M.Sc. BIOINFORMATICS

REGULATIONS AND SYLLABI
(Effective from 2007-2008)

Centre for Bioinformatics
SCHOOL OF LIFE SCIENCES
PONDICHERRY UNIVERSITY
PUDUCHERRY
<table>
<thead>
<tr>
<th>Semester</th>
<th>Course Code</th>
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<th>Credits</th>
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<tbody>
<tr>
<td>I</td>
<td>BINF 401</td>
<td>Cell and Molecular Biology</td>
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<td>BINF 402</td>
<td>Physics and Chemistry for Biologists</td>
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<td>Mathematics for Biologists</td>
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<td>BINF 404</td>
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<td>Data Structures and Programming Concepts</td>
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<td>BINF 451</td>
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<td>BINF 452</td>
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<td>BINF 453</td>
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<td>BINF 421</td>
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<td>Statistics for Biologists</td>
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<td>BINF 425</td>
<td>Programming in Java</td>
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<td>BINF 426</td>
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<td>BINF 504</td>
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SEMESTER - I
BINF 401 – CELL AND MOLECULAR BIOLOGY

Unit-I 7 Lectures
Architecture of prokaryotic and eukaryotic cells and tissues. Dynamics of the eukaryotic cell-Molecules of life- Cellular evolution- assembly of macromolecules and Origin of life- integrated structural organization of prokaryotic and eukaryotic cells- Concept of a composite cell and Molecular composition of cells; Cell division – mitosis and meiosis, eukaryotic cell cycle and its regulation

Unit-II 6 Lectures
The mitochondrion – structure, electron transport chain, oxidative phosphorylation, Chemiosmotic process; Chloroplasts – photosynthesis – photosystems, Calvin cycle, Dark reactions

Unit-III 7 Lectures
Cell Communication – membrane transport – principles, active transport, ion channels ; Protein sorting – an overview of targeting proteins to mitochondria, nucleus, endoplasmic reticulum, lysosome and plasma membrane

Unit-IV 7 Lectures
Organisation of eukaryotic genome- components of eukaryotic chromatin- chromatin and chromosome structure- DNA-supercoiling -linking number- satellite DNA-possible functions- Cot curve- C- value paradox.

DNA replication- Prokaryotic and eukaryotic DNA replication, mechanism of replication. Enzymes and necessary proteins in DNA replication. Telomeres, telomerase and end replication. Role of telomerase in aging and cancer.

Unit-V 9 Lectures
Transcription- Prokaryotic and eukaryotic Transcription- RNA polymerases- general and specific transcription factors- regulatory elements- mechanism of transcription regulation- Transcription termination; Post transcriptional modification

Translation- Genetic code- Prokaryotic and eukaryotic translation- translational machinery- Mechanism of initiation- elongation and termination- Regulation of translation.

Recommended Texts:

Reference Books

SEMESTER - I
BINF 402 – PHYSICS AND CHEMISTRY FOR BIOLOGISTS

Unit-I 8 Lectures

Unit-II 5 Lectures

Unit-III 7 Lectures

Unit- IV 11 Lectures

Unit- V 5 Lectures
Spectroscopy of organic molecules – Spectroscopic identification of simple organic molecules - Infrared Spectroscopy, nuclear magnetic resonance Spectroscopy, mass spectrometry

Recommended Texts:
SEMESTER - I
BINF 403 – MATHEMATICS FOR BIOLOGISTS

Unit I
Algebra - Logarithms – Quadratic equations – Simple problems on cubic equations – Solution of a system of linear equations using determinants

Unit II
Matrices and Vectors - Different types of matrices – Addition, Subtraction and Multiplication of matrices – Transpose of a matrix – Singular matrix - Inverse of a matrix

The concept of a vector – Dot product – Cross product – Angle between two vectors - Scalar triple product – Divergence – Curl – Equation of a normal

Unit III
Trigonometry and Analytical Geometry - Trigonometric ratios- De Moivre’s theorem; Cartesian coordinates in two dimensions – Distance formula - Straight line – Slope of a line – Intercepts of a line – Equation of a line - Intersection of two lines – Angle between two lines - Circle, ellipse and parabola

Unit IV
Calculus: The concept of limit – Derivatives of simple, standard functions – Geometrical application of differentiation - Maxima and minima – Partial differentiation
Definite and indefinite integrals – Numerical integration

Unit V
Differential equations: First order ordinary differential equations – Laplace transform and its application

Recommended Texts:


Reference Books

SEMESTER - I
BINF 404 – BIOINFORMATICS – I

Unit I
Bioinformatics: an overview - Introduction to Computational Biology and Bioinformatics; Emergence of bioinformatics as a separate discipline; some of the biological problems that require computational methods for their solution; Role of internet and www in bioinformatics.

