Bioinformatics Syllabus

Course Description:

BINF 701/702 is the bioinformatics core course developed at the KU Center for Bioinformatics. The course is designed to introduce the most important and basic concepts, methods, and tools used in Bioinformatics. Topics include (but not limited to) bioinformatics databases, sequence and structure alignment, protein structure prediction, protein folding, protein-protein interaction, Monte Carlo simulation, and molecular dynamics. Emphasis will be put on the understanding and utilization of these concepts and algorithms. The objective is to help the students to reach rapidly the frontier of bioinformatics and be able to use the bioinformatics tools to solve the problems on their own research.

Instructors:

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- Ilya Vakser, Email: vakser@ku.edu, Phone: 785-864-1057
- John Karanicolas, Email: johnk@ku.edu, Phone: 785-864-4683

Schedule:

2:00-2:50pm, MWF

Homework & Exams:

There will be several homework assignments that will constitute 50% of your grade. The final examination constitutes another 50% of your grade.

Student evaluation and grades:

The grading scale will be:
A = 90-100%
B = 80-89
C = 70-79
D = 60-69
F = below 60

Textbook:

A textbook is not required for this course. Assigned materials will either be handed out to the class or posted on the blackboard website.
Course policies:

Attendance and class participation are expected. Repeated absences without approval or valid justification will result in the reduction of the grade for the course.

Late assignments will be docked 10% for being late, and an additional 10% for each additional day they are late.

Cheating and Plagiarism will be considered academic misconduct and therefore subject to the University Senate Rules and Regulations Section 2.6.1-7. Briefly, if a student represents someone else’s work for their own (either by cheating or plagiarism) in any classroom examination or assignment without making the proper acknowledgement of that work, it will be deemed academic misconduct. All work, either in class or on an assignment, is expected to be your own work. Homework: the penalty for the first offense will be a reduction in grade to a zero (F) for that specific work. The penalty for a second offense will be a reduction in grade assignment to F for the course. Exams: the penalty for the first offense will be a reduction in grade to F for the course. For more information on academic misconduct, please see

Table of content

PART I: BIOINFORMATICS BASICS

1. Introduction (Ilya Vakser)
   1.1. What is bioinformatics
   1.2. Principles of protein structure
      1.2.1. Tertiary structure
      1.2.2. Qaternary structure
      1.2.3. Similarity of ternary and quaternary structure

2. Bioinformatics databases (John Karanicolas)
   2.1. Introduction
   2.2. Nucleotide sequence databases
   2.3. Protein sequence databases
   2.4. Sequence motif databases
   2.5. Protein structure databases
   2.6. Other relevant databases

3. Alignment (Ilya Vakser)
   3.1. Similarity and Homology
   3.2. Types of divergence
   3.3. Conserved regions
   3.4. Methodological principles
   3.5. Substitution scores
   3.6. Insertion/deletion scores
   3.7. Statistical significance
   3.8. Database search
   3.9. Multiple alignment
   3.10. Structure alignment
   3.11. Matching algorithms
   3.12. Searching 3D Databases
   3.13. Classifying 3D shapes

PART II: BIOMOLECULAR SIMULATIONS

4. Basic concepts (Wonpil Im)
   4.1. Units and derivatives
   4.2. Force field and energy landscape
   4.3. Truncation of nonbonded interactions

5. Conformational Sampling (Wonpil Im)
   5.1. Introduction
   5.2. Minimization and algorithms
   5.3. Molecular dynamics
5.4. Ensembles (statistical mechanics)
5.5. Monte Carlo simulations

6. Solvation (Wonpil Im)
   6.1. Introduction
   6.2. Periodic boundary condition
   6.3. Ewald summation
   6.4. Implicit solvent model and continuum electrostatics
   6.5. Monte Carlo simulation on parallel computers

7. Advanced Techniques (Wonpil Im)
   7.1. Introduction
   7.2. Replica-exchange simulations
   7.3. Restraint potentials
   7.4. Free energy calculations
   7.5. Membrane simulations

PART III: PROTEIN STRUCTURE AND DESIGN

8. Protein secondary structure (John Karanicolas)
   8.1. Introduction
   8.2. Hydrogen bond
   8.3. Defining a secondary structure element
   8.4. Methods for predicting secondary structure

9. Experimental methods for protein structure determination (John Karanicolas)
   9.1. X-ray crystallography
   9.2. Nuclear magnetic resonance (NMR)

10. Protein tertiary structure modeling (John Karanicolas)
    10.1. Basic concepts
    10.2. Protein folding and dynamic simulation
    10.3. Modeling protein sidechains
    10.4. Comparative modeling
    10.5. Threading
    10.6. Ab initio modeling
    10.7. Combined modeling approaches
    10.8. CASP: A blind protein structure prediction competition

11. Introduction to protein design (John Karanicolas)
    11.1. “Rational” design efforts
    11.2. Experimental methods (directed evolution)
    11.3. Computational protein design
PART IV: PROTEIN INTERACTION

12. Protein quaternary structure modeling (Ilya Vakser)
   12.1. Basic concepts
   12.2. Energy landscapes
   12.3. Docking algorithms – foundation
   12.4. Docking algorithms – current & future
   12.5. Docking example
   12.6. CAPRI
   12.7. Protein Structure Initiative
   12.8. Computational proteomics

13. Designing protein-protein interfaces (John Karanicolas)
   13.1. Designing for affinity
   13.2. Designing for specificity