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 chemistry, biology, and more.

- Graph Neural Networks for Chemistry and Biology
- 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)

WORK EXPERIENCE

University of Illinois at Urbana-Champaign, Urbana, IL, USA — Sep 2023 – Present

- Visiting Scholar in Computer Science Department
  - Host: Prof. Jimeng Sun
  - 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

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

[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 Workshop on Computational Biology (**WCB 2023**)

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

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 - 2023
- CoE202: Basics of Artificial Intelligence — Fall 2021

PROFESSIONAL SERVICES

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

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

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

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

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