Unit II
Biological Data Acquisition – The form of biological information; DNA sequencing methods – basic DNA sequencing, automated DNA sequencing, DNA sequencing by capillary array and electrophoresis; Types of DNA sequences – genomic DNA, cDNA, recombinant DNA, Expressed sequence tags (ESTs), Genomic survey sequences (GSSs); RNA sequencing methods; Protein structure determination methods; gene expression data.

Unit III
Databases: Format and Annotation – Conventions for databases indexing and specification of search terms; Common sequencing file formats – NBRF/PIR, FASTA, GDE; Files for multiple sequence alignment – multiple sequence format (MSF), ALN format; Files for structural data – PDB format and NMR files; Annotated sequence databases – primary sequence databases (GenBank-NCBI, the nucleotide sequence database-EMBL, DNA sequence databank of Japan-DDBJ; Subsidiary data storage (ESTs, dbESTs, GSSs), unfinished genomic sequence data, organisms specific databases (EcoGene, SGD, MatDB, TAIR, FlyBase, OMIM, etc.); Protein sequence and structure databases (PDB, SWISS-PROT and TrEMBL); List of Gateways (NCBI, GOLD, MIPS, TIGR, UniGene)

Unit IV
Data: Access, Retrieval and Submission – Data access – standard search engines, Data retrieval tools – Entrez, DBGET and SRS (sequence retrieval systems); Software for data building; Submission of new and revised data.

Unit V
Sequence Similarity Searches – Sequence homology as product of molecular evolution; Sequence similarity searches; Significance of sequence alignment; Sequence alignment – global, local and free-space; Alignment scores and gap penalties; Measurement of sequence similarity; Similarity and homology.

Recommended Texts:


Reference Books
SEMESTER - I
BINF 405 – DATA STRUCTURES AND PROGRAMMING CONCEPTS

Unit - I
Concepts in Computing

Unit – II
Elementary Data Structures
Arrays, Stacks, Queues, Dequeues, Order Lists, Generalized List, Linear List, Linked lists, Circular Linked Lists, Doubly-Linked Lists, Infinite Lists, Hash tables, Hash functions, Recursive functions

Unit – III
Computing Algorithms
Algorithms in Computing, Analyzing algorithms, Designing algorithms – Sorting and Searching techniques: Bubble Sort, Merge Sort and Insertion sort – Binary Search

Unit IV
C
Algorithms, flow-charts, programming languages, compilation, linking and loading, testing and debugging, documentation – C programming – variables and identifiers, data types, Conditional statements and loops – if, if-else statements, while, do-while, for loop, switch case, Structured Programming, Library Functions

Unit V
Object Oriented Programming Concepts
C++ – Abstract Data type, Encapsulation, Object, Message, Method, class, Inheritance, Polymorphism, Virtual Functions, Abstract Classes, Interface, Constructors & Destructors, Overloading & Overriding, Copy Instructor

Reference Books

SEMESTER - I
BINF 406 – GENERAL BIOLOGY (Elective)

Unit I 7 Lectures
Molecules and Macromolecules of the Cell - Elements, molecules and macromolecules of the cell; Formation of macromolecules; Types of bonds; Structure of carbohydrates, lipids, DNA, RNA and proteins

Unit II 7 Lectures
Cell Structure and Functions – Unity and diversity in life forms; Structure of virus and bacteria; Features of prokaryotic and eukaryotic cells; Levels of biological organization – cell, tissue and organs.

Unit III 7 Lectures
Supramolecular Assemblies of the cell – Self assembly of macromolecules – ribosomes, chromosomes, membrane, collagen, actin and cellulose

Unit IV 8 Lectures
Energy and Cellular Work – Energy input and output in cell; The role of ATP; Electron transfer reactions; Electron transfer molecules; Electron transport chains; Light-driven electron flow; Catabolism and Metabolism; Metabolic pathways

Unit V 7 Lectures
Cell Cycle – Different phases of cell cycle; mitosis and meiosis; Regulation of cell cycle; Apoptosis

Recommended Texts:


Reference Books

SEMESTER - I
BINF 407 – COMPUTERS FOR BIOLOGISTS (Elective)

Unit I
7 Lectures
**Computer Organization**

Unit II
7 Lectures
**Network Basics**

Unit III
7 Lectures
**Introduction to Database systems**

Unit IV
8 Lectures
**Ms-Office**
Introduction to M.S. office package - Word – creating a new document – templates and wizards – scientific data representation and basic calculations with EXCEL - Creating Tables and databases using Access – interactive presentations creating using Power Point

Unit V
7 Lectures
**Internet Technologies**
Web Services – WWW, URL, DNS - Servers-E-mail server, WEB servers, Browsers-IP Addressing, IPV6.

Reference Books
Exercises in Cell Biology

1. Paper Chromatography of Chlorophyll pigments
2. Estimation of Chlorophyll
3. Ascorbic acid estimation in different tissues of plants and animals.
5. Estimation of cell mass of bacteria.

