

# Tien Dat Nguyen

Waterloo, Ontario

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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

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, enhancing controllability and generation quality.

### 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 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

Waterloo, Ontario, Canada

#### Reading to Learn Laboratory

- 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

Daejeon, South Korea

#### Vision and Learning Laboratory

- 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

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### Vector Scholarship in AI (Offered)

September, 2024

Vector Institute

Ontario, Canada

- An entrance award of 17,500\$ for top students pursuing AI master's in Ontario

### 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 5<sup>th</sup> 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

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**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)