Seonghyun Park

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Summary

I'm a second-year Ph.D. candidate at Graduate School of AI at KAIST, advised by Sungsoo Ahn ⬈. My Master's research focused on addressing the over-squashing phenomenon in Graph Neural Networks (GNNs) to capture long-range interactions in molecule graphs. Currently, my research focuses on AI for Science (AI4Science), specifically integrating machine learning with biomolecular modeling and molecular dynamics (MD). Recently, I led a project on machine learning–based collective variables (CVs) for enhanced sampling of proteins, by repurposing 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 2024, 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 Graduate School of Artificial Intelligence — Seoul, South Korea — Feb 2025 – present
- Structured and Probabilistic Machine Learning Lab ⬈ @ Sungsoo Ahn
- Interest: Bio-molecules, Molecular dynamics (MD)

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
- Interest: Graph Neural Networks (GNNs), Over-squashing

E.S. **Institut National des Sciences Appliquées (INSA) Lyon**, Bioinfomatics — Lyon, France — Jan 2022 – June 2022
Exchange Student

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