Exercises in Molecular Biology

1. Isolation & Purification of genomic DNA from bacteria
2. Isolation & Purification of plasmid DNA
3. Agarose gel electrophoresis of chromosomal & plasmid DNA
4. Restriction Digestion of chromosomal & plasmid DNA
5. Isolation of DNA fragment from agarose gel
Exercises:

1. Entrez and Literature Searches.
   a. PubMed
   b. PubMed central
   c. OMIM / OMIA
   d. Citation matcher

2. SRS of Biological Databases
   a. Nucleotide/ Genome Databases.
   b. Protein Sequence Database.
   c. Structure databases.
   d. Protein Pattern Databases

3. File format conversion
   a. FmtSeq
   b. ReadSeq
   c. Sequence manipulation Suite

4. Sequence Analysis
   a. Dot Plot
   b. Pairwise alignment
   c. Multiple Sequence Alignment

5. Phylogenetic analysis using PHYLIP, Phylodraw, PAUP, Treeview, JalView.

6. Softwares
   b. GeneDoc
   c. ClustalW / X, MEGA, MEME

7. Visualization Tool
   a. RasMol
   b. Cn3D
   c. MolMol
Exercises:

1. **DOS Commands - Internal Commands**: Viewing a directory, Changing Directory, Renaming a Directory - File operations: Creating files, removing a file, renaming files, viewing a file - External commands: Copying a disk, Comparing disks


3. **Working with Programs**: Basic Program Layout, WordPad Program, Scrolling in Documents, Moving Insertion Point, Delete & Insert Key, Selecting Text, Cut, Copy & Paste, Working with Multiple Programs.

4. **Files & Folders**: Organization, View Folder Structure, Working with Folders Search for Files, Organizing Workspace - Personal Desktop, Shortcuts, Start Menu, Start Properties, Display as Menu, Taskbar, Quick Launch.

5. **Windows Properties** - Navigating Control Panel, Changing Theme, Desktop Settings, Screen Saver Settings, Appearance Settings, Display Settings, Mouse Settings

6. **Working with documents**: Creating a document, Manage files and folders for documents, working with icons, editing documents - Text formatting and alignment, Indentation.

7. **Paragraph formatting** - Margins, tabs and page numbering.

8. **Working with tables and borders** - Printing - Working with Images and Text - Find and replace text - Mail merge.

9. **Creating and formatting a presentation** - Creation of a new Presentation, Adding Slides and Text to a Presentation, Editing Slide Text, Saving a Presentation, and Running a Slide Show - Adding Tables and charting data – Modifying objects and adding Images, Preparing to deliver a presentation.

10. **Creating and modifying a worksheet** - Formatting Worksheets – Working with multiple worksheets – Performing Calculations

11. **Surfing information using Search Engines**: Saving web pages to a disk, Composing E-mail, Sending E-mail.
SEMESTER- I  
BINF 454 – LAB - PROGRAMMING IN C/ C++

Exercises:


2. **C Programming:** Flowcharts, Algorithm, Keywords, Identifiers, variables, Constants, Scope of Life of variables- Local and Global variables. Data types, Expressions, Operators - Arithmetic operators, Logical operators, Relational, conditional, Bitwise operators - Input / Output Library functions.

   Declaration statement, Conditional statement: If statement, If…Else statement, Nesting of If…Else statement, Switch statement – Iteration statements - Arrays: Concept of Single and Multi-dimensional arrays, Array declaration, and initialization of arrays. Functions: User defined and library functions - File Handling: Opening a file, Closing a file, Reading and Writing into a file, Appending to a file

3. **C++:** I/O statements- Escape sequences- Comment lines - Expressions and Statements- Standard libraries - Prototype of main() function - Data types – Conditional Statements - Functions and variables - Classes and objects – Constructors and Destructors – Inheritance.
SEMESTER - II
BINF 421 – GENOMICS AND PROTEOMICS

Unit-I
7 Lectures
Organization of the prokaryotic and eukaryotic genomes; Genome maps and types; current sequencing technologies; partial sequencing; gene identification; gene prediction rules and softwares; Genome databases; Annotation of genome. Genome diversity: taxonomy and significance of genomes – bacteria, yeast, Caenorhabditis, Homo sapiens, Arabidopsis, etc.

Unit-II
7 Lectures
Microarray - Gene Expression, methods for gene expression analysis; DNA array for global expression profile; Types of DNA array, Array databases; Applications of DNA microarray – analysis of gene expression, differential gene expression under different conditions and during development of organisms.

Unit-III
7 Lectures
Human Genome - Mapping of Human Genome; Construction of physical maps; Basics of radiation hybrid maps; Sequencing of the entire human genome, annotation and analysis of genome sequences: sequence repeats, transposable elements, gene structure, pseudogenes; Gene analysis; gene order; chromosome rearrangement; compositional analysis; clustering of genes; composite genes. Implications of the Human Genome Project; Basics of Single Nucleotide Polymorphisms, detection and its implications.

