School of Computational & Integrative Sciences, JNU

[PH.D IN COMPUTATIONAL BIOLOGY AND BIOINFORMATICS / COMPLEX SYSTEMS](https://jnu.ac.in/scis-program-study#superhero_tab_content_3)

Syllabus (All Courses)

IT-422 **Research Methodology**

**Course Code**: IT422

**Credits**: 3 (42 h)

**Course offered to**: Ph.D. and M.Sc.- 3rd Semester

**Objective:** To make the students understand the foundation and concept of interdisciplinary research, research design and methodology, teach how to plan experiment, draw conclusions from results, judge reliability and validity of experiments, provide knowledge appropriate format for research articles, manuscript editing and presentation skills, to use tools for reference management and check for plagiarism.

**Course content**:

1. Introduction to research methodology: meaning, objective and motivation in interdisciplinary research area; simple research rules for graduate students, computational biologists
2. Research project selection and design: problem identification and hypothesis testing, experiment design, feasibility, method selection, sampling and variables
3. Scientific literature: Search, reading and interpretation of relevant articles
4. How to make a good and effective presentation
5. Writing and presentation of research proposal: Basic components and ethical concerns (human/animal and biosafety).
6. Report/Manuscript writing and presentation: format for research articles and reviews, language editing, reference management, plagiarism, scientific presentation tips and citing relevant scientific literature
7. Reference management: Collection and management of references; formatting styles; reference managers (Mendeley, Endnote etc.)
8. Scientific publishing: Journal selection; formatting; plagiarism; figure/table composition, reviewing, addressing reviewer comments
9. Importance of research collaborations and networking; research start-up and/or commercialization
10. Basic methods for quantitative data analysis: Basic statistical tools; data visualization methods (graphs, histograms, heat maps etc.); Data normalization and scaling; Tests for significance analysis (P-value, ANOVA etc.); Univariate and bivariate analysis; Machine learning methods for model development; Principal component analysis etc.

**Suggested readings:**

1. ROIG (M). Avoiding plagiarism, self-plagiarism, and other questionable writing practices: A guide to ethical writing (2006)
2. VAUGHAN (L). Statistical methods for the information professional: A practical, painless approach to understanding, using and interpreting statistics (Ed. 2), (2004) Information Today, Medord.
3. Kothari C.K. (2004) 2/e, Research Methodology – Methods and Techniques (New Age International, New Delhi)
4. Mathews. “Successful scientific writing: A step-by-step guide for Biomedical Scientists”, Second edition, Cambridge University Press, 2001.
5. Research Methodology and Scientific Writing by C. George Thomas (2016) Ane Books Publisher
6. RETHINKING PHDS, BY ALISON MCCOOK, 280 | NATURE | VOL 472 | 21 APRIL 2011
7. Estimating the reproducibility of psychological science, Open Science Collaboration, Science, 28 AUGUST 2015 • VOL 349 ISSUE 6251
8. Scientific Writing Made Easy: A Step-by-Step Guide to Undergraduate Writing in the Biological Sciences, Turbek et al 2016 published in Bulletin Ecological society of America
9. 1,500 scientists lift the lid on reproducibility by Monya Baker (2016) NATURE VOL 533, 452-454
10. Ten Simple Rules for Reproducible Computational Research (2013) Sandve et al PLOS Computational Biology Vol 9, Issue 10, e1003285

**IT-719 - Course Title: Research and Publication Ethics (RPE)**

**Credits:** 2 Credits (30 h)

**Course offered to:** Ph.D. students of SCIS

**Objective:** Course for awareness about the publication ethics and publication misconducts. This course is focused on basics of philosophy of science and ethics, research integrity, publication ethics. Hands-on-sessions are designed to identify research misconduct and predatory publications. Indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor, etc.) and plagiarism tools will be introduced in this course.

**Course content:**

PHILOSOPHY AND ETHICS: Introduction to philosophy: definition, nature and concept, branches; Ethics: definition, moral philosophy, nature of moral judgments and reactions

SCIENTIFIC CONDUCT: Ethics with respect to science and research; Intellectual honesty and research integrity; Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP), Consequences of scientific misconducts, measure to maintain research ethics and avoid scientific misconducts; Redundant publications: duplicate/overlapping publication and simultaneous submission, salami slicing; Selective reporting and misrepresentation of data (methods and/or results)

PUBLICATION ETHICS: Publication ethics: definition, introduction, and importance; Best practices/standards setting initiatives and guidelines: Committee on Publication Ethics (COPE), World Association of Medical Editors (WAME), International Committee of Medical Journal Editors (ICMJE); Conflicts of interest; Publication misconduct: definition, concept, problem that lead to unethical behaviour and vice versa, types; Violation of publication misconduct, complaints and appeals; Predatory publishers and journals

OPEN ACCESS PUBLISHING: Open access publications and initiatives (Introduction, open access vs subscription journals, advantages); Broader impact of open access publications, Compliance with funding mandates, Open access resources for researchers and students; SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies; Software tool to identify predatory publication developed by SPPU; Journal finder / journal suggestion tools viz, JANE. Elsevier Journal Finder, Springer Journal Suggester, etc.

PUBLICATION MISCONDUCT: FFP; Scientists Fabricate and Falsify Research, Subject specific ethical issues, authorship; Conflicts of interest; Complaints and appeals: example and fraud from India and abroad; Retraction; Use of plagiarism software like Turnitin, Urkund and other open source software tools.

