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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	2026
Seonghyun Park , Kiyoung Seong, Soojung Yang, Rafael Gomez-Bombarelli, Sungsoo Ahn	
ICLR 2026	
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	Seoul, South Korea
Graduate School of Artificial Intelligence	Feb 2025 – present
<ul style="list-style-type: none"> 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
<ul style="list-style-type: none"> Machine Learning Lab @ Sungsoo Ahn Interest: Graph Neural Networks (GNNs), Over-squashing 	Feb 2023 – Feb 2025
E.S. Institut National des Sciences Appliquées (INSA) Lyon , Bioinfomatics	Lyon, France
Exchange Student	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
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