Unit-IV
7 Lectures
The proteome and Proteome technology – Introduction; Expression proteomics (express profile); Cell map proteomics; Protein separation technology - 2D-Gel Electrophoresis, liquid chromatography, affinity chromatography (for cell map proteomics); mass spectroscopy and its uses in protein identification; Forward and Reverse Proteomics

Unit-V
8 Lectures
Protein-Protein Interactions – Yeast two hybrid, Co-Precipitation, Phage Display, Phylogenetic Profile, Domain fusion, Gene Neighborhood, Gene Cluster, Mirror Tree, Analysis of genome wide Protein-Protein Interactions in yeast, Genome wide yeast two hybrid analysis of other organisms, Protein fragment complementation assays.
Recommended Texts:

Reference Books
Unit-I  
**Classical and quantum mechanics** – Elementary introduction to Lagrangian and Hamiltonian formulation of mechanics; breakdown of classical mechanics; Planck theory of blackbody radiation; photoelectric effect; Bohr model of the atom; atomic spectra; De Broglie theory of matter waves; Schrodinger wave equation; interpretation of wave function; atomic orbitals; molecular orbitals; hybrid orbitals; valency of carbon atom; covalent bond; bond order; resonance structure of benzene; partial double bond; character of peptide bond.

Unit-II  
**Thermodynamics and energetics** – Thermodynamics systems; laws of thermodynamics; statement and applications; concepts of entropy and enthalpy; chemical potentials; free energy; Gibb and Helmholtz free energy; ATP as energy currency in biological systems; free energy of hydrolysis of ATP and other organophosphates.

Unit-III  
**Molecular Mechanics and Dynamics** – Basic principles; molecular representations; force fields; atom; atom pair potentials; bond length and bond angle and torsion angle potential; van der Waals and electrostatic potential – hydrogen bonding terms – MM3, AMBER, GROMOS, ECEPP/3 force fields; minimization techniques; line search and elementary introduction to gradient techniques; concepts of molecular dynamics.

Unit-IV  
**Protein and Nucleic Acid Structure** – Levels of protein structure – primary, secondary, tertiary and quaternary with examples; alpha helix, beta sheet and beta turn; domains and structural motifs; Rossmann fold, Immunoglobulin fold; Double helical structure of DNA – DNA polymorphism; RNA secondary and tertiary structure, with viruses – TMV, TBSV and HIV.

Unit-V  
**X-Ray Crystallagraphy and Spectroscopy** – Elementary description of crystallography; crystal growth, data collection, structure solution, refinement and interpretation; concept of resolution, IR spectroscopy, UV-visible spectroscopy; hyperchromism and hypochromism; Raman Spectroscopy; ‘finger printing’ using Raman spectra; complementarity of Raman and IR spectroscopy Fluorescence spectroscopy; NMR spectroscopy chemical shift; Fourier transform NMR spectroscopy; protein structure determination using NMR.

**Recommended Texts:**

Reference Books
Unit I 7 Lectures
Sequence Analysis – Methods of sequence alignment: graphic similarity comparison; Dot plots; Hash tables; Scoring matrices – identify matrix, genetic code matrices (GCM); Substitution matrices, Mutation Data Matrices (MDM), Percentage accepted Mutation (PAM). Block Substitution Matrices (BLOSUM), mutation probability matrices; Sequence similarity searches and alignment tools – dynamic programming algorithms; Needleman-Wunch and Smith Waterman; alignment scores and gap penalties; measurement of sequence similarity; percentage of identically aligned residues; Optimal global alignment and optimal local alignment;

Unit II 7 Lectures
Pairwise Sequence Alignment – Concept; Programmes (Dot matrix, Dot plot, Dynamic programming); Similarity Searches; Sequence repeats and inversion; Database searching (BLAST and FASTA).

Unit III 7 Lectures
Multiple Sequence alignment (MSA) – significance; softwares (PIMA, Clustal, Pileup, ClustalW, Meme, MACAW); Considerations while choosing a MSA software for analysis; sensitivity and specificity of each software.

Unit IV 8 Lectures
Comparative Genome Analysis – Relevance of comparative genomics; orthologs and paralogs; Comparative genomics of prokaryotes; Minimal genome; Vertical and horizontal gene transfer. Comparative genomics of organelles; Comparative genomics of eukaryotes. Differences and similarities in genomes of organisms; Evolution of protein families; Applications of comparative genomics in reconstruction of metabolic pathways.

