4/22
Weekly Update

- Elie
  - Progress
    - Visualization plots
    - Meeting with AMPL team
    - Working on the integration of the AMPL score
  - Blocker
    -
  - Plan
    -

- Arjun
  - Progress
    - Analyzing and visualizing GMD output files
    - Working on poster draft
    - Meeting with AMPL team
    - Working on the integration of the AMPL score
    - Hyperparmeter tunning and trying different data sets out
  - Blocker
    -
  - Plan
    -

- Gauri
  - Progress
    - Worked on Poster Draft
    - Working on AMPL integration
    - Created initial population EDA for score distributions to predict novelty and create subsets
    - Ran 10 epochs of data to compare to initial population
    - Currently creating subsets to train as well
  - Blocker
    -
  - Plan
    -

- Nicole
  - Progress
    - Analyzing GMD output files
    - Working on poster draft
    - Meeting with AMPL team
    - Working on integration of AMPL scoring
  - Blocker
    - Singularity installation
  - Plan
    -

4/15/2024
Weekly Update
- Gauri
  - Progress
    - Looked into BayesianOptimization
    - Novelty Score, Synthesizability options
    - Initial population EDA
    - Organizing capstone repository
  - Blocker
    - Current BayesianOptimization is dependent on Theano
  - Plan
    - Switch to Pytorch/bay_opt implementation for Bayesian Optimization
- Nicole
  - Progress
    - Organizing capstone repository
    - Starting some comparison of results
  - Blocker
    - Originally had some permission issues but those should be resolved now
  - Plan
    -
- Elie
  - Progress
    - Tried integrate AMPL score
  - Blocker
    -
  - Plan
    -
- Arjun
  - Progress
    - Organizing repository
    - Continuing test with GMD
  - Blocker
    - Git hub repo issues
  - Plan
    -

4/1/2024
Weekly Update

- Gauri
    - Progress
        - Completed AMPL Tutorial Evaluations
        - Ran GMD on sample logP_JTVAE data
    - Blocker
        -
    - Plan
        -
- Nicole
    - Progress
        - AMPL Tutorial Evaluation
        - Run GMD on new data
    - Blocker
        -
    - Plan
        -
- Elie
    - Progress
        - Completed AMPL Tutorial Evaluations
        - Read the reference paper on LogP
        - Read the report of AMPL team
        - Ran AutoGrow4 of FNLGMD on the new LogP dataset
    - Blocker
        -
    - Plan
        -
- Arjun
    - Progress
        - AMPL Tutorial Evaluation
        - Reference Added
        - Read reference paper on LogP
        - Ran AutoGrow4 on the LogP dataset
    - Blocker
        -
    - Plan
        -

3/25/2024
Weekly Update

- Elie
  - Progress
    - Prepared for presentation
    - Reference Added
    - Ran code for Autogrow4 from FNLGMD github repo on google cloud
  - Blocker
    -
  - Plan
    -
- Arjun
  - Progress
    - Prepared for presentation
    - Reference Added
    - Ran code for Autogrow4 from FNLGMD github repo on google cloud
  - Blocker
    -
  - Plan
    -
    -
- Nicole
  - Progress
    - Reference Added
    - Ran code for FNL_JTVAE and icml18-jtnn repos on google cloud
  - Blocker
    -
  - Plan
    -
- Gauri
  - Progress
    -
  - Blocker
    -
  - Plan

3/18/2024
Weekly Update

- Gauri
  - Progress
    - Prepared JTVAE presentation
    - Worked on midterm progress report
    - Reference Added
    - Installation of JTVAE via icml github
    - Set up JTVAE on google cloud
  - Blocker
    - Database access
    - This JTVAE version is written in Python2.7 and has RdKit as a requirement. But, RdKit no longer supports Python2.
  - Plan
    -

- Nicole
  - Progress
    - Prepared for presentation
    - Worked on midterm progress report
    - Running software using sample data
  - Blocker
    - Full NExT database can be downloaded?
  - Plan
    -

- Elie
  - Progress
    - Worked on midterm progress report
    - Reference added
  - Blocker
    - Testing AutoGrow4 with Docker
  - Plan
    -

- Arjun
  - Progress
    - Worked on midterm progress report
    - Reference added
  - Blocker
    - Database access
  - Plan
    -

