Samuel C. Hoover

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Skills

- Languages & tools: Python, Rust C, PyTorch, scikit-learn, NumPy, XGBoost, Git, AWS, SQL, Spark, Docker, HTML
- Methods: machine and deep learning, optimization, NLP, computer vision, object-oriented design, data wrangling

Experience

Muthu Polymer Group (Graduate Research Assistant) *UMass Amherst, Amherst, MA* Jan 2021 - Present

- Created >260k row dataset and novel representation to accurately learn ($R^2 > 0.95$) the conformations of macromolecules
- Cleaned datasets using physical principles, determining 5% of samples as candidates for recalculation or removal
- Designed explainable machine learning model that extracted sequence-property relationships of 6,500 polymers
- Developed theory for macromolecule complexation, determining mechanism for critical behavior over 8 parameters
- Refactored group free energy minimization script to be 10x faster by implementing C backend with a Python wrapper

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

- Led design of induction heating coil to selectively desorb VOCs for molecular sensing device (< 1 ppm sensitivity)
- Created an application for design optimization, facilitating faster design and improving productivity for 5+ member team

Bai Research Group (Graduate Research Assistant) *UMass Amherst, Amherst, MA* Jan 2019 - Dec 2020

- Trained neural networks on geometric descriptors and volumetric data for 100,000+ materials property prediction
- Wrote custom PyTorch modules to process large (> 1 GB/sample) data for computer vision aided virtual screening
- Developed deep learning pipeline to ETL, train MLPs & CNNs, and ensure reproducibility for 8 person research team

Selected Projects

2D Ising Model in Rust
Efficient (>100M steps/s) implementation of a 2D Ising Model in Rust, leveraged integer calculation for faster compute

Automating Teaching Assistant Duties
Saved 8+ hours over the semester by automating routine tasks like anonymizing, aggregating, and emailing peer feedback

Publications & Ongoing Work

- **Hoover, S. C.**, Li, S.-F. & Muthukumar, M. Learning the sequence effects on the microphase separation transition of charged heteropolymers. **In preparation**.
- **Hoover, S. C.**, Margossian, K. O. & Muthukumar, M. Theory and quantitative assessment of pH-responsive polyzwitterion-polyelectrolyte complexation. *Soft Matter* **20**, 7199-7213. (2024) doi: 10.1039/D4SM00575A.
- Liu, Y., Perez, G., Cheng, Z., Sun, A., **Hoover, S. C.**, Fan, W., Maji, S., Bai, P. ZeoNet: 3D convolutional neural networks for predicting adsoprtion in nanoporous zeolites. *J. Mater. Chem. A* **11**, 17570-17580. (2023) doi: 10.1039/D3TA01911J.

Education

University of Massachusetts Amherst *Amherst, MA* Sep 2018 - Present
Ph.D. in Chemical Engineering (awarded PPG Fellowship and Teaching Assistant Award)
Thesis: "Study of Charged Macromolecule Phase Behavior using Conventional and Modern Modeling Methods"

Clarkson University *Potsdam, NY* Aug 2014 - May 2018
B.S. in Chemical Engineering (with distinction); Minors in Mathematics and Cross-Cultural & International Perspectives