Samuel C. Hoover, Ph.D.

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Summary

I am a research scientist, PPG Fellow, and Chemical Engineering Ph.D. with 6 years of experience building data-driven models to answer complex, scientific problems. Proven track record of success through peer-reviewed publications, interdisciplinary internships, and open-source projects. Adept at wearing many hats, working in fast-paced cross-functional teams, and effectively communicating difficult subjects. Enthusiastic about applying my experience to deliver results in data science roles.

Education

University of Massachusetts Amherst *Amherst, MA* Sep 2018 - Dec 2024
Ph.D. in Chemical Engineering (awarded PPG Fellowship and Teaching Assistant Award)
Dissertation: "Study of Charged Macromolecule Phase Behavior using Conventional and Modern Modeling Methods"
Relevant coursework: Machine Learning, Neural Networks, Mathematical Modeling, Statistical Mechanics, Adv. Mathematical Analysis

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), SQL (SQLite, Postgres), Rust, C/C++, Git, Docker
- **Methods:** machine learning, statistical modeling, high-performance computing, data science, NLP, regression, biophysics

Experience

Muthu Polymer Group (Research Assistant; Data science & biophysics) *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
- Trained a machine learning model that accurately predicts ($R^2 > 0.95$) protein behavior 90x quicker than traditional methods
- Developed theory that allows scientists to design cargo-releasing materials with specific properties
- Rewrote the group's free energy minimization code, increased productivity by reducing compute time and cost by 90%
- Integrated **Transformers** into genomic sequencing pipeline and benchmarked against other available third-party sequencing tools
- Automated extracurricular duties so I could focus on important tasks, required managing unstructured and structured data
- Fostered a collaborative and open environment by mentoring junior lab members and giving multiple seminars each semester

Triton Systems, Inc. (Technology & Signal Processing Intern) *Chelmsford, MA* Jun 2023 - Sep 2023
- Optimized design of electromagnetic components for a handheld viral detection device in collaboration with engineers
- Developed an application for product testing, enabled users to make on-the-fly design changes and estimate performance
- Supported design best practices by reviewing current literature on data acquisition and **signal processing** for breath analysis
- Worked with key stakeholders, meeting monthly to present research updates and respond to questions from financial sponsors

Bai Research Group (Research Assistant; ML & computational chemistry) *Amherst, MA* Jan 2019 - Dec 2020
- Applied **convolutional neural networks** for 20,000x quicker materials property predictions than traditional methods, enabling researchers to focus on promising candidates
- Built custom **PyTorch** framework for processing large datasets (>1 GB/sample), training, model analysis, and experiment logging; ensured reproducibility and reliability for 8 person research team
- Created an automated pipeline in **MATLAB** to process, analyze, and visualize over 100,000 3D materials
- Computed forcefield parameters and phase diagrams for small molecules using Gibbs ensemble **Monte Carlo** simulations

SI Group, Inc. (Global Manufacturing Technology Intern) *Schenectady, NY* May 2017 - Aug 2017
- Strengthened institutional knowledge by identifying root causes of loss events and determining impact on revenue and production
- Standardized the block flow diagrams of 19 key company assets, reduced potential errors by improving consistency and clarity
- Aided PI Asset Framework implementation for real-time process monitoring, enabled quick decisions and eliminated guesswork

Publications

- Hoover, S., et al. Learning the sequence effects on the microphase separation transition of charged heteropolymers. *In preparation.*
- Hoover, S., et al. Theory and quantitative assessment of pH-responsive polyzwitterion-polyelectrolyte complexation. *Soft Matter*.
- Liu, Y., et al. ZeoNet: 3D convolutional neural networks for predicting adsorption in nanoporous zeolites. *J. Mater. Chem. A*.