DATABASES AND RESEARCH METRICS: Indexing databases; Citation databases: Web of Science, Scopus, MEDLINE; General and discipline-specific scholarly indexing data bases; Research Metrics: Need of Research Metrics system, Impact factor of journal as per JCR, SNIP, SJR, IPP, Cite Score); Metrics: h-index, g-index, i10 index, altmetrics.

**Suggested readings:**

Bird, A. (2006). Philosophy of Science. Routledge.

MacIntyre, Alasdair (1967) A history of ethics. London.

P. Chaddah, (2018) Ethics in competitive research: Do not get scooped; do not get plagiarized, ISBN: 978-9387480865

Gross, C. (2016). Scientific Misconduct. Annual Review of Psychology, 67(1), 693–711. doi:10.1146/annurev-psych-122414-033437.

Committee on Publication Ethics (COPE). (2009). COPE code of conduct. http://publicationethics.org/code-conduct.

Steen, R. G., Casadevall, A., & Fang, F. C. (2013). Why Has the Number of Scientific Retractions Increased? PLoS ONE, 8(7), e68397.

Wang, X., Liu, C., Mao, W. & Fang, Z. (2015). “The Open Access Advantage Considering Citation, Article Usage and Social Media Attention.” Scientometrics 103 (2): 555–64.

Garfield, E. (2010). The evolution of Science Citation Index, International microbiology, 10(1), 65-69.

**IT-763 : Advanced Computational Methods for Optimizations (ACMO)**

Credits 3

**Course offered to**: M,Sc./Ph.D. (Common for CS-Track & CB-Track)

**Course Description**: The development of fast, efficient and in computers has significantly increased the range of complex problems specially biological/complex networks that can be solved reliably. Computational techniques use computers to solve problems by step-wise, repetitive and iterative solution methods, which would otherwise be tedious or unsolvable by hand calculations. This course is designed to give an over of computational methods of interest to model biological network for optimal solution(). A part will be class room teaching and other part will be working exercise with project assigned to the students along with the demonstrations of some mathematical software(s) for problem solving (if the software is available).

**Pre-requisites**: Must complete the semester one and at least credited the course on Computational Biology and Bioinformatics. A part will be classroom teaching and other part will be working exercise (assignments/practicals) with project assigned to the students.

**Course Outcomes) (CO):** Upon finishing the course, the student is expected to be able to:

1. Knowledge of errors analysis in computation problems.
2. Knowledge of solving system of linear equations by various mathematical methods.
3. To find the optimal solutions of complex/wide networks problems.

4, This paper helps to understand various decision making optimization techniques such as game theory, AHP, etc.

**Tentative plan**:

|  |  |  |
| --- | --- | --- |
| Week number | Lecture topic | CO met |
| (1s-)2 | Introduction : Motivation and applications.  Computation and Error Analysis: Accuracy and precision; Truncation and round-off errors; Binary Number System; Error propagation. | CO 1 |
| 3-5 | Linear Systems and Equations: Matrix representation; Cramer's rule; Gauss Elimination; Matrix Inversion; LL: Decomposition; Iterative Methods; Relaxation Methods; Eigen Values. | CO 2 |
| 6-8 | Optimization - Introduction, Formulation of LPP , Geometry of LPP and Graphical Solution of LPP, Solution of LPP : Simplex Method,  Big-M Method, Two-Phase Method, Special Cases in Simple  Applications | CO 3 |
| 9-10 | Introduction to Duality Theory, Dual Simplex Method, Post Optimallity Analysis | CO 4 |
| 11-12 | Introduction to TYansportation Problems *&* Assignment Problems Solving Various types of 'flansportation Problems and Assignment Problems | CO 5 |
| 12-14 | Analytic Hierarchy Process, Multi Objective Decision Making,Game  Theory (Introduction) | CO 6 |

**Note:** To encourage and motivate the students, topic related to further studies can be included/change in the syllabus to maintain the quality of research,

**Some Text Books and References:**

1. Gupta S. K. (1995) Numerical Methods for Engineers, New Age International.
2. Chapra S. C. aid Canale RR (2006) Numerical Methods for Engineers, 5th Ed;

McGraw Hill

3, I, A. Taha, Operations Research: An Introduction, 8th Edition, Prentice Hall, 2006, 4. 0, Hadley, Linear Programming, Narosa. 1987 (2002 reprint available).

1. F.S. Hillier SzO.J. Lieberm, An: Into Operations Research Concepts and Cases, 9th

Edition, to M cG raw Hill. 2010,

1. R.E. Sty per, Multiple Criteria. Optimization; Theory, Computation and Application, John Wiley, New York, 1986.

7, Ravindran A., Phillips, D.T,, Solberg J.J.,, - Operations Research: Principles and Practice, 2nd ed.,2001, John Wiley k Sons,

1. Related articles from journals
2. Hyperlinks: en.wikipedia.org/wiki/Operations Research

**IT-764: Stochastic Simulations in Biological Physics (SSBP)**

**Pre-requisites:**

Must complete the semester one and at least credited the course on "Computational Biology & Bioinformatics".

Objective: This course will introduce students to stochastic simulation techniques as used in solving biological problems. Theory of stochastic processes will be briefly discussed along with the example of random walk problem. The basis of stochastic simulations will be rigorously elucidated using the method of master equations. This course will emphasize kinetic Monte Carlo simulations that are able to capture dynamical aspects, complex details in biological problems (such as spatial heterogeneity) and fluctuation effects. We plan to discuss stochastic modeling of important cellular (as mediated by gene regulatory networks and signal transduction networks) and immunological processes.

