Donald Loveland

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RESEARCH INTERESTS

I am a third year PhD student at the University of Michigan, Ann Arbor. My research focuses on fundamental questions in **machine learning**, **graph representation learning** and **graph neural networks (GNNs)**. Broadly, I study how to improve the interpretability and fairness of GNNs with respect to a graph's structural characteristics.

EDUCATION

University of Michigan, Ann Arbor Aug. 2021 - May 2026
Ph.D. in Computer Science (3.93/4.00 GPA) Ann Arbor, MI

- **Advisor**: Danai Koutra - Graph Exploration and Mining at Scale (GEMS) Lab
- **Fellowships:** NSF Graduate Research Fellowship (GRFP), Rackham Merit Fellowship

California Polytechnic State University, San Luis Obispo Aug. 2014 - June 2018
B.S. in Physics (3.61/4.00 GPA) San Luis Obispo, CA

- **Minors**: Computer Science, Mathematics, Astronomy, Ethnic Studies

RECENT RESEARCH EXPERIENCE

MIT Lincoln Laboratory May 2023 - Sep. 2023
Research Intern - Advised by Dr. James Usevitch & Dr. Rajmonda Caceres

- Developed an efficient GNN architecture to solve bipartite assignment problems. GNN leverages a line graph transformation and novel pruning strategy to achieve improvements of up to 30% in the optimization objective over previous baselines. Work submitted to the International Conference on Autonomous Agents and Multiagent Systems (AAMAS).

MIT Lincoln Laboratory May 2022 - Aug. 2022
Research Intern - Advised by Dr. Rajmonda Caceres

- Developed a gradient-based optimization method to efficiently edit graph structures and improve task performance. Demonstrated the capabilities of this method on newly proposed shortest path and substructure manipulation datasets. Proposed method studied across different GNNs, demonstrating improvements of up to 60% over baselines. Work accepted for oral presentation at the Twelfth International Conference on Complex Networks and Their Application.

Lawrence Livermore National Lab Feb. 2019 - Sept. 2021
Applied Machine Learning Researcher

- Developed an XAI method for counterfactual introspection of DL models in PyTorch. Method was applied to materials science problems to extract domain-specific concepts learned by convolution neural networks. US patent recieved.
- Explored the relationship between adversarial training and post-hoc XAI methods for GNNs in PyTorch Geometric. Additionally Created an inverse design method for molecular graphs through a GNN-based RL model. New molecules were designed through an interpretable graph editing policy.

PREPRINTS

- **D. Loveland**, J. Usevitch, R. Caceres, Z. Serlin, D. Koutra, "Efficient Optimization of Bipartite Assignment Problems via Pruned Graph Neural Networks", *Submitted to AAMAS 2023*
- **D. Loveland**, J. Zhu, M. Heimann, B. Fish, M. Schaub, D. Koutra, "On Performance Discrepancies Across Local Homophily Levels in Graph Neural Networks", *Submitted to Learning on Graphs 2023*

PUBLICATIONS

- **D. Loveland**, R. Caceres, "Network Design through Graph Neural Networks: Identifying Challenges and Improving Performance", *International Conference on Complex Networks and Their Applications*, 2023
- **D. Loveland**, J. Zhu, M. Heimann, B. Fish, M. Schaub, D. Koutra, "On Graph Neural Network Fairness in the Presence of Heterophilous Neighborhoods", *KDD Workshop on Deep Learning on Graphs*, 2022
- J. Zhu, J. Jin, **D. Loveland**, M. Schaub, D. Koutra, "On the Relationship Between Heterophily and Robustness of Graph Neural Network", *KDD*, 2022
- **D. Loveland**, S. Liu, B. Kailkhura, A. Hiszpanski, Y. Han, "Reliable Graph Neural Network Explanations Through Adversarial Training", *ICML Workshop on Theoretic Foundation, Criticism, and Application Trend of Explainable AI*, 2021
- P. Nguyen*, **D. Loveland***, J. Kim, P. Karande, A. M. Hiszpanski, Y. Han, "Predicting Energetics Materials' Crystalline Density from Chemical Structure by Machine Learning", *Journal of Chemical Information and Modeling*, 2021
- **D. Loveland**, B. Kailkhura, P. Karande, A. M. Hiszpanski, Y. Han, "Automated Identification of Molecular Crystals' Packing Motifs", *Journal of Chemical Information and Modeling*, 2020
- B. Gallagher, M. Rever, **D. Loveland**, T. N. Mundhenk, B. Beauchamp, et al, "Predicting Compressive Strength of Consolidated Molecular Solids using Computer Vision and Deep Learning", *Materials and Design*, 2020
- S. Liu, B. Kailkhura, J. Zhang, A. M. Hiszpanski, E. Robertson, **D. Loveland**, Y. Han. "Actionable attribution maps for scientific machine learning", *ICML Workshop on ML Interpretability for Scientific Discovery*, 2020
- S. Liu, B. Kailkhura, **D. Loveland**, Y. Han, "Generative Counterfactual Introspection for Explainable Deep Learning", *IEEE Global Conference on Signal and Information Processing*, 2019
- V. N. Bennert, **D. Loveland**, E. Donohue, M. Cosens, S. Lewis, et al, "Studying the [OIII]λ 5007Å emission-line width in a sample of 80 local active galaxies: a surrogate for σ*?", *Monthly Notices of the Royal Astronomical Society*, 2018

TECHNICAL SKILLS

- **Programming Languages**: Python, Java (Basic)
- **Packages**: Pytorch, Pytorch-Geometric, Scikit-Learn, NetworkX

ADDITIONAL EXPERIENCE

Cambridge Coaching Dec. 2021 - Present

Computer Science and Math Tutor

- Tutoring students at various academic stages in courses such as high school AP computer science, undergraduate calculus, and graduate machine learning.

Cal Poly College of Science and Math August. 2016 - Dec. 2017

Peer Mentor/Advisor

- Mentored first-year students on academic probation with the goals of improving study skills, promoting time management, and helping with general adjustment to college.

*Denotes equal contribution