Thien Le

Curriculum Vitae

Postdoctoral Fellow in Applied Mathematics
Harvard University, Cambridge, MA
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Research Interests

Theory of geometric deep learning; learning under invariances and equivariances; neural algorithmic reasoning and combinatorial optimization; continuous optimization; mathematical and algorithmic biology.

Academic Appointments

Oct. 2025–present **Postdoctoral Fellow in Applied Mathematics**, Harvard University.
Working with Prof. Melanie Weber.

Oct. 2024–Jan. 2025 **TILOS Visiting Researcher**, Halıcıoğlu Data Science Institute, University of California San Diego.
Host: Prof. Fan Chung Graham.

Education

2019–2026 **Ph.D., Electrical Engineering and Computer Science**
Massachusetts Institute of Technology, Cambridge, MA.
Advisor: Prof. Stefanie Jegelka.
Modern Graph-Theoretic Approaches to the Theory of Graph Machine Learning.

S.M., Electrical Engineering and Computer Science
Massachusetts Institute of Technology, Cambridge, MA.
Advisor: Prof. Stefanie Jegelka.

2016–2019 **B.S., Mathematics and Computer Science**
University of Illinois Urbana-Champaign, Champaign, IL.
Research mentor: Prof. Tandy Warnow.

Preprints

2026 **MPNNs implement family-specific graph coloring algorithms.**
Manuscript submitted to the Learning on Graphs Conference (LoG) 2026.

2026 **Thien Le** and Melanie Weber.
Powers of the Vandermonde determinant are eventually non-SNP.
arXiv:2607.23828.

2026 **Thien Le**, Tianyu Zhao, and Melanie Weber.
Contrastive Neural Algorithmic Reasoning for Graph Coloring.
arXiv:2606.03923. Extended abstract submitted to LoG 2026.

2026 **Thien Le** and Melanie Weber.
Towards Distillation Guarantees under Algorithmic Alignment for Combinatorial Optimization.
arXiv:2605.20074.

Publications

Conferences and Journals

2024 **Thien Le**, Luana Ruiz, and Stefanie Jegelka.
A Poincaré Inequality and Consistency Results for Signal Sampling on Large Graphs.
International Conference on Learning Representations (ICLR). *Spotlight.*

2024 Bobak T. Kiani*, **Thien Le***, Hannah Lawrence*, Stefanie Jegelka, and Melanie Weber.
On the hardness of learning under symmetries.
International Conference on Learning Representations (ICLR). *Spotlight.*
*Equal contribution.

2023 **Thien Le** and Stefanie Jegelka.
Limits, approximation and size transferability for GNNs on sparse graphs via graphops.
Advances in Neural Information Processing Systems (NeurIPS), 36.

2022 **Thien Le** and Stefanie Jegelka.
Training invariances and the low-rank phenomenon: beyond linear networks.
International Conference on Learning Representations (ICLR).

2021 Xilin Yu, **Thien Le**, Sarah A. Christensen, Erin K. Molloy, and Tandy Warnow.
Using Robinson-Foulds supertrees in divide-and-conquer phylogeny estimation.
Algorithms for Molecular Biology, 16, Article 12.

2021 **Thien Le**, Aaron Sy, Erin K. Molloy, Qiuyi Zhang, Satish Rao, and Tandy Warnow.
Using Constrained-INC for large-scale gene tree and species tree estimation.
IEEE/ACM Transactions on Computational Biology and Bioinformatics, 18(1):2–15. First published online in 2020.

2020 Xilin Yu, **Thien Le**, Sarah Christensen, Erin K. Molloy, and Tandy Warnow.
Advancing Divide-and-Conquer Phylogeny Estimation using Robinson-Foulds Supertrees.
Workshop on Algorithms in Bioinformatics (WABI), LIPIcs 172, 15:1–15:17.

2019 **Thien Le**, Aaron Sy, Erin K. Molloy, Qiuyi Zhang, Satish Rao, and Tandy Warnow.
Using INC within Divide-and-Conquer Phylogeny Estimation.
International Conference on Algorithms for Computational Biology (AlCoB), pp. 167–178.

2018 Si Chen, **Thien Le**, Brendan A. C. Harley, and P. I. Imoukhuede.
Characterizing Glioblastoma Heterogeneity via Single-Cell Receptor Quantification.
Frontiers in Bioengineering and Biotechnology, 6:92.

Workshop Papers

2025 **Thien Le** and Melanie Weber.
Towards distillation guarantees under algorithmic alignment.
NeurIPS Workshop on Differentiable Learning of Combinatorial Algorithms (DiffCoAlg).

Research Talks

2026 **Algorithmic alignment.**
Research talk, Prof. Yusu Wang's group, Halıcıoğlu Data Science Institute, University of California San Diego.

2025 **On the approximation theory of graph neural networks.**
Joint Mathematics Meetings (JMM), AMS Special Session on Algebraic Methods in Machine Learning and Optimization, Seattle, WA.

2024 **On the hardness of learning under symmetries.**
EnCORE Workshop on Computational vs. Statistical Gaps in Learning and Optimization, Institute for Pure & Applied Mathematics (IPAM), UCLA.

2023 **On graphon signal sampling.**
Contributed talk, DeepMath 2023, Johns Hopkins University.

Poster Presentations

2026 **Contrastive Neural Algorithmic Reasoning for Graph Coloring.**
Boston Symmetry Day, Boston, MA.

2026 **Neural algorithmic reasoning for graph coloring via Lovasz-ϑ with contrastive learning.**
NetSci 2026, International School and Conference on Network Science, Boston, MA.

Honors and Awards

2024 **Two ICLR Spotlight presentations**: *On the hardness of learning under symmetries* and *A Poincaré Inequality and Consistency Results for Signal Sampling on Large Graphs*.

2019 **Most Outstanding Undergraduate Major Award in Mathematics & Computer Science**, Department of Mathematics, University of Illinois Urbana-Champaign.

Professional Service and Mentoring

2020–present Reviewer: NeurIPS, ICML, ICLR, AISTATS, ICASSP, LoG, and ECML-PKDD.

2024 **MIT EECS GAAP**: Ph.D. admissions mentoring.

2023–2024 **ML Tea**: Co-organized a student seminar on machine learning research at MIT.

2021–2024 **Weekly reading group on learning with invariances**, for students at MIT, Harvard, and Northeastern.

2022–2023 Initial review of graduate applications for MIT EECS/AI+D Ph.D. admissions.

2019–2021 **Projects in Mathematics & Applications**, Ho Chi Minh City, Vietnam: taught and mentored high school students in machine learning.

Teaching Experience

Fall 2023 **6.S898 Deep Learning**, Massachusetts Institute of Technology.

Summer 2023 **18.6501x Fundamentals of Statistics**, Massachusetts Institute of Technology.

Spring 2018 **CS374 Introduction to Algorithms and Models of Computation**
CS473 Algorithms, University of Illinois Urbana-Champaign.