**Syllabus:**

1. Stochastic modeling approach to solve problems of biological and biomedical relevance (broad overview) (3+1 hours)
2. Introduction to stochastic processes Chapman-Kolmogorov formalism; Master equation (equations defined in probability space); Continuum limit and Fokker-Planck equation; Langevin equation (fast and slow time scales). Master equations for random walk problem and chemical kinetics Monte Carlo method to obtain solution of master equations (9+3 hours)
3. Stochastic simulation of the random walk problem (Statistical analysis of simulation data obtained from many parallel runs) Parallel computation based on task dependency. Kinetic Monte Carlo simulations, Metropolis Algorithm, rejection free algorithms (Gillespie's SSA) (9+3 hours)
4. Some basics of statistical mechanics, concept of ensembles, MC simulation in canonical ensemble, detailed balance in MC moves Kinetic Monte Carlo simulation that captures biological dynamics as well as spatial heterogeneity (simulation of receptor ligand binding and clustering); Langevin (Brownian) dynamics approach (9+3 hours)
5. Brief discussion of relevant biological applications and experiments. Kinetic Monte Carlo based in silico studies as a tool for mechanistic data analysis for biological / clinical data (such as NGS data): integration of big data with mechanistic models. Stochastic Modeling of Ligand-Receptor Binding process — applications to various two state biological problems. Research Projects. (12+4 hours)

**Suggested readings:**

Software: Programming and data analysis will be done in MATLAB or C/C++ **Texts:**

1. Stochastic Methods: A Handbook for the Natural and Social Sciences by C W Gardiner

(Springer)

1. Theory and Applications of Monte Carlo simulations ed. By Victor Chan (InTech).
2. **References:**
3. Monte Carlo Simulations in Statistical Physics by K Binder and DW Heermann (Springer).
4. Understanding Molecular Simulation by D Frenkel and B Smit (Elsevier)
5. Essential Cell Biology by B Alberts, 13 Bray, K Hopkin, AD Johnson, J Lewis, M Raff, K Roberts, P Walter (Garland Science)

**IT-765 : Computational Biophysics**Credit 3

The objective of the course is to introduce the subject of Computational Biophysics using theoretical & computational methods to explain and unfold basic topics like physicochemical properties of macromolecules, primary organization of interactive macromolecules , structure function relationship evolving different cellular functions and growing towards the thermodynamics of cell. A part will be classroom teaching and other part will be working exercise with project assigned to the participants.

**Prerequisites and Restrictions:**

Must complete the semester oneand at least credited the course on "Computational Biology &

Bioinformatics". Strong in Mathematics & Programing/Matlab/Python

Physical & chemical aspects in Biological systems at each level like, cellular, tissue organization, construction of parts & physiology of living system, Hierarchy in living system. Information ,. construction & Function ,a

self assemble system. (5)

Structure of Biomolecules, heterogeneous, disorderd & glass like molecules , Flexibility, plasticity and functional deformations , assembly in different levels , Protein ,DNA ,lipid & carbohydrate and how to

understand these phenomena theoretically using different models. (10)

Interaction & modeling of different macro & small molecules , tools for learning macro modeling some of the important biological systems like , single molecule dynamics to Biochemical pathway dynamics, role of noise in fluctuation and biochemical reactions, proof reading & noise reduction in genetic systems. (10)

Sequence ensembles , Designing structures from sequence for function in proteins, membranes & DNA/RNA . States of cell , long duration in neural network and ion chaqnnels, neuronal dynamics. (10)

Entropy vs. Information flow, Optimization of Information, Gathering information and modeling different biological functions like Genetic switch , Chemotactic , Control of metabolism, Signalling systems etc. (10)

Teaching will be interactive and through project work & journal papers.

**Books to follow:**

**Frauenfleder,** *Physics of Proteins*

**Bialek,** *Biophysics: Searching for Principles*

**Phillips,** *Physical Biology of the cell*

**1T-766 Genomics : Concepts, Methods and Applications (GCMA)**

3 Credits

**Examination: Mid-Sem (10 assignments + 40) & Final (10 assignments+ 40)**

**Pre-requisites:** Must complete the 1st semester and at least credited the course on "Computational Biology & Bioinformatics". Must have basic knowledge of Molecular Biology and Recombinant DNA Technology.

**Objective:** This course is an integrated presentation of genome organization, genome sequencing and characterization, comparative genomics, transcriptomics and introductory genomic data analysis. The course objective is to instil sufficient knowledge to the students to be conversant in all of the areas of genomics and provide a knowledge base that enables the student to successfully move on and master advanced topics in genomics. On the whole, the course will enhance the students' overall comprehension of the subject, improve their computational skills and eventually assist in proper planning, execution and analysis of their research work.

**Course content:**

**Next Generation Sequencing Technologies:** Methods and applications (4)

**Whole Genome Sequencing and Analysis:** Concept, methods, assembly (de novo and reference based), genome annotation (structural and functional), comparative genomics (10)

**High-throughput Transcriptome Profiling:** Concept, methods and applications; transcriptome construction (de novo and reference-based), differential gene expression (10)

**Non-coding RNAs:** Small RNAs, miRNAs, long non-coding RNAs; sequencing and prediction methods; biological relevance (10)

**Single nucleotide polymorphisms:** Genome resequencing; data processing and SNP prediction; applications in agriculture/human health (6)

**Suggested readings:**

1. Review and research articles in national and international journals 2. Online webpages/videos of various databases and sequencing platforms.

1. Principles of genome analysis and genomics - Sandy B. Primrose, Richard M. Twyman
2. Introduction to Bioinformatics: A theoretical and practical approach - Stephen A. Krawetz, David D. Wonmble
3. Fundamentals of data mining in genomics and proteomics - Werner Dubitzky, Martin Granzow, Daniel Berrar
4. A primer of genome science - Greg Gibson, Spencer V. Muse
5. Metzker ML (2010) Sequencing Technologies—The Next Generation. Nature Reviews Genetics 11: 31 PMID: 19997069
6. Mardis ER. (2008) Next-generation DNA sequencing methods. Annu Rev Genomics Hum Genet. 2008;9:387-402.

