Tien Dat Nguyen

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Overview

I am a Master's research student at the University of Waterloo, advised by Professor Victor Zhong. My foundational expertise was developed across 2.5 years of research at KAIST, centering on **Geometric Deep Learning** and **Graph Machine Learning**. My research focused on developing general-purpose deep learning algorithms for discrete and structure data, such as graphs, by leveraging the principles of geometry and equivariance. My past graduate research at Waterloo explored leveraging the reasoning capabilities of foundation models (VLMs) to develop a planning system for automating text-to-3D interior scene synthesis. I have recently pivoted my research focus towards two key areas: developing robust, controllable **AI Safety** systems and accelerating the pace of **Scientific Discovery** (with a particular interest in Drug Discovery applications).

Education

University of Waterloo — *September 2024 - December 2026*

Master of Mathematics in Computer Science — *Waterloo, Canada*

Korea Advanced Institute of Science and Technology (KAIST) — *September 2019 - February 2024*

Bachelor in Computer Science — *Daejeon, South Korea*

Experience

Reading to Learn Laboratory — *September 2024 - Present*

Graduate Research Assistant (Affiliated: University of Waterloo & Vector Institute) — *Ontario, Canada*

- Developed a VLM-based planning system for text-to-3D interior scene synthesis, enhancing controllability and generation quality.

Bionsight — *February 2024 - April 2024*

Machine Learning Engineer — *Seoul, South Korea*

- Developed an LC-MS quantification algorithm for measuring molecular abundance, supporting the drug discovery pipeline.

Vision and Learning Laboratory — *Daejeon, South Korea*

Research Assistant (Advisors: Phd Jinwoo Kim and Professor Seunghoon Hong) — *August 2021 - January 2024*

- In 2021, we investigated using Riemannian manifolds to enable neural networks to represent non-trivial graph properties.
- In 2022, we researched Graph Transformers for the molecular property prediction tasks.
- In spring 2023, we researched Equivariance Learning, leveraging data symmetries to improve neural network generalization.
- Since summer 2023, I carried out independent research with a focus on expanding the applicability of our prior work LPS..
- **Research duties:** developing and implementing ML models, addressing engineering challenges, conducting experiments (models training and evaluation), surveying literature, and proving theoretical results.

Publications

Learning Symmetrization for Equivariance with Orbit Distance Minimization [Paper][Code]

Tien Dat Nguyen*, Jinwoo Kim*, Hongseok Yang, Seunghoon Hong

NeurReps 2023 Workshop

Learning Probabilistic Symmetrization for Architecture Agnostic Equivariance [Paper][Code]

Jinwoo Kim, Tien Dat Nguyen, Ayhan Suleymanzade, Hyeokjun An, Seunghoon Hong

NeurIPS 2023 (**Spotlight Award, Top 3% of Submissions**)

Pure Transformers are Powerful Graph Learners [Invited Talk] [Paper][Code]

Jinwoo Kim, Tien Dat Nguyen, Seonwoo Min, Sungjun Cho, Moontae Lee, Honglak Lee, Seunghoon Hong

NeurIPS 2022

Research Projects

Text to 3D interior scene synthesis — *September 2024 - August 2025*

Reading to Learn Laboratory — *Waterloo, Ontario, Canada*

- Researched automatic 3D interior scene design from user-provided textual descriptions.
- Developed a planning system leveraging the visual reasoning capability of VLM to enhance the quality and controllability of scene planning.

Learning Symmetrization for Equivariance with Orbit Distance Minimization — *June 2023 - October 2023*

Vision and Learning Laboratory — *Daejeon, South Korea*

- Developed a novel symmetrization method built upon proposals of Kim et al. (2023) but introduced a framework modification to extend its applicability to a broader range of symmetry groups.
- Empirically showed competitive performance on image classification task with rotation symmetry and for the first time in literature, successfully applied symmetrization for task with Lorentz symmetry.

Probabilistic Symmetrization for Architecture Agnostic Equivariance *November 2022 - May 2023*

Vision and Learning Laboratory *Daejeon, South Korea*

- Developed the novel Probabilistic Symmetrization (PS) technique to make arbitrary base networks equivariant to group symmetries by performing a weighted average over a probability distribution of group transformations.
- Decoupled the handling of equivariance and expressiveness by parameterizing this probability distribution with a separate, equivariant network, trainable end-to-end with the base model.
- Formulated the theoretical weighted average as an expectation over this learned distribution, enabling practical estimation via a differentiable sampling-based approximation.
- Demonstrated competitive performance on graph learning (permutation symmetry) and particle dynamics (Euclidean symmetry) tasks by experimenting with general-purpose base networks (MLP, Transformer).

Graph Transformers for OGB-LSC@NeurIPS Molecular Property Prediction Challenge *September 2022 - October 2022*

Vision and Learning Laboratory & LG AI Research *Daejeon, South Korea*

- Tokenized extra geometric features, such as molecular rings, and provided as additional tokens for Graph Transformers.
- Achieved competitive performance on PCQM4Mv2 leaderboard

Pure Transformers for Graph Learning *February 2022 - August 2022*

Vision and Learning Laboratory & LG AI Research *Daejeon, South Korea*

- Proposed TokenGT, a standard Transformer model without graph-specific architectural modifications, proving to be both theoretically expressive and practically high-performing.
- Proved theoretically that TokenGT is more expressive than all message-passing Graph Neural Networks (GNNs).
- Achieved significantly better performance than GNN baselines on the large-scale PCQM4Mv2 molecular dataset and competitive performance against Transformer variants with sophisticated graph-specific inductive bias.

Riemannian Manifold for Graph Representation Learning *August 2021 - January 2022*

Vision and Learning Laboratory *Daejeon, South Korea*

- Explored using Riemannian manifold parameterized by neural networks for learning graph embeddings, capturing non-trivial geometry.

Honors and Awards

Undergraduate Research Program (URP) Excellence Award *August, 2022*

College of Engineering, KAIST *South Korea*

- Granted to students with outstanding research outcomes among 60 participants in the URP program.

Dean's List award *August, 2021*

School of Computing, KAIST *South Korea*

- Granted to students with outstanding academic performance ranked within top **3%** of School of Computing.

Shortlisted for the Vietnam International Mathematical Olympiad (IMO) Team (TST) *April, 2018*

Ministry of Education and Training *Vietnam*

- National Finalist: Top 42 students nationwide selected to compete in the final IMO team selection round.

First prize in the National Olympiad Mathematics *February, 2018*

Ministry of Education and Training *Vietnam*

- Ranked **5th** nationwide in the National Mathematics Olympiad competition. This prize is equivalent to the Golden medal.

Third prize in the National Olympiad Mathematics *February, 2017*

Ministry of Education and Training *Vietnam*

- This prize is equivalent to the Bronze medal

Skills

Programming	TensorFlow, Pytorch, Pytorch Geometric, Python
Machine Learning	Geometric Deep Learning, Graph Machine Learning, Natural Language Processing, Computer Vision
Mathematics	Probability and Statistics, Linear Algebra, Calculus
Research	Problem solving, Critical thinking, Research communication
Languages	Vietnamese (Native), English (Fluent, IELTS 8.0)