

M. Tech. Bioinformatics

Course Structure

Scheme of Evaluation

&

Syllabus



Indian Institute of Information Technology

Allahabad -211012

M. Tech. (Bioinformatics)

Proposed Course Structure and Syllabi

I Semester (Total credits=20)

Course Code	Course Name	Theory (Credits)	Practicals (Credits)	Sem-Total (Credits)
FCI ¹	Fundamental of computers	3	2	20
BS ²	Biological Systems-I	3	2	
DSA	Data Structure and Algorithms	3	2	
IGP	Introduction to Genomics and Proteomics	3	2	
MBS	Mathematics and Biostatistics	3	2	

II Semester (Total credits=20)

Course Code	Course Name	Theory (Credits)	Practicals (Credits)	Sem-Total (Credits)
BDS	Biological Databases	3	2	20
LAT	Language Algorithm and Tools	3	2	
Electives (Any 2)				
	Elective 1	3	2	
	Elective 2	3	2	
	Elective 3	3	2	

III Semester (Total credits=20)

Course Code	Course Name	Theory (Credits)	Practicals (Credits)	Sem-Total (Credits)
	Mini Project	10	0	20
Electives (Any 2)				
	Elective 4	3	2	
	Elective 5	3	2	
	Elective 6	3	2	

IV Semester (Total Credits= 20)

Course Code	Course Name	Theory (Credits)	Practicals (Credits)	Sem-Total (Credits)
	Semester Project	20	0	20

List of Electives**Semester II**

Elective 1: Computer Aided Drug design (CADD-232)

Elective 2: Molecular structure Prediction and Visualization (MSPV-232)

Elective 3: Data Mining in Biological Systems (DMBS-232)

¹ For students who are not from Computer Science/Information Technology

² For students who are not from Biology stream

Semester III

Elective 4: Systems Biology (SB-332)

Elective 5: Chemi-informatics (CIF-332)

Elective 6: Machine Learning for Biological Systems (MLBS-332)

Fundamentals of Computers (FC-132)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Computer basics Flowcharts, Algorithms, Data representation Characters, Integers, Fractions, Hexadecimal & Binary conversions

UNIT II:

Input/output units, Computer memory, Computer architecture, Computer languages

UNIT III:

Operating systems, Batch operating system, Multiprogramming O.S., Time shorting O.S., PC operating system, Unix O.S, Microkernel Based O.S., On-line and Real time Systems

UNIT IV:

Computer generations and classification, Computer networks, Communication protocols, Local area networks, Inter connecting Networks, Future internet technologies,

UNIT V:

C programming, The art for programming, Sequences and strings, condition checking and loops, file handling

UNIT VI:

HTML, Introduction, Get Started, Basic, Elements, Attributes, Headings, Paragraphs, Formatting, Styles, Links, Images, Tables, Lists, Forms, Frames, Colors, Color names, Color values, Quick List, CSS, Head, URL Encode

Text/Reference Books:

1. V.Rajaraman, Fundamentals of Computers, Estern Economy Edition
2. The C Programming Language by Brian W. Kernighan, Dennis M. Ritchie
3. HTML and CSS: Design and Build Websites,Jon Ducket.

Guide lines for practicals:

A two credit lab is to be conducted by covering the most relevant and useful topics from afore mentioned syllabus.

Data Structures and Algorithms (DSA-132)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Algorithms and problem solving, Computer programming for problem solving: basic idea of C language, C data types, control structure, pointers, arrays, structures: self referential structures.

UNIT II:

Data structures: linear list, array implementation of lists, linked lists, implementation of linked lists, list and linked list applications, stack data structure: array implementation of stacks, applications of stack: recursive programming, queue data structure: array implementation of queues, applications of queues: job scheduling, linked list implementation of stack and queues.