I T— 770 **Neural networks and deep learning for biological data**

**Pre-requisites**: Students opting for this course must be familiar with basics of machine learning

and artificial intelligence.

**Objective**: This course is aimed at introducing cutting edge artificial neural network techniques

applied to biological problems. Different types of neural networks, their training and validation

strategies and limitations will be discussed. Specific examples from published literature such

sequence specificity predictions will be taken up.

**Syllabus**:

* Background of machine learning methods: Regression and classification (2 hrs)
* Overview of discretization and data representation techniques (3 hrs)
* Introduction to neural networks architecture and training methods: Multilayer perceptron

backpropagation, quick propagation and other learning methods. Batch and online training. (5 hrs)

* Neural network applications in Bioinformatics: Secondary structure, solvent accessibility, side chain orientation predictions. Gene ontology predictions. Functional annotation prediction using neura networks and other machine learning methods. (5 hrs)
* Introduction to Time delay neural networks, RBF neural networks. Self organizing maps and

Kohonen learning. (3 hrs)

* Fundamentals of Deep learning strategies. Boltzman machine and auto-encoders. Denoising

autoencoders. Amino acid autoencoder and dimensionality assessment. (4 hrs)

* Inferring nucleic acid sequence specificity and other biological applications of deep learning (2 hrs)

**Suggested readings:**

1. Deep Learning Made Easy with R: A Gentle Introduction for Data Science CreateSpace

Independent Publishing Platform (ISBN-13: 978-1519514219)

1. Predicting the sequence specificities of DNA- and RNA-binding proteins by deep learning,

Alipanahi B, Delong A, Weirauch MT, Frey BJ, Nature Biotechnol. 2015 Aug;33(8):831-8.

doi: 10.1038/nbt.3300.

1. Deep learning for regulatory genomics, Park Y, Kellis M, Nature Biotechnol. 2015

doi: 10.1038/nbt/.3313.

1. Reversible auto-encoding of amino-acid residues in reduced space: an application to

predicting DNA-binding proteins, Shandar Ahmad, Third IAPR International Conference

on Pattern Recognition in Bioinformatics (PRIB) (2008, Melbourne, Australia) Monash

University Research Repositories (http://arrow.monash.edu. au/hdl/1959.1/63725)

1. Dimensionality of amino acid space and solvent accessibility prediction with neural networks,Marcos J. Arafizo-Bravo , Shandar Ahmad, , Akinori Sarai, Computational Biology and Chemistry, 2006, 30, 160—168

IT-771 **Information theory and Molecular biology**

**Pre-requisites:** Students, who successfully completed Pre. PhD. Program in Computational Biology

and Bioinformatics are eligible.

**Objective:** This course aims to introduce information contents in biological molecules, sequence

and surveys technical and biological aspects of information theory.

**Detailed syllabus:**

* Concepts of uncertainty/ information — entropy definition — Shannon entropy Joint entropy and conditional entropy (6 hrs)
* Relative entropy and mutual information (2 hrs)
* Overview of the applications of entropy concepts to communication networks (2 hrs)
* Overview of Markov chain - Hidden Markov models (4 hrs)
* Jansen's inequality - Maximum entropy principles (2 hrs)
* Parametric entropy — Renyi , Tsallis and their relation to Shannon entropy (4hrs)
* Molecular biology — The Genetic code - Central dogma and information flow (2hrs)
* Randomness — complexity — information content (4 hrs)
* Applications of Shannon's entropy to molecular data — Sequence, structure and gene expression ratios (8 hrs)
* Entropic divergence and its application (2)
* Information theory and evolution of living systems (4 hrs)

**References:**

1. Thomas Cover and Joy A Thomas. Elements of Information theory (2nd Edition) Wiley

InterScience 2006.

2. Hubert P Yockey Information theory and Molecular biology. Cambridge University Press .

1992.

3. John Avery Information theory and evolution. World scientific 2003.4. Applebaum. Probability

and Information: An integrated approach. Cambridge 1996.

**IT-772 : Data mining and modeling (DMM)**

**Pre-requisites:** There is no additional pre-requisite for the course, as students having passed Pre Ph.D. semester **I** exam are considered suitable for the course.

**Objective:** This course is aimed at training students in general principles of data mining, specially applied to biological data analysis.

**Syllabus:**

Introduction to Data Mining: Data Mining Techniques, Knowledge Representation Methods, Applications, Examples of sequence, PSSM data in biological systems.

Data pre-processing: Data cleaning transformation and reduction. Discretization and generating concept hierarchies

Attribute-oriented analysis: Attribute generalization, relevance and comparison, Statistical tests for assessment.

Data mining algorithms: Association rules, item sets, Generating item sets and rules efficiently, Correlation analysis. Classification, Basic learning tasks, Inferring rudimentary rules: 1R algorithm, Decision trees, Covering rules. Prediction, Statistical (Bayesian) classification, Bayesian networks, Instance-based methods (nearest neighbour), Linear models. Evaluating models. Estimating classifier accuracy (holdout, cross-validation, leave-one-out). Combining multiple models (bagging, boosting, stacking), Minimum Description Length Principle (MLD). overfitting, regularization

Clustering: Basic issues in clustering, Partitioning methods: k-means, expectation maximization (EM), Hierarchical methods: distance-based agglomerative and divisible clustering

Advanced techniques: Text mining: extracting attributes (keywords), structural approaches (parsing, soft parsing). Bayesian approach to classifying text. Web mining: classifying web pages, extracting knowledge from the web

**Suggested readings:**

1. Ian H. Witten and Eibe Frank, Data Mining: Practical Machine Learning Tools and Techniques (Second Edition), Morgan Kaufmann, 2005, 1SBN:0-12-088407-0
2. Introduction to Information Retrieval, Christopher D. Manning, Prabhakar Raghavan and Hinrich Schtitze, Cambridge University Press. 2008.