Unit V 7 Lectures
Phylogenetic analysis – Phylogenetics, cladistics and ontology; Phylogenetic representations – graphs, trees and cladograms; Classification and ontologies; Steps in phylogenetic analysis; Methods of phylogenetic analysis – similarity and distance tables, distance matrix method; Method of calculation of distance matrix (UPGMA, WPGMA); The Neighbour Joining Method; The Fitch/Margoliash method; Character-based Methods – maximum parsimony, maximum likelihood; Reliability of Phylogenetic trees; Steps in constructing alignments and phylogenies; Limitations of phylogenetic algorithms; Phylogenetic softwares – PAUP, PHYLIP, MacClade.
Recommended Texts:


Reference Books

SEMESTER - II  
BINF 424 – STATISTICS FOR BIOLOGISTS

Unit-I  
**Measures of central tendency**: Tabulation of data - Construction of a frequency table - Measures of central tendency – Arithmetic Mean, Median and Mode – Quartiles, Deciles and Percentiles – Geometric mean and Harmonic mean – Weighted arithmetic average – Crude and standardized death rate

Unit-II  
**Measures of dispersion**: Range – Inter quartile range – Mean deviation - Standard deviation and Coefficient of variation – Application of Lorenz curve

Unit-III  
**Linear correlation and regression**  
Scatter diagram – Correlation – Types of correlation - The coefficient of correlation – Properties of the coefficient of correlation – Rank correlation - Estimation using time series data - Linear regression - Fitting a straight line – Multiple regression

Unit-IV  
**Probability and probability distributions**: The concept of probability – Sample space – Independent events – Mutually exclusive events – Addition law of probability – Conditional probability – Bayes formula – Expected value – Variance – Binomial distribution – Poisson distribution – Normal distribution – Chi squared distribution – Students t distribution

Unit-V  
**Theory of Sampling and Theory of Queues**: The concept of sampling – Types of sampling – Techniques of probability sampling – Techniques of non-probability sampling – Sample size – Sampling error

Queues – Types of queues – Markov chains - The concept of dynamic programming – The use of statistics in information systems - The use of spreadsheets

**Recommended Texts:**


**Reference Books**

SEMESTER - II
BINF 425 – PROGRAMMING IN JAVA

Unit I 6 Lectures
Java Basics - Importance and features of java, Modifiers, Access Controls, Data types, Expressions, Declarations, Statements & Control Structures, Program Structures, String handling, Packages, Interfaces, Working with java util Package, Garbage Collection, Object Class

Unit II 8 Lectures
Exception Handling, I/O & JDBC – Exception Handling: Fundamentals exception types, uncaught exceptions, throw, throw final, built in exception, creating your own exceptions, Input Stream & Output Stream: Streams, Byte and Character stream, Predefined streams, Reading and Writing from Console and Files, Buffered Reader & Writer, Serialization, Data Compression, Using Standard Java Packages (lang, util, io, net) Database: JDBC Architecture, JDBC Basics, JDBC Drivers, Connecting to Database and accessing databases

Unit III 7 Lectures

Unit IV 7 Lectures

Unit V 8 Lectures
BioJava - Installing BioJava, Symbols, Basic Sequence Manipulation (DNA to RNA, Reverse Complement, motif as regular expression), Translation (DNA to Protein, Codon to amino acid, Six frame translation), Proteomics (Calculate the mass and pl of a peptide), Sequence I/O (File Formats conversions), Locations and Features (PointLocation, RangeLocation, Feature modifications), BLAST and FASTA (Blast and FastA Parser, extract information from parsed results), Counts and Distributions, Weight Matrices and Dynamic Programming, User Interfaces.

Reference Books

SEMESTER - II
BINF 426 – RELATIONAL DATABASE MANAGEMENT SYSTEM

Unit-I

Unit-II
Data models – ER Model: Keys, Constraints, Design Issues, Extended ER features, Reductions of ER Schema to Tables. Relational Model: Structure, Relational Algebra; Hierarchical Model, Network Model, Object Oriented Model

Unit-III
Structured Query Language – Basic Structure, Set Operations, Aggregate Functions, Null Values, Nested Sub queries, Views, Integrity: Domain constraints, Joined Relations, Data-Definition Language, Embedded SQL, Dynamic SQL

Unit-IV

Unit-V
Concurrency control techniques & Information retrieval – Locking techniques, Granularity of Data Items – Database System Architecture and Information retrieval: Centralized and Client-Server Architecture, Distributed DBMS, Data Mining, Data Integration, Data Warehousing

Recommended Texts:
SEMESTER - II  
BINF 427 – FUNDAMENTALS OF ALGORITHMS

Unit – I  
Computing Algorithms  
7 Lectures
Algorithms in Computing, Analyzing algorithms, Designing algorithms, Asymptotic notation, Standard notations, Big ‘O’ notations, Time and space complexity of algorithms and common functions
Sets: Union and Intersections, Differences, Disjoint Sets, Counting Elements, Relations
Matrices: Adding and Multiplying, Extracting a sub-matrix, Combining, Inverting

