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***, Sngwoo Mo, Sungsoo Ahn
neurips.cc/virtual/2023/poster/72405 (NeurIPS 2023)

Education

Ph.D. **Korea Advanced Institute of Science and Technology (KAIST)**, Kim Jaechul Gradudate School of Artificial Intelligence — Seoul, South Korea, 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 Computer Science and Engineering (CSE) — Pohang, South Korea, 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**, Bioinfomatics Exchange Student — Lyon, France, Jan 2022 – June 2022

B.S. **Pohang University of Science and Technology (POSTECH)**, Computer Science and Engineering (CSE) — Pohang, South Korea, Feb 2019 – Feb 2023

Experience

Bagelcode, Buisness Analyst (BA) intern — Seoul, South Korea, June 2021 – Aug 2021
KPI routines automation and game economy management

Seller Hub, Product Manager (PM) intern — Seoul, South Korea, July 2020 – Aug 2020
Task priority management and landing page renewal