Introduction to Data Mining, Pang-Ning Tan, Michael Steinbach and Vipin Kumar, Addison-Wesley, 2006.

**IT- 773: Bimolecular Simulation; Theory and application (BioSimulation)**

**Pre-requisite:** There is no strict pre-requisite but knowledge of mathematics, physics, chemistry up to class 12 is highly desirable.

**Objective**: Totake the students at the fore-front of research in biomolecular simulation start from basics.

**Syllabus:**

* Introduction to computational structural biology (2 hrs)
* Review of protein structure (2 hrs)
* Basic thermodynamics and statistical mechanics (8 hrs) Molecular mechanics (2 hrs)
* Computer simulation (5 hrs)
* Free energy calculations (3 hrs)
* Protein structure prediction(2 hrs)
* Protein-ligand interaction (3 hrs)
* Enzyme catalysis (2 hrs)
* Advanced sampling techniques (3 hrs)
* Illustration using molecular modeling softwares (8 hrs).

**Texts:**

* A, Leach, *Molecular Modeling: Principles and Applications,* 2' edition, Addison-Wesley publications, 2001.
* D. Frenkel and B. Smit, *Understanding Molecular Simulation,* 2" edition , Academic Press, 2001.
* Statistical Physics, F. Reif, Berkeley lecture series (volume 5). McGraw-Hill.

**References:**

- K. A. Dilland S. Bromberg, *Molecular driving forces: Statistical thermodynamics in Chemistry and Biology,* Garland Science, 2003.

**IT-774 : Molecular Technique in Genome Analysis**

**Pre-requisites**: There is no additional pre-requisite for the course, as students having passed Pre Ph.D. semester I exam are considered suitable for the course.

**Objective:** This course aims at covering the experimental techniques, which generate biological data. In particular, genomic-scale data generating techniques are discussed.

**Syllabus:**

Concept of Genome and genome evolution (2 hrs)

Methods in Genome Sequencing (2 hrs)

Detection of point mutations and SNPs (2 hrs)

Analysis of repeat based polymorphism caused by transposable and retrotransposable elements and their detection (4 hrs)

Genome-wide detection of DNA and Chromatin modification (4 hrs)

Detection of genome wide transcription, discovery of small RNAs and promoter elements (8 hrs) Proteomic approaches for expression analysis (6 hrs)

Methods for detection of glycoconjugate in large scale (4 hrs)

Methods used in metabolomics (4 hrs)

**Suggested Readings:**

Concepts and Techniques in Genomics and Proteomics, Saraswathy and Ramalingam (2016) Woodhead Publishing

**IT-776 : Petri nets: Theory and modeling forSystems (DPTMS)**

# Credit: 3 Course offered to: M.Sc./Ph.D. (Common Optional course for CS-Track *&* CB-Track),

**Course description:** The course will introduce the basic concepts of digraphs and discrete dynamical systems for

modelling of complex/biological/bioinformatics networks. The concept of digraph theory and Petri nets theory can be used to develop new algorithms and model a wide variety of systems such as data science, biological networks, computer hardware and software, chemical sciences, social sciences, life sciences, etc.

**Pre-requisites:** Must complete the semester one and atleast credited the course on **'Computational Biology** **& Bioinformatics'.** A part will be classroom teaching and other part will be workingexercise(assignments/practicals) with project assigned to the students.

Course Outcome(s) (CO): Upon finishing the course, the student is expected to be able to:

1. Knowledge of basic concepts of digraphs and Petri nets,
2. Knowledge of analysis techniques and algorithms for biological networks.
3. Visualization of dynamics of discrete event driven systems
4. Understanding of Petri net modeling for many complex networks.

Tentative plan:

|  |  |  |
| --- | --- | --- |
| Week | Lecture topic | CO met |
| 1-5 | **Digraphs and Basic Concepts**: Elementary concepts, digraphs and structures, Joining and reaching, connectedness, point base, limited reachability, Acyclic digraphs, balance in structures properties, orientation of graphs and digraphs; and classifications of trees, decision tree, some algorithms for solving complex networks in diverse fields, | CO 1 |
| 6-8 | **Distances in Digraphs**: different types of distances in digraph and matrices, Introduction to flows in networks and applications, | CO 2 |
| 9- I I | **Petri Net Theory and Modeling**: Finite state machine, Idea behind  Petri nets, some formal basic definitions of Petri net, examples (theoretical and real life modeling), structural& behavioural properties and analysis methods. | CO 3 |
| 12-14 | **Classification of Petri nets**: Boolean Petri nets and crisp Boolean Petri nets, Boolean Petri nets applications in computational and Integrative Sciences. | CO 4 |

Note: To encourse and motivate the students, topic related to further studies can be included/changed in the syllabus to improvement the quality of research.

**Some Text books and References**:

1. S. Lipschutz, Set *Theory and Related Topics,* Schaum's Outlines, Second Edition, McGraw-Hill, 1998.
2. Frank Harary, *Graph Theory,* Addison-Wesley, Massacliusettes, Reading, 1969.

