Namkyeong Lee

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RESEARCH INTEREST

Applied Machine Learning

By leveraging the power of Machine Learning, I'm interested in bringing insights and advancements to various scientific fields, including biology, chemistry, and more, ultimately benefiting human society through scientific discovery.

- Graph Neural Networks for Biology and Chemistry
- Multi-Modal Large Language Model for Biology and Chemistry
- Graph Representation Learning

EDUCATION

KAIST (Korea Advanced Institute of Science and Technology)

• Ph.D. in Industrial and Systems Engineering

Mar 2023 – Present

- Research Interest: Graph Representation Learning, AI4Science
- Advisor: Prof. Chanyoung Park

KAIST (Korea Advanced Institute of Science and Technology)

M.S. in Industrial and Systems Engineering

Mar 2021 – Feb 2023

- GPA: 3.85/4.3
- Research Interest: Graph Representation Learning, Graph Mining
- Advisor: Prof. Chanyoung Park

Korea University

■ B.S. in Industrial Management Engineering

Mar 2015 - Feb 2021

- GPA: 3.9/4.5
- Dean's List (Spring 2019)

POSITIONS

Genentech, South San Francisco, CA, USA

Sep 2024 - Nov 2024

- Research Intern
 - Mentors: Dr. Ehsan Hajiramezanali, Dr. Edward De Brouwer, and Dr. Gabriele Scalia
 - Project: Knowledge Enhanced Large Language Models for Drug Discovery

University of Illinois at Urbana-Champaign, Urbana, IL, USA

Sep 2023 – Feb 2024

- Visiting Scholar in Computer Science Department
 - Host: Prof. Jimeng Sun
 - Project: Uncertainty Quantification for Polymorphic Crystalline Materials
 - Project: Large Language Models for Drug Discovery

NAVER, Seongnam, Korea

Dec 2022 – Feb 2023

- Research Intern
 - Mentors: Dr. Donghyun Kim and Dr. Min-Chul Yang
 - Project: Learning Continual User Representation for Recommendation

AISoftKorea, Seoul, Korea

Jun 2020 - Mar 2021

- Co-founder of an AI-based Legal Counseling Startup Company
 - Building AI model for providing qualified answers to Korean legal questions

PUBLICATIONS

CONFERENCES

 $(\dagger \colon Equal\ contribution)$

[C13] Subgraph Federated Learning for Local Generalization

Sungwon Kim, Yoonho Lee, Yunhak Oh, **Namkyeong Lee**, Sukwon Yun, Junseok Lee, Sein Kim, Carl Yang, Chanyoung Park

International Conference on Learning Representations (ICLR 2024)

and KDD 2024 Workshop on Federated Learning for Data Mining and Graph Analytics (FedKDD)

[C12] Implicit Precursor Extraction with Expert Retriever for Inorganic Retrosynthesis Heewoong Noh, **Namkyeong Lee**, Gyoung S. Na, Chanyoung Park Conference on Neural Information Processing Systems (**NeurIPS 2024**)