3/4/2024
Weekly Update

- Elie
  - Progress
    - Reference Added
    - Finished AutoGrow4 installation
  - Blocker
    -
  - Plan
    -
- Arjun
  - Progress
    - Reference Added
    - Worked on presentation
    - Finished AutoGrow4 installation
  - Blocker
    -
  - Plan
    -
- Gauri
  - Progress
    - Reference Added
    - Fixed AMPL docker setup_tutorials issue
    - JTVAE installation and exploration (Manual)
    - Uploaded annotated version of last week's journal club paper
  - Blocker
    - Google Cloud Platform (don't have the free trial) - do we subscribe or are we given resources?
    - JTVAE docker installation
      ```
      gaurisamith@Gauris-Air-8 dockerbuild % docker run -v /dockerbuild:/data gmd_0_9:demo /run_gmd.sh
      Unable to find image 'gmd_0_9:demo' locally
      docker: Error response from daemon: pull access denied for gmd_0_9, repository does not exist or may require 'docker login': denied:
      cess to the resource is denied.
      ```
  - Plan
    -
- Nicole
  - Progress
    - Reference Added
    - JTVAE Installation
  - Blocker
    -
  - Plan
    -

2/26/2024
Weekly Update
- Gauri
  - Progress
    - Prepared for journal club presentation
    - Installed AMPL through Docker and ran Curation Notebook
    - Installed GMD repo through Docker
    - Explored JTVAE github
  - Blocker
    - Docker doesn't have the original curation notebook from tutorials2023
    - Authorization for GMD repo
  - Plan
    -
- Nicole
  - Progress
    - Reference Added
    - Installed AMPL through Docker
    - Attempted to install GMD repo through Docker
    - Explored JT-VAE GitHub
  - Blocker
    - Same as Gauri's blockers above
  - Plan
    -
- Elie
  - Progress
    - Reference Added
    - Downloaded AutoGrow4
  - Blocker
    -
  - Plan
    -
- Arjun
  - Progress
    - Installed AMPL through Docker
    - Reference Added
    - Downloaded AutoGrow4
  - Blocker
    - Issues with docker
  - Plan
    -

2/19/2024
Weekly Update

- Gauri
  - Progress
    - Read the Research paper for JTVAE
    - Submitted all required Forms to Naomi
    - Data Curation
    - Reference Added
    - AMPL Docker Installation
  - Blocker
    -
  - Plan
    - JTVAE installation
- Nicole
  - Progress
    - Read the Research paper for JTVAE
    - Data Curation
    - Reference Added
  - Blocker
    -
  - Plan
    - JTVAE Installation
- Elie
  - Progress
    - Prepared for Journal Club presentation
    - Data Curation
    - Read AutoGrow4 paper
    - Reference Added
    - Installed AMPL using Docker
  - Blocker
    -
  - Plan
    - Install AutoGrow4
- Arjun
  - Progress
    - Data Curation
    - Reference Added
    - Read research paper
  - Blocker
    -
  - Plan
    - Install autogrow4

2/12/2024
Weekly Update

- Gauri
  - Progress
    - Completed Coursera
    - Sent Scientific Technical Slides
    - Reference Added
    - Installed AMPL
  - Blocker
    - Photo Release Form Doubts
  - Plan
    - Email Naomi with Doubts
- Nicole
  - Progress
    - Completed Coursera
    - Technical Slides
    - Prepared for journal club presentation
  - Blocker
    - None
  - Plan
    - Acquire reference for next week and email if there are any doubts
- Elie
  - Progress
    - Send required documents to Naomi
    - Completed Coursera
    - Installed AMPL
    - Reference added
  - Blocker
    - Docker
    - Tests don't work
  - Plan
    - Address Docker issue
    - Data Curation
- Arjun
  - Progress
    - Send required documents to Naomi
    - Completed Coursera
    - Installed AMPL
    - Reference added
  - Blocker
    - Photo Release Form
  - Plan
    - Will message Naomi with my question on the form.

Date
Weekly Update
- Gauri
  - Progress
    - ▪
  - Blocker
    - ▪
  - Plan
    - ▪
- Nicole
  - Progress
    - ▪
  - Blocker
    - ▪
  - Plan
    - ▪
- Elie
  - Progress
    - ▪
  - Blocker
    - ▪
  - Plan
    - ▪
- Arjun
  - Progress
    - ▪
  - Blocker
    - ▪
  - Plan
    - ▪