3, Narsingh Deo, Graph *Theory with* Applications ***to*** Engineering and Computer *Science,* PHI Learning Private Limited, New Delhi-110001, 2012, ISBN-978-81-203-01115-0.

1. Frank Haray, R.Z. Norman, *&* D. Cartwright, *Structure Models: An introduction to* the Theory *of* Directed *Gmphs,* John Wiley &C Solis Inc.,

1965,

1. Petri, C.A., Kommunikation *Mit* Automoten, Scliriften des Institutes fur Instrumentelle Mathematik, Bonn, 1962.
2. Peterson, Petri net *Theory and the Modeling of**Systems,* Englewood Cliffs, NJ: Prentice-Hall, Inc., 1981.
3. Reisig, W., Petri *Nets,* Springer-Verleg, New York, 1985.
4. *Petri* Nets-Manufacturing and Computer (Edited by Powel Powlcwskl), ISBN: 978-958-51-0700-2.
5. G.P. Singh, *Some Advanced in the theory of Petri Nets,* a Ph.D. thesis, Faculty of Technology, University of Delhi, Delhi, India, 2013.
6. Related articles from journals.
7. Related topics from authentic sources

IT-771 : Electromagnetics applications for Biology

(credit 04)

Advance research in electromagnetic theory has been a fundamental key driver to push the frontiers of biomedical technology. These studies include evaluation of health hazards of microwave field emission by ubiquitous wireless communication systems, interaction of electromagnetic waves with biological tissues and living systems, and also the therapeutic, diagnostic, and imaging applications of electromagnetics. Cancer detection using ultrawideband signal, hyperthermia of tumors, healthcare informatics, and wireless bio implants are some of the research topics using electromagnetic waves.

**Contents:**

1. **Review of Electromagnetic:**

Fundamental properties of electromagnetic fields, Electric Field and Flux Density, Magnetic Field and Flux Density;

Mathematical description of electromagnetic fields: Maxwell's Equations: Gauss law, Faraday's law, Displacement current, Ampere's law; Time varying potentials: scalar and vector potentials;

Electromagnetic Waves, Antennas and Near Field; Antennas: Fundamentals, Antenna Configurations, examples: Electric Dipole

1. **RF/Microwave Interactionsin Biological Materials:**

Penetration in Biological Tissues and Skin Effect;

Dielectric Measurements: RF Measurements, Microwave Measurements, Liquids, Applicators; Exposure;

Tissue Characterization: Ionization and Non-ionization, Dielectric Characterization: Dipolar

Orientation, Interfacial Relaxation, Ionic Diffusion: Counter ion Polarization Effects;

Dielectric Dispersion in Tissues: Conductivity, Permittivity, Measurements: Tissues, Liquids

Biological Effects: Absorption: Fundamentals, Dosimetry and SAR, Thermal Considerations; Radiation Hazards and Exposure Standards, Standards and Recommendations; Tissue Phantoms and SAR Measurements, Computational Methods for SAR Evaluation, Exposure of Body to Cell Phone and Base Station.

1. **RE/Microwave Delivery Systems for Therapeutic Applications** Introduction, Transmission Lines and Waveguides for Medical Applications:

Skin Effect, Example: Coaxial Cable for Microwave Balloon Angioplasty Microwave Measurement Techniques Examples: Method of Measuring Blood Perfusion (Flow) in Heart Muscle by Use of Microwave Energy; Lumen Measurement of Arteries Utilizing Microwave Apparatus.

1. **Wireless Body Area networks:**

Introduction to Wireless Sensor Networks, patient monitoring; Technical Challenges Facing wireless BAN and personalized healthcare;

Wireless biotelemetry: inductive coupling and RF communication in body; antenna design and testing for BAN/BSN;

Matching networks and tuning: RF Losses in Components and Layout Issues, parasitic effects;

Power consideration and battery challenges;

BAN Application Scenarios: stand-alone and global healthcare system, pervasive sensor networks;

WBAN/WPAN network technologies overview, regulatory environments and IEEE regulatory standards; Healthcare System Integration.

**Suggested readings:**

* Vorst, A. Rosen, Y. Kotsuka, "RF/Microwave Interaction with Biological Tissues", Wiley (2006)
* F. Barnes, B. Greenebaum, "Bioengineering and Biophysical Aspects of Electromagnetic Fields", CRC (2006)
* S. Grimnes, 0. Martinsen, "Bioelectricity and Bioimpedance Basics", Academic Press (2008)
* Body Sensor Networks, Guang-Zhong Yang (Ed.), Springer-Verlag London Limited 2006, ISBN-13: 978-1-84628-272-0

**IT-778 : Agriculture Bioinformatics**

* Course Name: **Agriculture Bioinformatics**
* Course Code:778
* Credit: 3
* Course offered to: M.Sc. and PhD

**Course description:**

The use of bioinformatics in agriculture has huge potential for speeding crop improvement. Through this course, students will be introduced with key challenges in agriculture and how advances inomic technologies and bioinformatics are helping to resolve them. The advances made so far by applying omics technologies in plant research and the key challenges ahead will be discussed. The detailed syllabus is as follows:

1. Introduction to agricultural bioinformatics
2. Sequencing of Plant genomes: Status and Challenges
3. Comparative genomics in major crop plants and prospects
4. Omics technologies for gene discovery and pathway analysis in plants
5. Concept and applications of phylogenomics in selecting targets for crop improvement
6. Overview of Plant microRNAs and analysis
7. Web tools and databases available for plant research

* Pre-requisite (Mandatory): must have credited course on "Fundamentals of Biological Sciences" OR should have knowledge about basic concepts of molecular and computational biology.
* Pre-requisite (Desirable): Knowledge and hands-on experience with concept and tools inplant biotechnology and next generation sequencing technologies will be very helpful.

