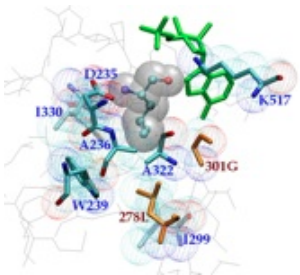
CS 89/189, Spring 2012
Computational Structural Biology



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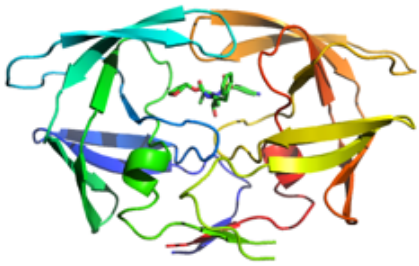
HIV-1 protease + drug


influenza hemagglutinin

Course description

This course will explore how computer science can help in the rational design of proteins, drugs, and vaccines. For example, in protein design we will look at approaches for optimizing mutations, or even entirely new proteins, to be harnessed in applications ranging from biofuels to biosensors. In drug design, we will study algorithms for discovering new lead compounds, and for mining the relationships between properties of molecules and their activities. In vaccine design, we will see how to train immunogenicity predictors and use them to develop specifically targeted vaccines. We will find that these and other such applications raise numerous interesting and challenging problems requiring the development of appropriate models and algorithms.

Prereqs: none. In particular, a background in biology / biochemistry is not required, and the basics will be introduced in context. At the same time, no specific CS courses are required as prereqs, though readings and discussions will often assume familiarity with core concepts (as in CS 5 and 8).

Administrative info

Instructor
Gevorg Grigoryan | 113 Sudikoff | office hours: by appointment

Class meetings
2A | TuTh 2:00-3:50 | 214 Sudikoff

Textbook
None recommended, we'll be reading papers. However, a decent book on the subject is "Introduction to Proteins: Structure, Function, and Motion" by Amit Kessel, Nir Ben-Tal (see Amazon link).

Course materials
Blackboard will serve as an exchange platform. I will set up the schedule, including topics and primary readings; presenters will post presentations; others will post critiques; all will share supplementary resources. Help develop a comprehensive survey of the material!
I've also set up a public page with the reading list.

Coursework

This seminar course will introduce and study topics by way of primary literature, from seminal papers to results hot off the presses. All students will present papers and participate in discussions; graduate students will also do paper critiques (undergraduates are welcome to, since it's good practice). The seminar will culminate in final projects offering the opportunity to dive more deeply into topics of interest.

Presentations (30% undergrad; 25% grad)
Critically present the material in and underlying the reading, addressing the following:

- The core problem and its context, including why other methods (computational and/or experimental) are insufficient.
- The approach, including how the computational methodology captures and helps address the problem.

- The validation of the approach, including how it is demonstrated to improve the state of the art.
- Strengths and weaknesses of the approach and the paper, and possible next steps.

Help everyone get the big picture and background (since much of the material will be new and challenging), and then provide your insights into the contribution. Try to engage everyone else in a discussion (see class participation below).

The slides and a brief summary are due on blackboard before class.

Follow general advice on how to give a good talk (e.g., by Bruce Donald, Hany Farid, and Simon Peyton-Jones).

I will set up a queue of papers and solicit your preferences for when and what to present. I'm also glad to take your suggestions for specific papers on these topics that you would like to present (or would like to add to the queue). In some cases, additional reading will be required to prepare a presentation; I'm glad to help identify materials.

Participation (20% undergrad; 15% grad)
Don't leave the presenter dangling up there! Read the paper(s) thoroughly before class, so that you also can have critical insights into the material. Give your perspectives, ask and respond to questions, raise additional points, etc.

Project (50% undergrad; 45% grad)
Do an in-depth exploration of a relevant topic, worthy of (about) half the grade for the course. The project may be done individually or in a group (recommended), and may include a project- & student-appropriate mixture of research, implementation, and application. A project proposal and a project update will ensure that we are on the same page as to the project's suitability; a project presentation will make for a fun class-wide exchange; a project report will document what was done and what was learned.

Critiques (extra credit undergrad; 15% grad)
For six different papers, not including what you present, write a *short* (2-3 paragraph) critique, including the points discussed above for presentations. Don't just repeat what you read in the abstract, introduction, and conclusion, but instead use your own background and experience for a unique critical perspective. Don't be overwhelmed by jargon and details, but try to cut through all that to the essence of the contribution.

The critique is due on the blackboard before class.

This is essentially a short review, and there's also plenty of general advice out there for reviewing papers (e.g., by Alan Jay Smith and Ian Parberry).

Honor code

Dartmouth's honor code applies to this course, and academic misconduct policies will be strictly enforced. If you have questions, ask!

As this is a seminar course, you are encouraged and expected to discuss the material with others. You are also encouraged to work in teams for the project. So the only real pitfalls are attribution: the work you present as your own must in fact be your own. In particular, you must write your critiques yourself, in your own words. You must also create your own presentation slides, though you may incorporate others' images and text, with citation. And in your project, while you certainly may use and build upon others' code, you must clearly indicate what part is your contribution.

Disabilities

Students with disabilities enrolled in this course and who may need disability-related classroom accommodations are encouraged to make an appointment to see the instructor before the end of the second week of the term. All discussions will remain confidential, although the Student Accessibility Services office may be consulted to discuss appropriate implementation of any accommodation requested.