CS612: Algorithms in Bioinformatics – Syllabus

Nurit Haspel

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Course Description and Objectives

This course will introduce students to bioinformatics – the area concerning the development and application of computational methods to address key problems in biology. It will introduce the students to a variety of methods and skills required to conduct research in this highly rising field. The emphasis of the course is structural bioinformatics with focus on various computational methods to simulate, analyze and model protein structure, dynamics and function. Other subjects such as systems biology, genomics and interaction networks will be introduced as well. The course is designed first and foremost for computer scientists but is also open to biology majors with adequate computational/mathematical background, subject to permission from the instructor.

Prerequisites

- CS210 (intermediate computing with data structures)
- MATH260 (linear algebra) or permission from the instructor.
- Knowledge in biology is not required but is an advantage. This is a CS graduate course but highly motivated undergraduate students and biology majors with adequate background are welcome to register.

Textbooks

All of the course materials will be available online. There is no required text book. The following books are highly recommended:

- Structural Bioinformatics, 2nd edition, Jenny Gu and Philip E. Bourne. Wiley - Blackwell, 2009.
- Introduction to Bioinformatics by A. Lesk, 3rd edition, Oxford University Press, 2008.

Topics (Approximate)

Week	Topic	Recommended
1	Introduction to molecular biology: basic concepts in biochemistry and bioinformatics, what are proteins and why they are important.	Gu chapter 1.
2-3	Database search and sequence alignment: BLAST and FASTA algorithms, the BLAST web server, Multiple sequence alignment.	Lesk chapter 1
4	Introduction to protein structure: Protein structure, the protein folding problem, protein structure visualization and classification.	Gu chapters 2,
5-6	Protein folding: Folding methods homology modeling, threading, ab-initio folding. Folding models, folding vs. protein structure determination, AlphaFold and LLM	 Gu chapters 28 Gu chapters 28
7-8	Biomolecular simulations: Molecular dynamics, monte carlo. Applications of MD, force fields and energy models. Geometry based methods: Transformations, distance measurement	Gu chapters 8, Gu chapter 37. Gu chapter 8,
9	introduction to geometric hashing. Geometry based methods (cont.): Geometric hashing in docking, Geometric hashing and its applications in protein structural alignment.	 Gu chapter 16.
10	introduction to Robotics applications in bioinformatics. Geometry based methods (cont.): Robotics-based methods and their applications in folding,	 Gu chapter 27.
11	flexible docking and conformational search.	Gu chapter 27.
12	Dimensionality reduction techniques	
13	Other topics in bioinformatics: Systems biology, networks.	Lesk chapter 7
14	Other topics in bioinformatics: Evolutionary biology, data mining. Course review and introduction to topic presentations.	 Lesk chapter 5

Assignments and Grading

The following grading scheme is subject to change (I will do my absolute best to not change it and if I do, I'll let you know):

- Homework assignments (4-5 of them) – 70% of your final grade.
- Course project and presentation – 30% of your final grade.

You must have a documented reason to schedule a makeup exam. I must know that you need a makeup exam within 2 days after the exam date.

Final Grade

Your final grade will be calculated using the following table. The minimum standard for passing a graduate course is a percentage score of 60% or C. Keeping this in mind, your grade for the course will be calculated using the following table. Assume your final percentage score for the course is P:

$P > 90$	A
$85 < P \leq 90$	A-
$80 < P \leq 85$	B+
$75 < P \leq 80$	B
$70 < P \leq 75$	B-
$65 < P \leq 70$	C+
$60 < P \leq 65$	C
$P < 60$	F

Accommodations

Section 504 of the Americans with Disabilities Act of 1990 offers guidelines for curriculum modifications and adaptations for students with documented disabilities. If applicable, students may obtain adaptation recommendations from the Ross Center for Disability Services, M-1-401, (617-287-7430). The student must present these recommendations and discuss them with each professor within a reasonable period, preferably by the end of Drop/Add period.

Student Conduct

Students are required to adhere to the University Policy on Academic Standards and Cheating, to the University Statement on Plagiarism and the Documentation of Written Work, and to the Code of Student Conduct as delineated in the catalog of Undergraduate Programs, pp. 44-45, and 48-52. The Code is available online at:

https://www.umb.edu/academics/seas/undergraduate-studies/academic-policies/code-of-student-conduct/

AI is prohibited

In this class, all work submitted by students must be generated by the students themselves. Students should not have another person or entity do the writing of any portion of an assignment; this includes hiring a person or a company to write assignments and using AI tools like ChatGPT. All work submitted must contain citations for any material that has been quoted or referenced. If students are unsure about whether or not a source is appropriate to use in the assignment, they should contact the instructor.

Class email

Should I need to send the class an e-mail, I will use your umb address (`firstname.lastname<number>@umb.edu`. The number is usually 001). Please make sure you check it regularly, including your junk mailbox.

Homepage

The course home page is `http://www.cs.umb.edu/ nurith/cs612`.