**Course Outcome (CO):**

1.Understand the impact of bioinformatics and next generation technologies in agriculture

1. Role of Comparative genomic and phylogenomics in candidate selection for crop improvement
2. Get acquainted with tools and resources available for plant research

**Tentative plan:**

|  |  |  |
| --- | --- | --- |
| Week number | Lecture topic | COs met |
| Wk I | Introduction to agricultural bioinformatics | Cos I |
| Wk2-3 | Sequencing of Plant genomes: Status and | Cos2 |
|  |  |  |
|  | Challenges |  |
| Wk4-5 | Comparative genomics in major crop plants and | Cos2 |
| Wk6-9 | Contribution of omics prospects technologies in gene | Cos2 |
| WkI0-11 | Concept and applications discovery and pathway of phylogenomics in | Cos2 |
| WkI2-13 | selecting targets for crop Overview of Plant  microRNAs and analysis | Cos2 |
| Wk14-16 | Web tools and databases available for plant | Cos3 |

research

**Resource Material:**

I. Review and Research Articles in National and International Journals

1. Web-based databases and tools
2. Agricultural Bioinformatics Edited by Kishor, P.B. Kavi, Bandopadhyay, Rain). Suravajhala. Prashanth
3. Phylogenomics: An Introduction by Christoph Bleidom
4. The role of bioinformatics in agriculture by Santosh Kumar
5. Plant Bioinformatics: Methods and Protocols; edited by David Edwards

**IT-779: Advanced Applied and Computational Complex Analysis**

Course Name : **Advanced Applied and Computational Complex Analysis**

Course Code: IT-779 : Ph.D

Credit: 3 Credits

Course offered to: Optional

* Course description: This course will fulfill the need of mathematical applications in Advance complex analysis as well as computational method to understand complex variables. The aim of this course is enhance the knowledge and understanding of the students for developing new mathematical real world problems for complex variables and functions and their solutions.
* Pre-requisite (Mandatory): Student should be able to understand mathematics at the +2 level.
* Pre-requisite (Desirable): Nil
* Course Outcome (COI-5):

Students should be able to understand:

Complex Variables, Complex functions and applications in biological systems. This topic will introduce the formulation of Complex Variable, limit continuity and differentiability of complex variables. Complex integral and its use in real word problems along with their solutions with applications.

Tentative teaching plan:

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| --- | --- | --- |
| **Week number** | **Lecture topic** | **CO met** |
| 1-3 | Function of Complex Variable, Limit of Complex Variable,  Continuity of complex Variable. Differentiability of Complex Variable. Analytic Function. Cauchy-Riemann Equations. Harmonic Functions, Conjugate Functions. Milne's Thomson Method (Applications). | COI |
| 4-6 | Complex Integration, Cauchy's Integral Theorem, Cauchy's  Integral Formula, Cauchy's Integral formula for the Derivatives, Cauchy's Inequality, Liouville's Theorem. Rouche's Theorem, Fundamental theorem of Algebra (Applications). | CO2 |
| 7-9 | Power Series, Radius of convergence of Power Series, Series of  Complex terms, Taylor's Series. Laurent's Series (Applications). | CO3 |
| 10-12 | Zero of an Analytic Function, Singularity, Types of Singularity, Poles. Types of Poles, Residue. Cauchy's Residue Theorem, Methods of finding Residue (Applications). | CO4 |
| 12-14 | Contour Integration, Residue theorem to evaluate  integrals, Complex Integrals when no zeroes on the real axis, Complex Integrals when zeroes are on the real axis, Jordan's Inequality, Jordan's Lemma (Applications). | CO5 |

References:

* 1. Current Topics in Pure and Computational Complex Analysis-Santosh Joshi, Michael Dorff, Indrajit Lahiri
  2. Applied and Computational Complex Analysis-Peter Henrici
  3. Higher Engineering Mathematics- B. S. Grewal
  4. Complex Analysis with Applications — Richard A. Silverman
  5. Introductory Complex Analysis - Boris Vladimirovich Shabat -
  6. Invitation to complex analysis- Ralph P. Boas, Harold P. Boas
  7. Complex Analysis for Mathematics and Engineering-John Mathews, Russell Howell -
  8. A Complex Analysis Problem Book-Daniel Alpay
  9. Fundamentals and Applications of Complex Analysis- Harold Cohen
  10. Complex Analysis with MATHEMATICAO-William T. Shaw
  11. Complex Analysis-Man Wah Wong
  12. A First Course in Complex Analysis with Applications-Zill

**IT-780 : Mathematical concept and methods for Biological Systems**

Course Name : **Mathematical concept and methods for Biological Systems**

Course Code: IT-780

Credit: 3 Credits

Course offered to: Optional

* Course description: This course will fulfill the need of mathematics application as well as advance so that the students can learn to apply mathematics for real world problems. The aim of this course is enhance the knowledge and understanding of the students for developing new mathematical real world problems and their solutions.
* Pm-requisite (Mandatory): Student should be able to understand mathematics at the +2 level.
* Pre-requisite (Desirable): Nil
* Course Outcome (CO):

Students should be able to understand:

I. Differential Equation and its applications in biological systems

* 1. Partial Differential equations: This topic will introduce the formulation of partial differential equation ant its solution as well as its application to biological problem.
  2. Numerical Analysis: Numerical methods are more accurate in comparison to analytical methods. And In research work numerical techniques have become indispensable tools in all the fields.
  3. Analytic functions: The Solution of differential equation using analytical techniques.
  4. Linear Programming: Optimization techniques to solve the maximization and minimization problem and its application in biological problems.

