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
- Graph Representation Learning
- Multi-modal Learning for Scientific Discovery

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

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

(†: Equal contribution)

CONFERENCES

[C9] Density of States Prediction of Crystalline Materials via Prompt-guided Multi-Modal Transformer
Namkyeong Lee†, Heewoong Noh†, Sungwon Kim, Dongmin Hyun, Gyoung S. Na, Chanyoung Park
Conference on Neural Information Processing Systems (**NeurIPS 2023**)

[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, Chanyoung 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 Park
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-Parametric 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 2022 Short Paper**)

[C1] Augmentation-Free Self-Supervised Learning on Graphs
Namkyeong Lee, Junseok Lee, Chanyoung Park
AAAI Conference on Artificial Intelligence (**AAAI 2022**)

JOURNALS

[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)

[J1] Self-Supervised Graph Representation Learning via Positive Mining
Namkyeong Lee, Junseok Lee, Chanyoung Park
Information Sciences (2022)

WORKSHOPS

[W5] Molecule Language Model with Augmented Pairs and Expertise Transfer
Namkyeong Lee, Siddhartha Laghuvarapu, Chanyoung Park, Jimeng Sun
ACL 2024 Workshop on Language and Molecules

[W4] Subgraph Federated Learning for Local Generalization
Sungwon Kim, Yoonho Lee, Carl Yang, Yunhak Oh, **Namkyeong Lee**, Sukwon Yun, Junseok Lee, Sein Kim, Chanyoung Park
KDD 2024 Workshop on Federated Learning for Data Mining and Graph Analytics (**FedKDD**)

[W3] Stoichiometry Representation Learning with Polymorphic Crystal Structures
Namkyeong Lee, Heewoong Noh, Gyoung S. Na, Tianfan Fu, Jimeng Sun, Chanyoung Park
NeurIPS 2023 Workshop on AI for Scientific Discovery: From Theory to Practice (**AI4Science**)

[W2] Deep Single-cell RNA-seq data Clustering with Graph Prototypical Contrastive Learning
Junseok Lee, Sungwon Kim, Dongmin Hyun, **Namkyeong Lee**, Yejin Kim, Chanyoung Park
ICML 2023 Workshop on Computational Biology (**WCB**)

[W1] Predicting Density of States via Multi-modal Transformer
Namkyeong Lee[†], Heewoong Noh[†], Sungwon Kim, Dongmin Hyun, Gyoung S. Na, Chanyoung Park
ICLR 2023 Workshop on Machine Learning for Materials (**ML4Materials**)

PROJECTS

Retrosynthesis Analysis for Inorganic Materials 2023
- Collaboration with Korea Research Institute of Chemical Technology (KRICT)

Learning Continual Universal User Representation for Recommendation 2022
- Collaboration with NAVER Shopping

Predicting Molecular Properties after Chemical Interaction 2022
- Collaboration with Korea Research Institute of Chemical Technology (KRICT)

Predicting Density of States based on the Structure of Materials 2021
- Collaboration with Korea Research Institute of Chemical Technology (KRICT)

Sentence Similarity Model for Korean Legal Sentences 2020
- 1st Awarded project at Seoul R&D research center

AWARDS & SCHOLARSHIPS

NeurIPS Scholar Award 2023

KDD Travel Award 2023

CIKM Travel Award 2022

Grand Prize at Seoul Innovation Challenge 2020, Seoul Business Agency 2021
- Building AI model for providing quantified answers to Korean legal questions
  - Awarded for the best team among 444 teams

Dean's List, Korea University Spring 2019
- Academic Excellence Award for attaining a semester GPA of 4.5 / 4.5

Special Scholarship for the Student Affairs Office, Korea University Fall 2019, Spring 2020

Veritas Scholarship, Korea University Spring 2020
- Research on optimize drone routing with trucks for on-demand services
  - Advisor: Prof. Taesu Cheong

Certificate, Korea National Police Agency 2018
- An exemplary auxiliary police.

TEACHING EXPERIENCE

Teaching Assistant
- IE343: Statistical Machine Learning Spring 2021 - 2024
- CoE202: Basics of Artificial Intelligence Fall 2021

PROFESSIONAL SERVICES

Conference Reviews
- AAAI Conference on Artificial Intelligence (AAAI) 2023 - 2025
- Conference on Neural Information Processing Systems (NeurIPS) 2023 - 2024
- International Conference on Learning Representations (ICLR) 2024
- International Conference on Machine Learning (ICML) 2024
- Learning on Graphs Conference (LoG) 2023 - 2025

Journal Reviews
- ACM Transactions on Knowledge Discovery from Data (TKDD)
- IEEE Transactions on Neural Networks and Learning Systems (TNNLS)
- World Wide Web
- Information Sciences

Workshop Reviews
- New Frontiers of AI for Drug Discovery and Development (AI4D3) @ NeurIPS 2023
- Computational Biology (WCB) @ ICML 2023
- Structured Probabilistic Inference & Generative Modeling (SPIGM) @ ICML 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 (KAIST)
E-mail: cy.park@kaist.ac.kr

Prof. Jimeng Sun
Health Innovation Professor, University of Illinois at Urbana-Champaign (UIUC)
E-mail: jimeng@illinois.edu

Prof. Tianfan Fu
Assistant Professor, Rensselaer Polytechnic Institute (RPI)
E-mail: fut2@rpi.edu

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