Samuel C. Hoover, Ph.D.

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Summary

I am a research scientist and PPG Fellow with 6 years of experience building computational models and using statistical analysis to answer complex problems. Specializing in predictive modeling and data visualization with a focus on translating insights from data and models into solutions. Proven track record of success through peer-reviewed publications, interdisciplinary internship experiences, and personal projects. Seeking to apply my expertise to meaningfully contribute to data science roles in cross-functional teams.

Education

University of Massachusetts Amherst *Amherst, MA* Sep 2018 - Dec 2024
Ph.D. in Chemical Engineering (awarded PPG Fellowship and Teaching Assistant Award)

Clarkson University *Potsdam, NY* Aug 2014 - May 2018
B.S. in Chemical Engineering (with distinction); Minor in Mathematics

Skills

- **Languages & Tools:** Python (PyTorch, scikit-learn, pandas, Matplotlib, XGBoost, PySpark), SQL (SQLite, Postgres), Git
- **Methods:** machine learning, predictive modeling, statistics, data science, data visualization, data wrangling, data reporting

Experience

Muthu Polymer Group (Research Assistant - Polymer Physics) *Amherst, MA* Jan 2021 - Dec 2024

- Created a dataset with 260k samples and 11 hand-engineered features from real-world data using **pandas** and improved data quality by identifying 5% of samples as unreliable
- Developed a molecular fingerprint that accurately predicts molecular behavior ($R^2 > 0.95$) using **XGBoost** and then found important learned interactions with **SHAP** values
- Developed statistical theory that captured newly discovered experimental observations, findings are relevant to molecular design for industrial and pharmaceutical applications
- Rewrote the group's free energy minimization code with an optimized **NumPy** and **SciPy** implementation, reducing compute time by 90% and allowing for quicker experimentation
- Developed an automation script for routine teaching assistant duties, saved 8 hours so I could focus on important tasks
- Fostered a collaborative and well-rounded environment by mentoring junior lab members on interdisciplinary topics and giving seminars twice yearly

Triton Systems, Inc. (Technology & Signal Processing Intern) *Chelmsford, MA* Jun 2023 - Sep 2023

- Led modeling of electromagnetic components for a molecular sensing device for viral detection in collaboration with engineers
- Improved team productivity by developing an easy-to-use **COMSOL** application for complex finite element method modeling, enabled users to make on-the-fly design changes and estimate performance
- Supported design best practices by reviewing current literature on instrumentation, data acquisition, and signal processing for breath analysis
- Worked by key stakeholders, meeting monthly to present research updates and respond to questions from DHS sponsors

Bai Research Group (Research Assistant - Computational Chemistry) *Amherst, MA* Jan 2019 - Dec 2020

- Trained **convolutional neural networks** for 20,000x quicker materials property predictions than traditional methods, enabling researchers to focus efforts on promising candidates
- Built custom **PyTorch** framework for preprocessing of large datasets (>1 GB/sample), neural network training, model analysis, and experiment logging; ensured reproducibility and reliability for 8 person research team
- Created an automated pipeline to process, analyze, and visualize over 100,000 materials in **HDF5** format using **MATLAB**