

Seonghyun Park

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Summary

I'm a 1st-year Ph.D. candidate in at KAIST AI, advised by [Sungsoo Ahn](#). My master's research focused on solving the over-squashing phenomenon in graph neural networks (GNNs). Currently, I am integrating machine learning with molecular dynamics (MD) to advance scientific discovery. Most recently, I led a project on machine learning-based collective variables for enhanced sampling simulations of proteins, leveraging foundation models.

Publication

- Learning Collective Variables from BioEmu with Time-lagged Generation** 2025
Seonghyun Park, Kiyoung Seong, Soojung Yang, Rafael Gomez-Bombarelli, Sungsoo Ahn
 Preprint, under review
- Transition Path Sampling with Improved Off-Policy Training of Diffusion Path Samplers** 2025
 Kiyoung Seong, **Seonghyun Park**, Seonghwan Kim, Woo Youn Kim, Sungsoo Ahn
iclr.cc/virtual/2025/poster/29361 (ICLR 2025)
- Non-backtracking Graph Neural Networks** 2024
Seonghyun Park*, Narae Ryu*, Gahee Kim, Dongyeop Woo, Se-Young Yun**, Sungsoo Ahn**
arxiv.org/abs/2310.07430 (TMLR, NeurIPS 2023 GLFrontiers Workshop (Oral))
- Diffusion Probabilistic Models for Structured Node Classification** 2023
 Hyosoon Jang, **Seonghyun Park**, Sangwoo Mo, Sungsoo Ahn
neurips.cc/virtual/2023/poster/72405 (NeurIPS 2023)

Education

- Ph.D. Korea Advanced Institute of Science and Technology (KAIST)**, Kim Jaechul Seoul, South Korea
 Graduate School of Artificial Intelligence Feb 2025 – present
- [Structured and Probabilistic Machine Learning Lab](#) @ Sungsoo Ahn
 - Topic: Molecular dynamics (MD), Collective Variables (CVs)
- M.S. Pohang University of Science and Technology (POSTECH)**, Graduate School of Pohang, South Korea
 Computer Science and Engineering (CSE) Feb 2023 – Feb 2025
- [Machine Learning Lab](#) @ Sungsoo Ahn
 - Topic: Graph Neural Networks (GNNs), Over-squashing
- E.S. Institut National des Sciences Appliquées (INSA) Lyon**, Bioinformatics Lyon, France
 Exchange Student Jan 2022 – June 2022
- B.S. Pohang University of Science and Technology (POSTECH)**, Computer Science Pohang, South Korea
 and Engineering (CSE) Feb 2019 – Feb 2023

Experience

- Bagelcode**, Buisness Analyst (BA) intern Seoul, South Korea
 KPI routines automation and game economy management June 2021 – Aug 2021
- Seller Hub**, Product Manager (PM) intern Seoul, South Korea
 Task priority management and landing page renewal July 2020 – Aug 2020