UNIT III:

Sorting: bubble sort, selection sort, insertion sort, merge sort, quick sort, heap sort, Searching: Linear (sequential) and binary search

UNIT IV:

Graphs and Trees: Basic terminology, trivial graph, directed and undirected graph, path, loop (closed path), implementation of graph using linked list; Graph traversal: DFS and BFS; Trees: trivial tree, binary tree, mway tree, conversion of graph into tree, DFS and BFS based spanning trees, Kruskal's algorithm, Prim's algorithm, applications of graphs; Shortest path algorithm, applications in Bioinformatics

UNIT V:

Search trees: Binary and m-way search trees (introduction), binary search and binary tree search, linked list implementation of binary trees, height balance trees (AVL) for searching (introduction), B tree (introduction); applications of trees and search trees

UNIT VI:

Heaps: Heap as binary tree, generation of heaps, heap sorting, Hashes: Hashing by chaining

Text/Reference Books:

1. Introduction to Algorithms, Thomas H. Cormen, Charles E. Leiserson, Ronald L. Rivest, Clifford Stein
2. Data Structures Using C and C++, Yedidyah Langsam, Moshe J. Augenstein, and Aaron M. Tenenbaum
3. The C Programming Language (2nd Edition), Brian W. Kernighan and Dennis Ritchie

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Introduction to Genomics and Proteomics (IGP-132)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Introduction to bio-informatics, Basic concepts, Cell Structure, Difference between Prokaryotes and Eukaryote genomes, Gene cloning, Blotting Techniques: Southern, Northern, Western, Gene structure and its Expression: Promoter, Exons, Intron, ORF, Gel Electrophoresis, Restriction mapping, Site directed Mutagenesis, copy-number variation, single-nucleotide polymorphisms,

UNIT II:

Polymerase Chain Reaction, Primer Design and evaluation, Human Genome project, Cloning and Contig assembly and analysis, Structural Genomics: Linkage, PFGE, Human-rodent somatic Cell hybrid, High resolution chromosome mapping, Meiotic mapping by recombination.

UNIT III:

Structural Genomics: Linkage, PFGE, Human-rodent somatic Cell hybrid, High resolution chromosome mapping, Meiotic mapping by recombination.

UNIT IV:

Physical Mapping, Radiation Hybrid Mapping, Hybridization and Amplification, Plasmid, Cosmid, BAC, PAC and YAC, Chromosome specific library, STSs, ESTs, Macro & micro satellite markers, FISH, Rearrangement break points, Radiation Hybrids, Genome maps for genetic analysis, Positional cloning 2.QTLs.

UNIT V:

Genetic Mapping: RFLP, SSLP, ISSRs, SNPs, RAPD & AFLP, Functional Genomics: Proteome by ORF analysis, Gene disruption knockouts, yeast two-hybrid system, Comparative Genomics, Micro Array Technique: Micro Array chip synthesis, Hybridization, Data capturing and analysis, Overview of data analysis, Transcriptomics: RT-PCR, RNAi

UNIT VI:

Proteomics: Basic Concept, 2D-PAGE, MOLDI-TOF, MS/MS Analysis, Protein-protein interaction (Two hybrid interaction screening), Protein engineering, Protein chips and functional proteomics, Metabolomics: Biochemical Pathways, System Biology.

Text/Reference Books:

1. Principles of Genome Analysis and Genomics, Third Edition (2003) S.B. Primrose and R.M. Twyman, Blackwell Publishing Company, Oxford, UK.
2. Introduction to proteomics – Tools For The New Biology, First Edition (2002) D.C. Liebler, Humana Press Inc, New Jersey, USA.

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Mathematics and Biostatistics (MBS-132)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Review of the basic concepts of Probability (up to Baye's Theorem) and Statistics (Central tendencies and standard deviations).

UNIT II:

Probability Distribution functions: Binomial, Poisson and Normal distributions.

UNIT III:

Correlation and Regression analyses, Correlation Coefficients, Least square method and curve fittings, Single and multivariable regression.

UNIT IV:

Test of hypotheses, Z-test, t-test, the chi-square test, F-test and ANOVA test.

UNIT V:

Area and averages as integrals, Numerical techniques for Integration, Concept of a differential Equation and formulation of some problems in the language of differential equations, Numerical solution of differential equations.

UNIT VI:

Representation of a system of linear equations as a matrix equation, Finding inverse of a matrix, Numerical solutions of system of linear equations, Determinants, Eigen values and Eigen vectors and methods to find them.