[C11]	Vision Language Model is NOT All You Need: Augmentation Strategies for Molecule Languag Models Namkyeong Lee, Siddhartha Laghuvarapu, Chanyoung Park, Jimeng Sun		
	ACM International Conference on Information and Knowledge Management (CIKM 2024) and ACL 2024 Workshop on Language and Molecules		
[C10]	Debiased Graph Poisoning Attack via Contrastive Surrogate Objective Kanghoon Yoon, Yeonjun In, Namkyeong Lee , Kibum Kim, Chanyoung Park ACM International Conference on Information and Knowledge Management (CIKM 2024)		
[C9]	Density of States Prediction of Crystalline Materials via Prompt-guided Multi-Modal Transforme Namkyeong Lee [†] , Heewoong Noh [†] , Sungwon Kim, Dongmin Hyun, Gyoung S. Na, Chanyoun Park Conference on Neural Information Processing Systems (NeurIPS 2023) and ICLR 2023 Workshop on Machine Learning for Materials (ML4Materials)		
[C8]	Shift-Robust Molecular Relational Learning with Causal Substructure Namkyeong Lee, Kanghoon Yoon, Gyoung S. Na, Sein Kim, Chanyoung Park ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD 2023)		
[C7]	Task Relation-aware Continual User Representation Learning Sein Kim, Namkyeong Lee , Donghyun Kim, Min-Chul Yang, Chanyoung Park ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD 2023)		
[C6]	Task-Equivariant Graph Few-shot Learning Sungwon Kim, Junseok Lee, Namkyeong Lee , Wonjoong Kim, Seungyoon Choi, Chanyour Park ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD 2023)		
[C5]	Conditional Graph Information Bottleneck for Molecular Relational Learning Namkyeong Lee, Dongmin Hyun, Gyoung S. Na, Sungwon Kim, Junseok Lee, Chanyoung Par International Conference on Machine Learning (ICML 2023)		
[C4]	Heterogeneous Graph Learning for Multi-modal Medical Data Analysis Sein Kim, Namkyeong Lee , Junseok Lee, Dongmin Hyun, Chanyoung Park AAAI Conference on Artificial Intelligence (AAAI 2023 Oral Presentation)		
[C3]	Relational Self-Supervised Learning on Graphs Namkyeong Lee, Dongmin Hyun, Junseok Lee, Chanyoung Park ACM International Conference on Information and Knowledge Management (CIKM 2022)		
[C2]	GraFN: Semi-Supervised Node Classification on Graph with Few Labels via Non-Parametri Distribution Assignment Junseok Lee, Yunhak Oh, Yeonjun In, Namkyeong Lee , Dongmin Hyun, Chanyoung Park ACM SIGIR Conference on Research and Development in Information Retrieval (SIGIR 20 2 Short Paper)		
[C1]	Augmentation-Free Self-Supervised Learning on Graphs Namkyeong Lee, Junseok Lee, Chanyoung Park AAAI Conference on Artificial Intelligence (AAAI 2022)		
JOURNA	LS		
[J2]	Deep Single-cell RNA-seq data Clustering with Graph Prototypical Contrastive Learning Junseok Lee, Sungwon Kim, Dongmin Hyun, Namkyeong Lee , Yejin Kim, Chanyoung Park Bioinformatics (2023) and ICML 2023 Workshop on Computational Biology (WCB)		
[J1]	Self-Supervised Graph Representation Learning via Positive Mining Namkyeong Lee, Junseok Lee, Chanyoung Park Information Sciences (2022)		
NeurIPS	S Scholar Award 202		
KDD Tr	avel Award 202		
CIKM T	CIKM Travel Award		

AWARDS & SCHOLARSHIPS

	 Grand Prize at Seoul Innovation Challenge 2020, Seoul Business Agency Building AI model for providing quantified answers to Korean legal questions Awarded for the best team among 444 teams 	2021
	Dean's List , Korea University ■ Academic Excellence Award for attaining a semester GPA of 4.5 / 4.5	Spring 2019
	Special Scholarship for the Student Affairs Office, Korea University	Fall 2019, Spring 2020
	 Veritas Scholarship, Korea University Research on optimize drone routing with trucks for on-demand services Advisor: Prof. Taesu Cheong 	Spring 2020
TEACHING EXPERIENCE	Teaching Assistant■ IE343: Statistical Machine Learning■ CoE202: Basics of Artificial Intelligence	Spring 2021 - 2024 Fall 2021
PROFESSIONAL SERVICES	 Conference Reviews AAAI Conference on Artificial Intelligence (AAAI) Conference on Neural Information Processing Systems (NeurIPS) International Conference on Learning Representations (ICLR) International Conference on Machine Learning (ICML) Learning on Graphs Conference (LoG) 	2023 - Now 2023 - Now 2024 - Now 2024 - Now 2023 - Now
	Journal Reviews ACM Transactions on Knowledge Discovery from Data (TKDD) IEEE Transactions on Neural Networks and Learning Systems (TNNLS) IEEE Transactions on Artificial Intelligence (TAI) World Wide Web Information Sciences The Journal of Supercomputing	
	 Workshop Reviews AI for New Drug Modalities @ NeurIPS New Frontiers of AI for Drug Discovery and Development (AI4D3) @ NeurIPS Computational Biology (WCB) @ ICML Structured Probabilistic Inference & Generative Modeling (SPIGM) @ ICML 	2024 2023 2023 2023
TALKS AND SEMINARS	Conditional Graph Information Bottleneck for Molecular Relational Learning ■ Learning on Graphs and Geometry (LoGG) Reading Group	2024
	Relational Self-Supervised Learning on Graphs • Top Conference Session of Korea Software Congress (KSC)	2022
	Augmentation-Free Self-Supervised Learning on Graphs ■ Top Conference Session of Korea Computer Congress (KCC)	2022
REFERENCES	Prof. Chanyoung Park Assistant Professor, Korea Advanced Institute of Science and Technology (KAIS E-mail: cy.park@kaist.ac.kr	ST)
	Prof. Jimeng Sun Health Innovation Professor, University of Illinois at Urbana-Champaign (UIUC E-mail: jimeng@illinois.edu	E)
	Prof. Tianfan Fu Assistant Professor, Rensselaer Polytechnic Institute (RPI) E-mail: fut2@rpi.edu	

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