Donald Loveland

Email: dlovelan@umich.edu | **Website:** donaldloveland.com | **LinkedIn:** donald-loveland

RESEARCH INTERESTS

I am a fourth year PhD student at the University of Michigan, Ann Arbor, focusing on fundamental questions in **machine learning**, **graph representation learning** and **graph neural networks (GNNs)**. Broadly, my research explores the generalization capabilities of GNNs with respect to a graph's structural characteristics. Currently, I am investigating graph-based recommendation systems and personalization techniques to enhance user experience.

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 and Awards:** 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

RESEARCH EXPERIENCE

Snap Research at Snap Inc. May 2024 - Aug. 2024
Research Intern - Advised by Dr. Clark Ju, Dr. Tong Zhao & Dr. Neil Shah Bellevue, Washington

- Developed an efficient training strategy for large context-free recommendation systems. Studied cost-effective regularization methods to enhance convergence properties and mitigate over-fitting. Conducted comprehensive analyses to demonstrate accelerated training while maintaining high performance. Work submitted to WWW '25

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

- Developed an efficient GNN architecture, MAGNET, to address bipartite assignment problems, utilizing a line graph transformation and a novel pruning strategy. This approach achieved up to 30% improvement in the optimization objective compared to previous baselines. Work submitted to AAMAS '25.

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

- Developed a gradient-based optimization method, ORE, to efficiently edit graph structures and improve task performance. ORE's capabilities were demonstrated on newly proposed shortest path and substructure manipulation datasets. Improvements of up to 60% were achieved over baselines. Work accepted for oral presentation at the Twelfth International Conference on Complex Networks and Their Applications.

Lawrence Livermore National Lab Feb. 2019 - Aug. 2021
Staff Scientist (Applied Machine Learning Researcher) Livermore, California

- 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 received.
- 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**, C. Ju, X. Wu, T. Zhao, N. Shah, D. Koutra, "Scalable Collaborative Filtering by Regularizing the Singular Values of Embedding Matrices", *Under Review*
- **D. Loveland**, D. Koutra, "Unveiling the Impact of Local Homophily on GNN Fairness: In-Depth Analysis and New Benchmarks", *Under Review*
- **D. Loveland**, J. Usevitch, R. Caceres, Z. Serlin, D. Koutra, "Efficient Optimization of Bipartite Assignment Problems via Pruned Graph Neural Networks", *Under Review*

PUBLICATIONS

- **D. Loveland**, J. Zhu, M. Heimann, B. Fish, M. Schaub, D. Koutra, "On Performance Discrepancies Across Local Homophily Levels in Graph Neural Networks", *Learning on Graphs 2023 (Spotlight Presentation, Top 5%)*, 2023
- **D. Loveland**, R. Caceres, "Network Design through Graph Neural Networks: Identifying Challenges and Improving Performance", *International Conference on Complex Networks and Their Applications (Oral Presentation)*, 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, **D. Loveland**, Y. Han, "Generative Counterfactual Introspection for Explainable Deep Learning", *IEEE Global Conference on Signal and Information Processing*, 2019

TECHNICAL SKILLS

- **Programming Languages**: Python
- **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.

*Denotes equal contribution