Text/Reference Books:

1. Choosing and using Statistics: A Biologist's Guide by Calvin Dytham.
2. An Introduction to Experimental Design and Statistics for Biology by David Heath.
3. Statistics for the life Sciences (4th Edition) By Myra L. Samuels, Jeffrey A. Witmer and Andrew Schaffner.
4. Biostatistics: Principles and Practice, By B. Antonisamy.
5. Fundamentals of Biostatistics, By Bernard Rosner.

Guide lines for practicals:

A two credit lab is to be conducted by covering the most relevant and useful topics from afore mentioned syllabus.

Biological Systems-I (BS-132)

(CREDIT HOURS Theory- 3 + Practical- 2)

UNIT I

Introduction to cell biology, Prokaryotic and Eukaryotic cell, Microscopy, Cell Chemistry, Plasma Membranes and its functions, Cytoskeleton of cells, Cytoskeleton filaments, Molecular motors, Transport across membranes, Ion channels, Mitochondria and Chloroplast.

UNIT II

Cell signaling, Cell Cycle, Cell division- Mitosis and Meiosis, Introduction to Germ cell, Cancer cell and Stem cells.

UNIT III

Overview of microbial world and development, Isolation, Characterization and growth of microorganisms, control of microbial growth, Gross time and structure of bacteria, viruses and eukaryotic Microbes, Introduction to *E. coli*, *M. tuberculosis*, *S. cerevisiae*, *Cyanobacteria*, *Plasmodium*, *Pox Virus*, *Influenza Virus* and phages.

UNIT IV

Overview of immune system, cells and organs of the immune system, Innate immunity, Adaptive immune response, T cell maturation, activation and differentiation, B cell generation, activation and development, Antigens, Immunoglobulin's structure and function, Antibody diversity, Antigen antibody reactions, Introduction to MHC Molecules and Immunodeficiency diseases.

UNIT V

Overview of Biochemistry, Amino acids and Proteins, Carbohydrates, Nucleotides and nucleic acids, Lipids, Vitamins, Hormones, protein structure, folding modification, targeting and degradation.

UNIT- VI

Protein function: enzymes, enzyme kinetics, enzyme regulation and inhibition, Metabolism and metabolic pathways, Glycolysis, TCA cycle, Fatty acids degradation.

Recommended books

1. Molecular biology of cell- Albert *et al.*
2. Brock Biology of Micro- organisms- Michal M. *et al.*
3. Microbiology- Michal J. Pelzar *et al.*
4. Kuby Immunology- Goldsby *et al.*
5. Lehninger Principles of Biochemistry- David L. Nelson *et al.*
6. Harper's Illustrated Biochemistry- Robert K. Murray *et al.*

Guide lines for practicals:

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Biological Databases (BDS-232)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Introduction to database, Database models, Flat model, Hierarchical model, & Network model, Profile & Block, Secondary and Tertiary sequence databases, Relational model, Codd's rule with explanation, 1st, 2nd and 3rd level normalization, Relational operations, Dimensional model and Object database models

UNIT II:

Database internals, Indexing and triggers, Binary tree and Hash-key based indexing, Transactions, concurrency, and Replication

UNIT III:

Applications of databases, Introduction to MySQL, Introduction to Database interfacing language, PHP, Introduction to PHP manipulating APACHE server

UNIT IV:

Applications: Introduction to Protein and Nucleic Acid Databases (PDB, NCBI etc.), PDB and NCBI database formalism, Further manipulation of PDB and NCBI data with the help of already acquired RDBMS knowledge based on PHP-MySQL manipulation, Pearl based data mining and linkage with databases (DBI)

UNIT V:

Data mining & Warehousing , Association, Clustering & Classification.

UNIT VI:

Next Generation Sequence Analysis, Phylogenetics, Highthroughput databases

Text/Reference Books:

1. Biological Databases by Attwood.
2. Programming the Perl DBI by O'Reilly
3. Essential of MATLAB for Scientist and Engineer by Hahn Brian D
4. Beginning PHP and MySQL 5: from novice to professional by W.Jason Gilmore

Guide lines for practicals:

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Language Algorithms and Tools (LAT-232)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Advanced Programming in PERL Packages, Object Oriented Programming, Difference between OOPs of PERL & C++

UNIT II:

BIOPERL; Handling Software Interfaces with BioPerl APIs Handling Sequences, database & structures

UNIT III:

Local & Global Alignment Algorithms, Differences, Dynamic Programming : Smith & Waterman Algorithm with proof, Needleman & Wunsch Algorithm with proof.

