

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 graph-structured data, such as molecules, by leveraging the principles of geometry and equivariance. My current graduate research at Waterloo focuses on improving the performance of **multimodal foundation models** on downstream tasks through automated prompt optimization.

Education

University of Waterloo

Master of Mathematics in Computer Science

September 2024 - December 2026

Waterloo, Canada

Korea Advanced Institute of Science and Technology (KAIST)

Bachelor in Computer Science

September 2019 - February 2024

Daejeon, South Korea

Experience

Reading to Learn Laboratory

Graduate Research Assistant (Affiliated: [University of Waterloo & Vector Institute](#))

September 2024 - Present

Ontario, Canada

- Developed a VLM-based planning system for text-to-3D interior scene synthesis, aimed at improving the quality, efficiency, and controllability of scene planning.
- Designing a multimodal prompt optimization framework to improve VLM reasoning and performance on visual benchmarks.

Bionsight

Machine Learning Engineer

February 2024 - April 2024

Seoul, South Korea

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

Vision and Learning Laboratory

Research Assistant (Advisors: [Phd Jinwoo Kim](#) and [Professor Seunghoon Hong](#))

Daejeon, South Korea

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 sample efficiency and generalization of neural networks.
- 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

[\[Valence Labs Talk\]](#) [\[Paper\]](#) [\[Code\]](#)

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

NeurIPS 2022

Research Projects

Automated Prompt Optimization for Vision-Language Models

January 2026 - Present

Reading to Learn Laboratory

Waterloo, Ontario, Canada

- Formulating a multimodal prompt optimization pipeline by extending the GEPA framework from text-only domains to visual benchmarks.
- Architecting the iterative prompt-refinement workflow using DSPy, implementing custom local modifications to the library to support Vision-Language Model (VLM) routing.

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 Orbit Distance Minimization, a novel symmetrization framework extending [Kim et al. \(2023\)](#) by replacing hand-designed contraction operators with gradient-based optimization to support broader symmetry groups.
- Established theoretical applicability to a diverse range of symmetry groups such as Permutation $S(n)$, Rotation $SO(n)$ and Lorentz $O(1, n-1)$.
- Empirically showed competitive performance on the image classification task with rotation equivariance $SO(2)$ and, for the first time in literature, successfully applied symmetrization to the particle scattering task with Lorentz equivariance $O(1, 3)$.

Probabilistic Symmetrization for Architecture Agnostic Equivariance

November 2022 - May 2023

Vision and Learning Laboratory

Daejeon, South Korea

- Developed Probabilistic Symmetrization (PS), a novel technique to make arbitrary base networks equivariant to group symmetries by performing a weighted average over a learned probability distribution of group transformations.
- Formulated the theoretical weighted average as an expectation over this learned distribution, enabling practical estimation via a differentiable sampling-based approximation.
- Achieved SOTA on the $S(n) \times E(3)$ n-body problem of predicting 3D coordinates of charged particles
- Adapted a pre-trained Vision Transformer to solve $S(n)$ equivariant node classification on graph-structured data, demonstrating novel cross-modal transfer and achieving SOTA on the PATTERN benchmark.
- Demonstrated competitive performance on real-world molecular benchmarks, establishing SOTA results on PCQM-Contact and Peptides-func.

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.
- 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 (Writing/Presenting)
Languages	Vietnamese (Native), English (Fluent, IELTS 8.0)