Final project description

Machine Learning for Molecular Dynamics
BMB961 – Sec 003

Overview

This project will allow you to show what you have learned in both the machine learning and molecular dynamics sections of the course by applying these skills to a system of your choice. This could be a system related to your research interests or a well-studied model system. There are three different possible "workflows" that you can follow for your project, based on your interest. **Note that Track 2 and Track 3 are labeled as "experimental" and might require more effort to implement.**

Track 1: Biomolecular simulation and analysis

- Set up a biomolecular system of your choice (CHARMM-GUI is recommended)
- Simulate a set of trajectories with OpenMM
- Compute features for each frame in the trajectory
- Use either tICA or VAMPnets to project onto long-timescale collective variables
- Visualize these motions, analyze and discuss

Track 2: "QM" simulations with neural network potential energy functions (experimental!)

- Set up a small system of atoms of your choice (10-200 atoms, [H, C, N, O only])
- Simulate a set of trajectories with TorchANI/ASE
- Compute features describing reactive events or structures of interest
- Analyze time-series data of features
- Visualize key events or structures, analyze and discuss

Track 3: Machine learning of dynamics from molecular dynamics simulations (experimental!)

- Set up one or more biomolecular systems of your choice (CHARMM-GUI is recommended)
- Simulate trajectories with OpenMM
- Train a machine learning model based on the simulations to predict what simulations would otherwise predict, e.g. the 'next' conformation based on a given snapshot or structural ensembles.
- Compare the ML predictions with the actual simulations, analyze and discuss

Components

The final project will consist of two components: a proposal and a project notebook.

Project Proposal: **(10 points)**
A concise **(limit two pages)** description of the proposed work that should contain the following elements:

- A title indicating "Track 1", "Track 2", or "Track 3"
- A description of the system you have chosen and your motivation for choosing it
- A description of the simulation conditions, including values of parameters such as temperature, box size and/or pressure, time step, initial conditions and velocities, number of steps, number of independent trajectories
- An outline of how you plan to prepare the inputs for simulation
- A description of the planned analysis techniques
- A description of the expected results: what do you hope to observe?

Project Notebook: **(40 points)**
You will summarize the results of your simulations in a Jupyter Notebook. This should contain, where possible, the code you used during setup, simulation and analysis, as well as informative descriptions of processes that occurred outside of the notebook (for instance, preparations of the system inputs with CHARMM-GUI). It should also contain the code used for analysis and visualization, including graphs. Additional files can be submitted along with the notebook if they cannot be embedded inside as images.

Due Dates

Project proposals due Thursday April 7, 11:59 PM
Project notebooks due Thursday April 28, 11:59 PM