UNIT IV:

Multiple Sequence Alignment, Concepts & Implementations.

UNIT V:

Amino Acid Substitution Matrices PAM & BLOSUM Derivation of Dayhoff Matrices

UNIT VI:

Profiles & Motifs General Tools, Techniques & Resources ClustalW, BLAST, FASTA, HMM.

Text/Reference Books:

1. David Mount, Bioinformatics Sequence and Genome analysis
2. Baxvanis, Bioinformatics.

Guide lines for practicals:

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Computer aided drug Designing (CADD-232)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Introduction, History of Drug Development, Basic pharmacodynamics and pharmacokinetics, Strategies for drug designing and drug development, Lead generation and Lead optimization Analogue and structure based methods, File format, conversion, Coordinate systems

UNIT II:

Identifying Cavities and Surface Matching, Shape Complementarity, Solvent-Accessible Surface, Connolly Surface, Lenhoff "Surface", Nussinov and Wolfson Method, Alpha Shapes.

UNIT III:

Docking and scoring methods for proteins-ligands, protein-protein, protein-DNA, DNA-ligand, Geometric Hashing, Generating a Coordinate System, Kuntz System, Clique detection, Docking Search and its Dimensionality, Evolutionary Algorithms (EA), Tabu Search (TS), Hybrid Global-Local Search, Lamarckian GA (LGA)

UNIT IV:

Docking Software: Dock, AutoDock, Flexx, GOLD, Optimization Technique: Gradient Descent Approach, Simulated Annealing, Metropolis Algorithm, Genetic Algorithm, Receptor mapping and active site finding

UNIT V:

Introduction, Pharmacophore Modeling, Structure Based Drug Designing (SBDD), Ligand Based Drug Designing (LBDD), Pharmacophore Generation, Hypogen Theory, HipHop Theory, Softwares Ex: Catalyst ect..

Text/Reference Books:

1. Drug Design: Structure and ligand-based approaches: Kenneth M. Merz, Dagmar Ringe, Charles H. Reynolds.
2. Bioinformatics-from genomes to drugs (Vol.2- Applications Lengauer, Thomas (ed.).
3. Burger's medicinal chemistry & drug discovery; Vol.-2(Drug discovery and drug development) Abraham, Donald J. (ed.)
4. Drug design : structure and ligand-based approaches: edited by Kenneth M. Merz, Dagmar Ringe, Charles H. Reynolds
5. Chemoinformatics; (Vol.-275 - Methods in molecular biology) : concepts, methods and tools for drug discovery : Bajorath, Jurgen (ed.)

Guide lines for practicals:

A two credit lab is to be conducted by covering the most relevant and useful topics from afore mentioned syllabus.

Molecular Structure Prediction and Visualization (MSPV-232)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Basic structural principles: Building blocks of life, Chemical properties of polypeptides & PDB Database, Intermolecular forces: Types of intermolecular forces, Entropy and temperature, Protein folding & Levinthal Paradox

UNIT II:

Levels of protein structure: Primary structure, Secondary structure, Tertiary structure & Quaternary structure, Motifs of protein structure: Hydrophobic and hydrophilic regions, Ramachandran plot Alpha-helix, Beta sheets, Loops, Topology diagrams & various structural motifs

UNIT III:

X-Ray crystallography and NMR: Structure determination methods & Structure evaluation methods

UNIT IV:

Protein structure prediction: Impediments, Secondary/fold recognition, Threading/tertiary structures, Sequence considerations, Structural considerations, Energy consideration, Energy landscape & Validation

UNIT V:

Structure prediction of small proteins using ab initio stochastic models: Lattice simulation, Random-walk model, Self-avoiding model & HP-models, Structure prediction of small proteins using ab initio deterministic models Ergodic hypothesis, Use of Newtonian equations of motion, Optimization techniques: Steepest descent, GA, simulated annealing & Force fields (Amber, CHARMM)

