YUNHUI JANG

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RESEARCH INTEREST

My research goal is to build generative models for structured data. Specifically, I focus on graph generative models, molecular generative models, AI4Science, etc. My previous research focused on

- AI4Science: C1, C2, C3, C4, C5, P1, P2, P4
- Generative models for structural data: C1, C2, C4, C5, P1, P4
- Large language models for science: C5, P1, P2, P4

WORK EXPERIENCE

Valence Labs, Research intern, (host: Emmanuel Noutahi) Montreal, Canada / Jul 2025 - Oct 2025
PuzzleData, Intern, Process mining & data analysis projects, Seoul, South Korea / May 2020 - Aug 2020
Netmarble, Research intern, RNN-based anomaly detection, Seoul, South Korea / Jul 2018 - Aug 2018
JoyCity, Intern, Data analysis on marketing KPIs, Seoul, South Korea / Jun 2017 - Aug 2017

EDUCATION

KAIST, Ph.D. student in Graduate School of AI (advisor: Prof. Sungsoo Ahn) Feb 2025 - present
POSTECH, M.S. in Graduate School of AI (advisor: Prof. Sungsoo Ahn) Sep 2022 - Feb 2025
RWTH, Exchange student in Computer Science Mar 2019 - Feb 2020
POSTECH, B.S. in Industrial & Management Engineering - cum laude Mar 2015 - Aug 2020

PUBLICATIONS

C: conference, J: journal, W: workshop, P: preprint / * equal contribution

[P4] Improving Chemical Understanding of LLMs via SMILES Parsing
Yunhui Jang, Jaehyung Kim, Sungsoo Ahn

[P3] Self-Training Large Language Models with Confident Reasoning
Hyosoon Jang, Yunhui Jang, Sungjae Lee, Jungseul Ok, Sungsoo Ahn

[P2] MT-MOL: Multi Agent System with Tool-based Reasoning for Molecular Optimization
Hyomin Kim, Yunhui Jang, Sungsoo Ahn

[P1] Can LLMs Generate Diverse Molecules? Towards Alignment with Structural Diversity
Hyosoon Jang, Yunhui Jang, Jaehyung Kim, Sungsoo Ahn

[C5] Structural Reasoning Improves Molecular Understanding of LLM
Yunhui Jang, Jaehyung Kim, Sungsoo Ahn
Annual Meeting of the Association for Computational Linguistics (ACL) (Main), 2025
NeurIPS AIDrugX Workshop, 2024

[C4] Pessimistic Backward Policy for GFlowNets
Hyosoon Jang, Yunhui Jang, Minsu Kim, Jinkyoo Park, Sungsoo Ahn
Conference on Neural Information Processing Systems (NeurIPS), 2024

[C3] Hybrid neural representations for spherical data
Hyomin Kim, Yunhui Jang, Jaeho Lee, Sungsoo Ahn
International Conference on Machine Learning (ICML), 2024

[C2] A simple and scalable representation for graph generation
Yunhui Jang, Seul Lee, Sungsoo Ahn
International Conference on Learning Representations (ICLR), 2024
NeurIPS GLFrontiers Workshop, 2023

[C1] Graph generation with K^2-trees
Yunhui Jang, Dongwoo Kim, Sungsoo Ahn
International Conference on Learning Representations (ICLR), 2024
ICML Structured Probabilistic Inference & Generative Modeling Workshop, 2023
Bronze Prize in 30th Samsung Humantech Paper Awards
Winner in 2024 Qualcomm Innovation Fellowship Korea

HONORS & AWARDS

Winner in Qualcomm Innovation Fellowship Korea, Qualcomm ($3,000) 2024
Presidential Science Scholarship, South Korea ($70,000) 2024-present
Travel Award, ICLR ($1,500) 2024
Bronze Prize in 30th Samsung Humantech Paper Awards, Samsung, ($4,000) 2023
POSTECHIAN Fellowship, POSTECH, ($3,000) 2022, 2023
RWTH Aachen University Exchange Scholarship, RWTH Aachen, ($3,900) 2019
Realize Your Dream Scholarship, Blizzard Entertainment, ($2,500) 2018
Presidential Science Scholarship, South Korea, ($16,000) 2015-2020

SERVICES

Conference Reviewer: NeurIPS 2023-2025, ICLR 2024-2025, ICML 2024-2025, AAAI 2025

TALKS

Graph Generation with K^2-trees, Qualcomm, Seoul 2025
Speaking the Structure: Generative Models in Molecular Science, MILA, Montreal 2024

TEACHING

Teaching Assistant, POSTECH, CSED105: Introduction to AI Sep 2023 - Dec 2023
Teaching Assistant, LAIDD, Introduction to Geometric deep learning Oct 2023 - Nov 2023
Teaching Assistant, POSTECH, CSED490B: Introduction to machine learning Sep 2022 - Dec 2022
Teaching Assistant, Hyundai Steel, AI expert course Oct 2022 - Nov 2022