https://mattaadams.github.io/

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EDUCATION

Carnegie Mellon University

Master of Science in Chemical Engineering

University of Tennessee, Knoxville

Bachelor of Science in Chemical Engineering

EXPERIENCE

U.S. Environmental Protection Agency

Data Modeling Specialist (Contractor)

Durham, NC Dec 2021 - Present

• Transformed a chemical fingerprinting method into a more universal format to allow for expanded applications in toxicology predictions of target chemical substances

- Performed in-depth pairwise comparison analysis across different chemical fingerprint sets to identify differences in information captured across chemical spaces.
- Analyzed the effect of chemical fingerprints on the performance of Generalized Read Across's (GenRA) predictive ability of chemical toxicity properties

Carnegie Mellon University

Pittsburgh, PA

Graduate Research Assistant

Aug 2019 - Dec 2020

- \circ Performed in-depth statistical analysis of composition effects on catalyst surface performance with computational calculations to reduce the required search space for screening by 70%
- \circ Designed a flexible framework with PyTorch for active learning with Deep Learning Neural-Network potentials leading to a reduction of 60% in computational time while maintaining accurate results
- o Manipulated large dataframes containing atomic structure information with MongoDB database in Python
- Collaborated in improvement of projects through implementation of continuous integration to improve code structure and reduce errors

Oak Ridge National Laboratory

Oak Ridge, TN

Research Intern

June 2019 - Aug 2019

- Constructed a unique framework through combining density functional tight binding with metadynamics which accelerated scanning of the free energy profile of a system by a factor of 1000
- $\circ\,$ Implemented neural-network assisted molecular dynamics simulations to reduce the error below 10%.
- Ran Python Jupyter notebook experiments for neural network hyper-parameter optimization.

Projects

For additional projects and source code, visit https://mattaadams.github.io/

Q-Wall Game | Python

o Developed a Deep Q-Learning agent in TensorFlow capable of accurate navigation inside a game environment

Sorting Algorithm Visualizer | JavaScript, HTML/CSS

• Developed a React App which visualizes popular sorting algorithms to aid in understanding of their functionality

Twitter Bot Detection | Python

- Utilized Twitter's API to extract and clean data into a readable format across thousands of individual accounts
- Implemented machine learning algorithms to obtain an overall accuracy of 85% for bot detection and classification.

Atomic Binding Energy Predictions | Python

 \circ Constructed and trained a model capable of predicting binding energies with an average error of less than 10%

SKILLS

- Languages: Python, JavaScript, SQL, CSS/HTML, Shell
- Frameworks: PyTorch, TensorFlow, Flask, NodeJS, ReactJS
- Technologies: Docker, Kubernetes, MongoDB, Git, CircleCI, VSCode

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Pittsburgh, PA

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Knoxville, TN

May 2019

Dec. 2020