UNIT VI:

Nucleic acid structures: DNA structures, RNA structures & Secondary structure prediction in RNA, Useful Tools: Visualization using VMD, PROCHECK, WHATIF & Simulation using Amber

Text/Reference Books:

1. Molecular Modelling: Principles and Applications (2nd Edition): Andrew R. Leach (Prentice Hall)
2. Introduction to Protein Structure: Carl Branden, John Tooze (Garland)
3. Proteins: Structures and Molecular Properties: Thomas E. Creighton (Freeman)
4. Principles of Nucleic Acid Structure Stephen Neidle (Academic Press)

Guide lines for practicals:

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Data Mining for Biological Systems (DMBS-232)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Biological Databases and Integration, Scientific Work Flows and Knowledge Discovery, Biological Data Storage and Analysis, The Curse of Dimensionality, Data Cleaning.

UNIT II:

Knowledge Discovery in Databases, Analysis of Data Using Large Database,. Challenges in Data Cleaning, Data Integration, Data Warehousing

UNIT III:

Feature Selection and Extraction Strategies , Over fitting, Data Transformation, Attributes Features and Relevance, Dataset/Distribution, Feature Selection, Reduction, Techniques for MS Data Analysis, Data Pre-processing, Association: Apriori, FP growth tree.

UNIT IV:

Clustering Techniques, Expressions for Co expressed Genes, Implementation of k-Means, Hierarchical Clustering, Microarray Data, Self-Organizing Maps Clustering, Hierarchical Clustering for Representation of Genes, Expectation Maximization Algorithm.

UNIT V:

Advanced Clustering Techniques, Graph-Based Clustering, Measures for Identifying Clusters, Graph-Based Algorithms, Graph Process, Kernel-Based Clustering, Identifying Stable and Tight Patterns, Problem in k-Means Clustering.

UNIT VI:

Classification Techniques in Bioinformatics, Support Vector Machines (SVMs) , Bayesian Approaches, Bayesian Networks, Expression Analysis, Decision Trees, Ensemble Approaches, Classifiers, Challenges of Supervised Learning, Validation and Benchmarking, Performance Evaluation Techniques, Classifier Validation, Performance Measures, Cluster Validation Techniques.

Text/Reference Books:

1. Data Mining for Bioinformatics (Text) Sumeet Dua, Pradeep ChowriappaCRC Press
2. Data Mining: Practical Machine Learning Tools and Techniques (Ed 3) (Ref)Ian Witten, Eibe Frank, Mark Hall, Morgan Kaufmann Publishers

Guide lines for practicals:

A two credit lab is to be conducted by covering the most relevant and useful topics from afore mentioned syllabus.

Systems Biology (SB-332)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Biological Systems, Introduction to Mathematical Modelling, Static Network Models

UNIT II:

Mathematical, Characterization of Network Capabilities, Biological Networks, Parameter Estimation

UNIT III:

Gene Systems , Protein Systems, Population Systems, Methods for Protein-Protein Interaction Analysis, Metabolic Systems and Networks, Regulatory networks, Signalling Systems / Networks

UNIT IV:

Integrative Analysis of genome, Protein and Metabolic Data, Physiological Modelling: The heart as an example

UNIT V:

Systems Biology in Medicine and Drug Development, Design of Biological Systems

UNIT VI:

Experimental Techniques for Systems Biology, Methods and Software platforms for System Biology, Emerging areas in Systems Biology.

Text/Reference Books:

1. A first Course in System Biology, Eberhard Voit, Mar 2012.
2. Introduction to System Biology, Sangdun Choi (Ed) , Jul 2007.
3. Systems Biology: A Text Book, Edda Klipp et al. Aug 2009.
4. The Music of life : Biology Beyond Genes, Denis Noble Apr 2008.

Guide lines for practicals:

A two credit lab is to be conducted by covering the most relevant and useful topics from afore mentioned syllabus.