Tentative teaching plan:

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| --- | --- | --- |
| Week  Number | Lecture topic | CO met |
| 1--3 | First order equations (linear and nonlinear); Higher order linear differential equations with constant coefficients; Second order linear differential equations with variable coefficients; Method of variation of parameters; Cauchy-Euler equation; Power series solutions; Legendre polynomials, Bessel functions of the first kind and their properties (Applications). | CO1 |
| 4-6 | Linear and quasilinear first order partial differential equations, method of characteristics; second order linear equations in two variables and their classification; Cauchy, Dirichlet and  Neumann problems; solutions of Laplace, wave in two dimensional Cartesian coordinates, Separation of variables method for solving wave and diffusion equations in one space variable; Fourier series and Fourier transform and Laplace transform methods of solutions for the above equations(Applications). | CO2 |
| 7-9 | Gauss elimination and Gauss-Seidel methods; Lagrange and Nev. ton's interpolations. Solution of polynomial and transcendental equations by Newton-Raphson method, Method of False Position; Numerical integration by trapezoidal rule, Simpson's rule and Gaussian quadrature rule; Numerical  Differentiation: solutions of first order differential equations by  Euler's method and 4th order Runge-Kuria method  (Applications). | CO3 |
| 10-12 | Analytic functions; Cauchy-Riemann equations; Line integral,  Cauchy's integral theorem and Cauchy's integral formula;  Taylor's series and Laurent series; Residue theorem  (Applications). | C04 |
| 12-14 | Linear programming problem and its formulation, convex sets and their properties, graphical method, basic feasible solution, simplex method, big-M and two phase methods; infeasible and unbounded LPP's. Dual problem and duality theorems, dual simplex method and its application in post optimality analysis; Balanced and unbalanced transportation problems, Vogel's approximation method for solving transportation problems; Hungarian method for solving assignment problems  (Applications). | CO5 |

1. Advanced Engineering Mathematics - by Kreyazig. E
2. Higher Engineering Mathematics - by 13. S. Grewal.
3. Engineering Mathematics - by Lazpath Roy.
4. I. M. J. Strauss. G. L. Bradley and K. J. Smith, Calculus (3rd Edition), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Delhi, 2007.
5. H. Anton, I. Bivens and S. Davis, Calculus (7th Edition), John Wiley and Sons (Asia) Pte. Ltd., Singapore. 2002.
6. Numerical Methods -by R.K. Jain,S.R.K. Iyengar, 2002
7. Integral Transform and their applications- B. Davies
8. Numerical Analysis- Doron Levy, 2010
9. Optimization Techniques- Godfrey C. On wubolu, B. V. Babu and
10. Engineering Optimization: Theory and Practice- S. S. Rao

**IT-781 : Advanced Fluid dynamics and its applications in biological** **systems**

Course Name: **Advanced Fluid dynamics and its applications in biological** **systems**

Course Code: IT-781

Credit: 3 Credits

Course offered to: Optional

Course description: This course will fulfill the need of hydrodynamics as well as advance mathematics for the solution of real world problems in biological systems. The aim of this course is enhance the knowledge and understanding of the students for developing new mathematical real world problems and their solutions in biological problems. The whole of the course will be embodied by different topic of mathematics which will develop student's conceptual knowledge along with the applications. The expected outcome of this course is to enhance the knowledge and understanding of mathematics and help out in their research work.

Pre-requisite (Mandatory): Student should be able to understand mathematics at the +2 level.

Pre-requisite (Desirable): Nil • Course Outcome (CO):

Students should be able to understand:

The concept of hydrostatics.

Methods to solve the fluid motion equations.

Applications of flow in different planes of different geometries.

Significance of non-dimensional parameters and their significance. 5 Solution of differential equations for different physical systems.

Tentative teaching plan:

|  |  |  |
| --- | --- | --- |
| **Week number** | **Lecture topic** | **CO met** |
| 1-2 | Viscosity, relationship between stress and strain-rate fo Newtonian fluids, incompressible and compressible flows, differences between laminar and turbulent flows. Hydrostatics:  Buoyancy, manometry, forces on submerged bodies. | r COI |
| 3-5 | Eulerian and Lagrangian description of fluids motion, concept of local and convective accelerations, steady and unsteady flows. | CO2 |
| 6-8 | Bernoulli's equation - assumptions and applications, potential function, Elementary plane flows - uniform flow, source, sink and doublet and their superposition for potential flow past simple geometries. | CO3 |
| 9-11 | Concept of geometric, kinematic and dynamic similarity, some common non-dimensional parameters and their physical significance: Reynolds number, Froude number and Mach number. | C04 |
| 12-14 | Differential equations of mass and momentum for incompressible flows: inviscid - Euler equation and viscous flows - Navier-Stokes equations, concept of fluid rotation, vorticity, stream function, Exact solutions of Navier-Stokes equation for Couette Flow and Poiseuille flow. | CO5 |

1. Fluid Mechanics L D Landau, E. M. Lifshitz -
2. A History and Philosophy of Fluid Mechanics— by G. A. Tokaty
3. Engineering Fluid Mechanics— by H. Yamaguchi
4. Advanced Fluid Mechanics: by William Graebel
5. Elementary Fluid Mechanics by Tsutomu Kambe
6. Cardiovascular Fluid Mechanics by Gianni Pedrizzetti, Karl Perktold
7. Recent Advances in Fluid Mechanics: P.L. Sachdev, M Vcnkatachalappa -