Final Project Instructions

CS/CME/BIOPHYS/BIOMEDIN 279

Due: December 4, 2015 at 3:00 PM

1 Description

The goal of this project is to allow you to explore something from the class in more detail. You can work *individually* or in groups of *up to three students*. The project is meant to involve the same amount of work as an average problem set.

To this end, projects will likely consist of one of the following:

- Implementing an algorithm discussed in class
- Use an existing software package to perform computational experiments and analyze the results.

You may also do a project that is mostly theoretical, but we’d recommend running it by Professor Dror or the CAs first.

2 Project Ideas

Below, we give a summary of some project ideas.

- Protein Structure Prediction: Explore Rosetta further or explore other methods / software packages for predicting structure
- Molecular Dynamics Simulations: Implement a basic MD simulation or use existing packages to see state-of-the-art predictions. (If you want to build on a project from CS 274, this is fine, but you must cite all starter code. Do not just re-submit this assignment for your project.)
- Docking: Lots of packages and databases of compounds to explore!
- Protein Design: Experiment with Rosetta design or other protein design software.
- Single-particle Electron Microscopy Reconstruction: Use existing software packages or implement some of the key algorithms involved in reconstruction
• Image Analysis of Cells: There are lots of other tasks you can perform on cellular images beyond what we did on the problem set, and good support in Matlab, ImageJ, and Python.

• Reaction-Diffusion Simulations: Extend the diffusion code from Assignment 3 to include reactions or use one of a number of existing packages to make more robust predictions

Anything else you’d like to explore (as long as its related to the topic of the class)! You're of course welcome to talk with any of us about your project ideas.

3 Deliverables

You are to turn in a written report summarizing the results of your project and your code. The report should be:

• 3-5 pages for individual projects
• 4-6 pages for groups of two
• 5-7 pages for groups of three

with 12pt font, double spaced, 1-inch margins, not including charts/figures.

Report Structure

The report should consist of the following sections:

• Identify the problem you wish to solve and the scope of your project
• Include a brief section on the background of the problem: why is it important and what techniques have people used to solve it?
• Give a description of your contributions to solving the problem.
• Analyze your work/results.
• If you are working in a team, describe each team member’s contribution.

The last section on the analysis of your project will vary slightly between projects that involve significant implementation and projects which use existing software.

Implementation Projects

In the analysis section, you should include some discussion of the following.

• Describe the major design decisions in your implementation.
• What challenges did you encounter?
• What did you learn through implementing the project? Any major takeaways?
• What are the “next steps” in the project (if you were to continue working on it)?

You will also be expected to submit your code and a description of how to build/run it.

Using Existing Software

In the analysis section, you should include results of your experiments as well as an analysis of their quality.

• How do the software packages you used work? Are there other approaches that might work? What are the tradeoffs between these approaches?
• What were the results of your experiments?
• Do these results seem reasonable? (Are they physically realistic? Do they match your intuition?)
• What did you learn by running the experiments?

In either case, you should give some explanation of how your project fits into the larger context of the class and computational biology.

4 Submission Instructions

Only one submission is required per group, so please be sure to indicate who is in your group at the top of your report. The submission script will ask you for writeup.pdf and code.zip. Please zip up your code and any data you used in code.zip. If you didn’t write any code, please write up a technical Read-Me (.txt file) describing the software packages you installed along with the commands you used — please zip the Read-Me file(s) and name it code.zip.

When you are ready to submit, upload your files to farmshare and use this submission script in project directory:

/afs/ir/class/cs279/scripts/submit.py project

You should see a message indicating a successful submission. If you have any issues submitting, let us know! You may resubmit if you discover things you would like to change in your work.