Cheminformatics (CIF-332)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Introduction to Cheminformatics in Drug Discovery. 2D Databases and Database searching: Substructure search, Virtual Screening, property searching, similarity searching, Representation and manipulation of 2D Molecular Structures, 3D Databases: experimental data sources, database searching, Representation and manipulation of 3D Molecular Structures, Selecting Diverse Sets of Compounds

UNIT II:

QSAR : Quantitative Structure and Activity Relationship, Historical Development of QSAR, Hammett Equation, Hansch Equation, Kubinyi bilinear model, Tools and Techniques of QSAR: Biological Parameters, Statistical Methods: Linear Regression Analysis,

UNIT III:

Parameters used in QSAR: Electronic Parameters, Hydrophobicity Parameters, Steric Parameters, Molecular Structure Descriptors, Quantitative Models: Linear Models, Nonlinear Models, Free-Wilson Approach, Applications of QSAR: Isolated Receptor Interactions, Interactions at the Cellular Level Interactions in-Vivo, Comparative QSAR: Database Development, Software: GRID, CoMFA.

UNIT IV:

QSPR : Quantitative Structure and Property Relationship, Octanol Water Partition Coefficient, Quantum Chemical Descriptor, HOMO/LUMO, Predictive Quantitative Structure –Activity Relationships Modeling: Data Preparation and General Modeling Workflow, Reaction network Generation, Open Source Cheminformatics Software and Database Technologies, Machine Learning based Bioinformatics Algorithms-Applications to Chemicals.

UNIT V:

Combinatorial Library Designing: Diverse and Focussed Libraries, Monomer Selection, Product based Library Design, Structure Based Library design.

UNIT VI:

High Throughput / Virtual screening Screening, Introduction, Basic Steps, Important Drug Databases, Database Designing Lipinski's Rule of Five, ADMET screening

Text/Reference Books:

1. Cheminformatics, Concepts, Methods & Tools for Drug Discovery; Ed. Jurgen Bajorath (Humana Press)
2. Cheminformatics Ed by Johann Gasteigen, Thomas Engel, Wiley-VCH
3. Molecular Modeling, Principles & Applications, Andrew R. Leach
4. Bioinformatics from Genomes to Drugs ; Vol I & 2
5. An Introduction to Cheminformatics, Andrew R. Leach, Valerie J. Gillet.
6. Hand Book of Cheminformatics Algorithms, Jean-Loup Faulon, Andreas Bender.

Guide lines for practicals:

A two credit lab is to be conducted by covering the most relevant and useful topics from afore mentioned syllabus.

Machine Learning for Biological Systems (MLBS-332)

(Credits: 3 Theory + 2 Lab)

UNIT I:

Foundation of Machine learning: Turing Machine, Concepts of John von Neumann, computation of amount of learning of a machine.

UNIT II:

Concept of supervised and unsupervised learning, concept of clusters and classes, concept of training and testing.

UNIT III:

Statistical Machine Learning:

1. Design of rule based expert system, knowledge engineering, forward chaining and backward chaining inference techniques, Application to discriminate intron from exon within eukaryotic DNA
2. Application of rule based system to discover knowledge from data, concept of clustering, condition to find best clusters. Various clustering techniques.
3. Important components of a classifier, Probabilistic classifier, Bayesian classifier, Nearest Neighbor Classifier, Discriminant Function Analysis (Linear and non-linear) as precursor to Artificial Neural Network

UNIT IV:

1. Hidden Markov Models and applications
2. Applications to discriminate Exon from Intron, to predict secondary structures of proteins, discover group of genes having similar up-regulation or down-regulation pattern from micro-array data.

UNIT V:

Soft computing method based machine learning

1. Artificial Neural Network for clustering and classification, local optimization of ANN weights, Back propagation network, Hopfield network.
2. Genetic algorithm for optimizing parameters of classifiers.
3. Support Vector Machine foundation, constrained local optimization using Lagrange Multiplier, application on 2 and more than 2 classes.
4. Over fitting and Cross validation

UNIT VI:

Application on the same items 3.v, as described above.

Text/Reference Books:

1. Pattern recognition and image analysis by Earl Gose.
2. Pattern Classification by Duda, Richard and David Stork
3. Machine Learning by Mitchell and Tom

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