Unit – II  
Sorting, Searching & Strings Matching  
8 Lectures
Sorting: Bubble Sort, Insertion sort, Selection sort, Quick Sort, Radix sort, Exchange sort, Shell sort, Mergesort. External sort (K-way mergesort, balanced mergesort, polyphase mergesort) Sorting in Linear time, Heaps (Binary Heaps, Janus Heap, Heap sort, Binomial Heaps, Fibonacci Heaps) Searching: Binary Search, Fibonacci Search, Hash Search, Lookup Searches, Generative Searches
String Matching: Naïve algorithm, Boyer-Moore algorithm, Knuth-Morris-Pratt algorithm

Unit – III  
Graphs  
7 Lectures
Representation of Graphs, Breadth First Search, Depth First Search, Topological Sort, Connected Components, Minimum Spanning Tree, Single-Source Shortest Path (Dijkstra’s and Bellman Fort Algorithm), All-Pairs Shortest Paths (Floyd-Warshall algorithm), Coloring of Graphs (Kruskal’s Algorithm, Prim’s Algorithm),

Unit – IV  
Trees  
7 Lectures
Forests, DAGs, Ancestors, and Descendants, Binary Search Trees, Querying a Binary search tree, Insertion and Deletion, Tree Traversals, Red-Black Trees, Properties of Red-Black Trees, AVL-Trees, Rotations, Insertion, Deletion, B+ Tree, B* Trees.

Unit – V  
Algorithm Design and Analysis  
7 Lectures
The substitution method, The iteration method, The master method, Divide and Conquer, Greedy Algorithms, Dynamic Programming (Traveling Sales Person Problem, Hamiltonian Path Problem), Backtracking Algorithms (8-queens Problem, Graph Coloring), Branch and Bound Algorithms

Recommended Texts

2. Ellis Horwitz, Sartaz Sahani and Sanguthevar Rajasekaran,(1999),“Computer Algorithms!”, Galgotia Publications
SEMESTER - II
BINF 455 – LAB - PROGRAMMING IN JAVA

Exercise in JAVA

2. Writing Pseudo Codes.
3. Working with Objects, Arrays, Conditionals and Loops.
4. Creating Classes and Applications in Java.
7. Managing Simple Events and Interactivity.
8. Creating User Interfaces with AWT, Modifiers.
9. Packages and Interfaces, Exception, Multithreading.
10. Streams and I/O, Using Native Methods and Libraries.
Exercise in RDBMS (MYSQL)

Data Definition Language (DDL) statements:
Creating database, Selecting database, Deleting database, Creating table, Modifying Table, Deleting table

Data Manipulation statements:
Inserting, updating and deleting records
Retrieving Records
Retrieving specific rows and columns
Use of MySQL operators – Arithmetic operators, Comparison Operators, Logical operators
Math functions, Aggregate functions
String operations
Limiting, Sorting and grouping query results
Handling null values
Renaming or aliasing table and column names
Using subqueries
Using Joins – joining a table to itself, joining multiple tables
Use of Indexes
Security Management
Granting and Revoking rights on tables
Exercises:

1. Sequence Analysis Packages – EMBOSS, NCBI ToolKit
2. Dynamic programming.
3. Analysis of Biological Sequences.
   a. Basic Blast
   b. Specialized Blast
4. FASTA
5. Multiple sequence alignment
6. MEME/MAST, eMotif, InterproScan, ProSite, ProDom, Pfam
7. Phylogenetic analysis – PAUP, PHYLIP, MacClade
8. Genome annotation – Artemis.
9. Hypothetical Protein analysis
10. Genome Comparison
SEMESTER - III
BINF 501 – STRUCTURAL BIOLOGY

Unit-I 7 Lectures
Structural features of biomolecules; techniques used to determine the structure of biomolecules;
Methods for single crystal X-ray Diffraction of macromolecules: molecular replacement method
and direct method – Fiber diffraction; analysis of structures and correctness of structures;
submission of data to PDB: atomic coordinates and electron density maps.

Unit-II 7 Lectures
Anatomy of proteins; Ramachandran Plot; secondary structures; motifs; domains; tertiary and

Unit-III 7 Lectures
Methods for prediction of secondary and tertiary structures of proteins – knowledge-based
structure prediction; fold recognition; ab initio methods for structure prediction, Comparative
protein modeling.

Unit-IV 7 Lectures
Methods for comparison of 3D structures of proteins; Methods to predict three dimensional
structures of nucleic acids, rRNA; Electrostatic energy surface generation.

Unit-V 8 Lectures
Molecular Mechanics and Molecular dynamics of Oligopeptides, Proteins, Nucleotides and small
molecules – Mechanism and dynamics of bio-macromolecules, Simulation of molecular
mechanics and dynamics, Simulations of Free energy changes; Force fields. Molecular
interactions of protein-protein, protein-DNA, protein-carbohydrate and DNA-small molecules.

Recommended Texts:

   Edition, Prentice Hall, USA
   Freeman and Company, New York, USA.

