Spring 2019
COMP-150 CSSB – Computational Systems Biology

Prof. Soha Hassoun
Department of Computer Science
School of Engineering
Tufts University

Course Overview
This course will provide an overview of computational systems biology focusing on select topics in biochem-informatics, metabolic network constructions and analysis, and metabolomics. Students will explore concepts through reading papers from the literature, using various toolboxes, and by writing software to design and/or collect and analyze data from biological databases. A term project will require students to define a computational challenge in systems biology and implement and evaluate a solution.

Instructor
Professor Soha Hassoun
email: soha@cs.tufts.edu; Office Telephone: x7-5177 (voice mail gets forwarded as email)
Office hours: By Appointment

Course Goals and Learning Objectives
1. Goal: Students will learn the organization of one or more biological databases in order to efficiently retrieve desired information. By the end of the course the student should be able to:
   • Explain the organization of the KEGG database
   • Augment existing biopython package functions to access various parts of the KEGG database
   • Implement and analyze a case study involving the use of data in a database

2. Goal: Students will learn fundamental concepts for representing and comparing molecular structures. By the end of the course the student should be able to:
   • Assess the merits and shortcomings of different molecular representations
   • Analyze various algorithms to compute molecular similarity
   • Evaluate molecular similarities using various metrics

3. Goal: Students will learn foundational concepts for metabolic network. By the end of the course the student should be able to:
   • Provide evidence why metabolic network are hierarchical and modular
   • Describe the process required for network construction
   • Create mathematical models that represent metabolic networks
   • Compute steady-state flux balance and variability analysis for a metabolic network using constraint-based techniques
   • Critique various synthesis pathway construction algorithms
   • Use the COBRA toolbox to evaluate steady-state behavior and the yield of various synthesis pathways

4. Goal: Students will learn fundamentals of measuring and identifying metabolites using mass spectrometry. By the end of the course the student should be able to:
   • Discuss tandem mass spectrometry technologies
   • Define the metabolite annotation problem
   • Critique algorithmic solutions for metabolite annotation
Prerequisites
Proficient in programming (Python and/or MATLAB) and background in algorithms.

Textbooks
The class has no required textbook; handouts will be made available through the class webpage. The following are recommended but not required:


Computing Resources
It is expected that you will use your own laptop for performing all the work. All toolboxes that will be used will run both on MAC and Windows. You may choose to run your project on the Tufts cluster if it is computationally intensive. If you do not have access to a reliable laptop, please notify the instructor ASAP and she can set you up to work in the PC Lab in Halligan.

Communication
We will use your email posted on the official SIS listing to contact you or post announcements. For the most part, we will rely on piazza for communication.

Lectures
Lectures will be used to introduce new concepts and case studies and to discuss solutions. Attendance is not mandatory, but highly recommended. If you will miss class, please drop the instructor a note ahead of time to explain your absence. Please see the class calendar for the materials that you missed.

Blogs (to be further discussed in class)
Each week, 50% of students are expected to write a weekly blog due on Thursdays at noon on Piazza. The other 50% of the class will have till Friday 4pm to comment on the blogs. A student can respond to a blog if they were blog writers for that week. A student may respond to more than one blog every week. The blog should focus on a concept/idea that is either biological or computational that is relevant to the material presented in class the prior week. The blog should cover any of the following:

a. Ask critical questions that were not answered by the article
b. A concept that was difficult for you to understand but you were able to understand either through the paper or through supplementary reading
c. A concept that intrigued you, where you did additional research on the topic (historical, comparative, ..)
d. A concept that connected with another concept from earlier material in the class
e. A result that surprised or that you would like to challenge. Detailed explanation of the experimental setup and analysis is required
f. A conceptual idea of a tool or a research study.

Once you start your project, that blog entry can be relevant to your project, including requesting feedback on parts of the project write-up.

Homework
We will have about 4 homeworks to introduce the various concepts. The homeworks will consist of mostly programming assignments, and some data analysis.

Exams
There will be no exams

**Project**
Each student is expected to define a problem relevant to the material taught in the class, implement a solution, and evaluate the implementation using real biological data. The project will have a write up similar to that found in a published paper.

**Paper Critiques**
Each student will be responsible for presenting one technical paper to the class using slides. The presentation must introduce the problem, explain why it is important, and include a detailed critique of the method and the results.

**Late Work Policy**
Late assignments are penalized at 15% per 24 hours. No assignments will be accepted after 5 days. For excused late work, you will need to provide documentation from health services or your dean.

**Cheating Policy**
The Faculty of the School of Arts and Sciences and the School of Engineering are required to report suspected academic integrity violations to the Dean of Student Affairs Office. Any cheating will be reported immediately. There will be no exceptions. Please see [http://students.tufts.edu/student-affairs/student-life-policies/academic-integrity-policy](http://students.tufts.edu/student-affairs/student-life-policies/academic-integrity-policy)

Collaborative work is encouraged when specified as such, and you should document who you collaborated with and how the work was divided.

**Course Grading**
Please get back to the instructor or TA regarding any disputes for grades within a week of handing out the grades. 100-90% = A, 90-80% = B, 80-70% = C, 70-60% = D, <60% = F.
- Blogs 20%
- Class participation 10%
- Homeworks 20%
- Paper Critique 10%
- Project 40%

**Feedback**
Your thoughts and concerns about this course are important. You are encouraged to give feedback to the instructor throughout the term.