Matthew Adams

https://mattaadams.github.io/

Email : mattaadams1@gmail.com
Mobile : +1-865-951-9994

Education

Carnegie Mellon University — Pittsburgh, PA
Master of Science in Chemical Engineering — *Dec. 2020*

University of Tennessee, Knoxville — Knoxville, TN
Bachelor of Science in Chemical Engineering — *May 2019*

Experience

U.S. Environmental Protection Agency — Durham, NC
Data Modeling Specialist (Contractor) — *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*

- 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%
- 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
- 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
- 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*

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

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*

- Performed Feature Engineering on molecular structures to enable predictions for chemical properties
- 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
- **Technologies**: Docker, Kubernetes, MongoDB, Git, CircleCI, VSCode