Reference Books

   Laboratory Press, New York.
   Publications, USA.
SEMESTER - III
BINF 502 – MOLECULAR MODELING AND DRUG DESIGNING

Unit-I 5 Lectures
Concepts in Molecular Modeling – Introduction; Coordinate System; potential energy surfaces molecular graphics; Computer hardware and software; Mathematical concepts – introduction of molecular mechanics & quantum mechanics.

Unit-II 8 Lectures
Molecular Mechanics – Features of molecular mechanics, force fields; Bond structure and bending angles – electrostatic, van der Waals and non-bonded interactions, hydrogen bonding in molecular mechanics; Derivatives of molecular mechanics energy function; Calculating thermodynamic properties using force field; Transferability of force field parameters, treatment of delocalised $pi$ system; Force field for metals and inorganic systems – Application of energy minimization.

Unit-III 7 Lectures
Molecular Dynamics Simulation Methods – Molecular Dynamics using simple models; Molecular Dynamics with continuous potentials and at constant temperature and pressure; Time-dependent properties; Solvent effects in Molecular Dynamics; Conformational changes from Molecular Dynamics simulation.

Unit-IV 8 Lectures
Molecular Modeling in Drug Discovery – Deriving and using 3D pharmacophore; Molecular Docking; Structure-based methods to identify lead compounds; de novo ligand design; Applications of 3D Database Searching and Docking

Unit-V 8 Lectures
Structure Activity Relationship - QSARs and QSPRs, QSAR Methodology, Various Descriptors used in QSARs: Electronic; Topology; Quantum Chemical based Descriptors. Use of Genetic Algorithms, Neural Networks and Principle Components Analysis in the QSAR equations.

Recommended Texts:


Reference Books
Unit-I 8 Lectures

Unit-II 7 Lectures
Regular expressions and Pattern Matching – Uses of Regular Expressions, Patterns, Single-Character Patterns, Grouping Patterns (Sequence, Multipliers, Parentheses as memory, Alternation) Anchoring Patterns, Precedence, Matching Operators, Ignoring Case, Different Delimiter, Variable Interpolation, Special Read-Only Variables, Substitutions, Split and Join Functions, Dynamic Programming, Approximate String Matching

Unit-III 7 Lectures
Common Gateway Interface - Gene.pm, Arrow notation (->), AUTOLOAD, Cleaning unused objects with DESTROY URL Encoding, CGI Environment Variables, Handling forms, Accessing form Input, Extra Path Information, CGI.pm Module, Passing Parameters via CGI, Less Typing, Sever Side Includes, Debugging CGI programs, Stepping through programs, Breakpoints, Line Action

Unit-IV 7 Lectures

Unit-V 7 Lectures
BioPerl – Installing Bioperl, General Bioperl Classes, Sequences (Bio::Seq Class, Sequence Manipulation), Features and Location Classes (Extracting CDS), Alignments (AlignIO), Analysis (Blast, Genscan), Databases (Database Classes, Accessing a local database), Implementing REBASE

Reference Books
SEMESTER - III
BINF 504 – APPLICATIONS OF BIOINFORMATICS

Unit-I 7 Lectures
Profile analysis – Expression profile analysis of cells, Mining data from Yeast. Microarray and genome wide expression analysis: transcriptomes, proteome: Genomics in medicine, disease monitoring, profile for therapeutic molecular targeting.

Unit-II 7 Lectures
Reconstruction of pathways and annotation – Reconstructing metabolic pathways from sequence and function information in microbial species; statistical profiling and function annotation of genomes with a microbial genome as an example.

Unit III 7 Lectures

Unit-IV 8 Lectures
Systems Biology - Objectives of Systems Biology, Strategies relating to In silico Modeling of biological processes, Metabolic Networks, Signal Transduction Pathways, Gene Expression Patterns. E-cell and V-cell Simulations and Applications.

Unit-V 7 Lectures

Recommended Texts:
SEMESTER - III
BINF 505 – NETWORKS AND DISTRIBUTED COMPUTING

Unit – I 6 Lectures
Nuts & Bolts in Networks
Reference Model, Network Topologies and Protocols, Types of Networks: Local Area Network (LAN), Wide Area Network (WAN), Metropolitan Area Network (MAN), Network Security (Firewall, Packet Filtering, VPN), Uses of Computer Networks

Unit – II 9 Lectures
Network Architecture
OSI & Internet Architecture, IEEE 802 standards, Physical Layer - Transmission Media, Switching. Data Link Layer - Design Issues, Example Data Link Protocols, Data Link layer in the Internet, Media Access Sub layer

Unit – III 8 Lectures
Network Layer and Transport Layer

Unit – IV 8 Lectures
Application Layer
Design Issues, Conventional Encryption, Classical and Modern Techniques, Encryption and Decryption Algorithms (RSA), Confidentiality, DNS, SNMP, RMON, WWW, E-mail, Digital Signatures

Unit – V 7 Lectures
Characteristics of Distributed Computing
Introduction to Distributed Computing, Examples, Key Characteristics, Historical background, Basic design issues, User requirements
Introduction to IPC, Building Blocks, Client Server Communication, Group Communication, Remote Procedure Call (RPC).

