles and Applications" By Andrew R Leach, 2nd Edition, 2001, Pearson Education Lim.
   2. Biostatistics: A foundation for Analysis in the Health Sciences. Wayne Daniel, Seventh Edition, Wiley-India Edition, 2005.

   Reference Books:

   1. "Molecular Modeling and Simulation - An Interdisciplinary Guide" By Tamar Schlick, Springer, New York, 2002
   2. "Introduction to Proteins" Amit Kessel & Nir Ben-Tal, CRC Press (Taylor & Francis Group)
   3. Introduction to Biostatistics and Research Methods. P.S.S. Sundar Rao and J. Richard, Fifth edition, PHI Learning Private Limited. 2018.

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)
3-6	Biomolecular structure and conformation	Protein structural hierarchy, Structural motifs, classification, Nucleic acids conformation	R-1 (3-5)
7	Molecular graphics	Introduction to graphic representation, Representation of molecular structure: macromolecules Database of macromolecular structures	Class notes/Databases website(s)
6	Visualization and modeling packages	Usages of freely available visualization packages like VMD, Rasmol, Pymol	Class-notes/ websites
7-10	Protein structure prediction	First principle methods for predicting protein structure, homology/comparative modeling, threading.	TB1(10) R-1(8-9)
11-12	Advanced homology modelling	Refined structure modeling	User guide to MODELLER
13-15	Quantum chemical approaches to solve biological problems	Basic quantum mechanics, H-F approximation, Basis set, application of quantum chemistry in Biological systems	TB1 (2-3)
16-18	Forcefield and Molecular Mechanics	Forcefields in understanding protein structures (salt bridge, long range interactions etc.)	TB1 (4)
18-20	Molecular dynamics	MD simulation techniques, simulated annealing	TB1 (6-7), class notes
21-22	Introduction to statistical analyses in biology	How statistical analyses are used in different facets of biology?	TB2 (1)
23-26	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	TB2 (2)
27-30	Probability: Estimating the likelihood of occurrence of an event	Understanding probability of occurrence of an event, Probability distributions.	TB2 (3-4)
31-34	Statistical Inference – I: Understanding statistical significance	Sampling Distributions, Estimation, Tests of Significance (Hypothesis Testing)	TB2 (5-7)
35-40	Statistical Inference – II: Estimating whether the obtained results conform to the null	Chi-Square test, Analysis of Variance, Non-parametric or Distribution-free statistical tests	TB2 (8,12)

	hypothesis		

5. Experiments:

1. Understanding Excel's statistical capabilities: Statistical analysis of descriptive data, drawing conclusions from data, modeling distributions, writing Macros for performing statistical tests
2. Computer experiments (Modeller/Gromacs,NAMD) for Biomolecular Modeling

6. Evaluation Scheme:

Component	Duration	Marks	%	Date and Time	Venue	Remarks
Mid-Sem	90 min	50	25	As per Timetable		Closed book
Laboratory Evaluation	-	30	15		-	Open book
Take home/in-class Assignment/Quiz	-	40	20		-	Open book
Comprehensive exam	120 min	80	40	As per Timetable		Partly Open book (50%)
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


innovate
achieve
lead