Recommended Texts:
This course is designed to introduce the bioinformatics students to standard scientific presentation formats and to provide a forum to practice/improve oral and written communication skills.

1. **Readings, writing exercises and in-class discussion** – Students (in small groups) will lead in-class discussions on assigned readings and writing exercises.

2. **Individual oral presentation** – Students select a research project/topic and present results as an oral presentation followed by a Q&A session.

3. **Individual Poster presentation** – Students select a research project/topic and present results as a poster followed by a Q&A session.

**Recommended Texts:**
Exercises

1. Advanced Visualization Software and 3D representations.

2. Coordinate generations and inter-conversions.

3. Secondary Structure Prediction

4. Fold Recognition, *ab initio* (Rosetta Server)


7. Validation of models.
   a. WHATIF
   b. PROSA
   c. PROCHECK
   d. VERIFY 3D

8. Protein Structure Alignment.

9. Modeller

10. Geno-3D

11. Discovery Studio Server.
Exercise:

1. Binding Site Identification.
2. Pharmacophore Identification
3. Rigid body Docking using AutoDock and ADT
4. Molecular dynamics simulations using Gromacs
5. Visual molecular Dynamics (VMD)
6. Docking with LigandFit (Discovery studio)
7. Receptor and Ligand Optimization.
8. Conformational Analysis
9. BABEL, MOPAC
SEMESTER - III
BINF 553 – LAB - PROGRAMMING IN PERL

Exercise in Structured Programming


Exercise in Regular Expressions

Uses of Regular Expressions, Patterns, Single-Character Patterns, Grouping Patterns (Sequence, Multipliers, Parentheses as memory, Alternation) Anchoring Patterns, Precedence, Matching Operators, Ignoring Case, Different Delimiter, Variable Interpolation, Special Read-Only Variables, Substitutions, Split and Join Functions, Dynamic Programming, Approximate String Matching

Exercise in CGI

URL Encoding, CGI Environment Variables, Handling forms, Accessing form Input, Extra Path Information, CGI.pm Module, Passing Parameters via CGI, Less Typing, Sever Side Includes, Debugging CGI programs, Stepping through programs, Breakpoints, Line Action

Exercise in CPAN Database Modules

DBM Databases and DBM Hashes, Design of DBI, DBI Methods, DBI Environment Variables, DBD Interface Modules, Fixed Length Random-Access Databases, Variable-Length Databases, Win32 Database Interface, Perl Graphics, Using the GD.pm graphics library

Exercise in Bioperl

Installing Bioperl, General Bioperl Classes, Sequences (Bio::Seq Class, Sequence Manipulation), Features and Location Classes (Extracting CDS), Alignments (AlignIO), Analysis (Blast, Genscan ), Databases (Database Classes, Accessing a local database), Implementing REBASE
SEMESTER - III
BINF 520 – BIOETHICS AND INTELLECTUAL PROPERTY RIGHTS

Unit-I 9 Lectures
The legal and socioeconomic impacts of biotechnology; public education of the process of the processes of biotechnology involved in generating new forms of life for informed decision making

Unit-II 6 Lectures
Biosafety regulation and national and international guidelines; rDNA guidelines; Experimental protocol approval; levels of containment

Unit-III 5 Lectures
Environmental aspects of biotechnology applications; Use of genetically modified organisms and their release in environment; Special procedures for rDNA-based product production.

Unit-IV 9 Lectures
General principles of Intellectual property rights (IPR); Patents and methods; application of patents; Legal implications; International treaties for protection of IP – Bern, Paris, TRIPS, WIPO treaties, Biodiversity convention, etc.

Unit-V 7 Lectures
Biodiversity and farmers rights; Beneficial applications and development of research focus to the need of the poor; Identification of directions for yield effect in agriculture, aquaculture, etc; Bioremediation

Recommended Texts:
Unit-I 5 Lectures
Team Work – Interpersonal skills, Behavioural attitude, People management – Intrapersonal skills, Personality development, Clean and healthy living tips.

Unit-II 4 Lectures
Organizational Behaviour – Goal setting, Individual goal, Organizational goal.

Unit-III 4 Lectures
Time Management – Planning, Scheduling

Unit-IV 4 Lectures
Ethics, Values, Attitudes.

Unit-V 4 Lectures
Indian Culture and Heritage
The course is designed to result in the satisfactory completion and defense of the Masters dissertation.

This process includes

a) the conceptualization of the independent research that will comprise the dissertation,
b) the preparation of and satisfactory defense of the dissertation proposal,
c) the collection, analysis, and interpretation of data,
d) presentation of findings in the dissertation format, and
e) oral defense of the dissertation.

Dissertation activity must be completed within prescribed time frame for the semester.
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