Sungsoo Ahn

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Education

MS/Ph.D Integrated Course in Electrical Engineering — Mar. 2015 – Mar. 2021
Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea
Advisor: Jinwoo Shin

BS in Electrical Engineering — Mar. 2011 – Mar. 2015
Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea

Employment

Assistant Professor — Jan. 2025 – Now
Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea

Assistant Professor — Dec. 2021 – Jan. 2025
Pohang University of Science and Technology (POSTECH), Pohang, South Korea
Graduate School of AI and Department of Computer Science and Engineering

Research Associate — Mar. 2021 – Nov. 2021
Mohamed Bin Zayed University of Artificial Intelligence (MBZUAI),
Abu Dhabi, United Arab Emirates
Supervisors: Le Song and Eric Xing

Research Intern — Jun. 2018 – Aug. 2018
Amazon Cambridge Development Center, Cambridge, England
Supervisor: Zhenwen Dai

Visiting Student — Mar. 2018 – May 2018
University of Cambridge, Cambridge, England
Host: Adrian Weller

Research Intern — Jun. 2017 – Aug. 2017
Los Alamos National Laboratory, New Mexico, United States
Host: Michael Chertkov

Research Intern — Jun. 2016 – Aug. 2016
Los Alamos National Laboratory, New Mexico, United States
Host: Michael Chertkov

Software Developer Intern — Jan. 2014 – Feb. 2014
Penta Security Systems Inc., Seoul, South Korea
Supervisor: Seonghwan Cho

Publications

Conference

1. Federico Berto, Chuanbo Hua, Junyoung Park, Laurin Luttmann, Yining Ma, Fanchen Bu, Jiarui Wang, Haoran Ye, Minsu Kim, Sanghyeok Choi, Nayeli Gast Zepeda, André Hottung, Jianan Zhou, Jieyi Bi, Yu Hu, Fei Liu, Hyeonah Kim, Jiwoo Son, Haeyeon Kim, Davide Angioni, Wouter Kool, Zhiguang Cao, Qingfu Zhang, Joungho Kim, Jie Zhang, Kijung Shin, Cathy Wu, **Sungsoo Ahn**, Guojie Song, Changhyun Kwon, Kevin Tierney, Lin Xie, Jinkyoo Park, RL4CO: an Extensive Reinforcement Learning for Combinatorial Optimization Benchmark, In *Knowledge Discovery and Data Mining (KDD) Datasets and Benchmarks*, 2025.

2. Yunhui Jang, Jaehyung Kim, **Sungsoo Ahn**, Structural Reasoning Improves Molecular Understanding of LLM, In *Annual Meeting of the Association for Computational Linguistics (ACL) Main*, 2025.

3. Dongyoon Hahm, Woogyeol Jin, June Suk Choi, **Sungsoo Ahn**, Kimin Lee, Enhancing LLM Agent Safety via Causal Influence Prompting, In *Annual Meeting of the Association for Computational Linguistics (ACL) Findings*, 2025.

4. Minsu Kim, Sanghyeok Choi, Taeyoung Yun, Emmanuel Bengio, Leo Feng, Jarrid Rector-Brooks, **Sungsoo Ahn**, Jinkyoo Park, Nikolay Malkin, and Yoshua Bengio, Adaptive Teachers for Amortized Samplers, In *International Conference on Learning Representations (ICLR)*, 2025.

5. Taewon Kim, Hyunjin Seo, **Sungsoo Ahn**, Eunho Yang, ReBind: Enhancing Ground-state Molecular Conformation Prediction via Force-Based Graph Rewiring, In *International Conference on Learning Representations (ICLR)*, 2025.

6. Kiyoung Seong, Seonghyun Park, Seonghwan Kim, Woo Youn Kim, **Sungsoo Ahn**, Transition Path Sampling with Improved Off-Policy Training of Diffusion Path Samplers, In *International Conference on Learning Representations (ICLR)*, 2025.

7. Nayoung Kim, Seongsu Kim, Minsu Kim, Jinkyoo Park, **Sungsoo Ahn**, MOFFlow: Flow Matching for Structure Prediction of Metal-Organic Frameworks, In *International Conference on Learning Representations (ICLR)*, 2025.

8. Seonghwan Seo, Minsu Kim, Tony Shen, Martin Ester, Jinkyoo Park, **Sungsoo Ahn**, Woo Youn Kim, Generative Flows on Synthetic Pathway for Drug Design, In *International Conference on Learning Representations (ICLR)*, 2025.

9. Hyosoon Jang, Yunhui Jang, Minsu Kim, Jinkyoo Park, **Sungsoo Ahn**, Pessimistic Backward Policy for GFlowNets, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2024

10. Seongsu Kim, **Sungsoo Ahn**, Gaussian plane-wave neural operator for electron density estimation, In *International Conference on Machine Learning (ICML)*, 2024.

11. Hyomin Kim, Yunhui Jang, Jaeho Lee, **Sungsoo Ahn**, Hybrid neural representation for spherical data, In *International Conference on Machine Learning (ICML)*, 2024.

12. Nayeong Kim, Juwon Kang, **Sungsoo Ahn**, Jungseul Ok, Suha Kwak, Removing multiple biases through the lens of multi-task learning, In *International Conference on Machine Learning (ICML)*, 2024.
13. Hyeonah Kim, Minsu Kim, **Sungsoo Ahn**, Jinkyoo Park, Enhancing sample efficiency in black-box combinatorial optimization via symmetric replay training, In *International Conference on Machine Learning (ICML)*, 2024.
14. Fanchen Bu, Hyeonsoo Jo, Soo Yong Lee, **Sungsoo Ahn**, Kijung Shin, Tackling complex conditions in unsupervised combinatorial optimization: cardinality, minimum, covering, and more, In *International Conference on Machine Learning (ICML)*, 2024.
15. Youngsik Yoon, Gangbok Lee, Sungsoo Ahn, Jungseul Ok, Breadth-first exploration in adaptive grid-based reinforcement learning, In *International Conference on Machine Learning (ICML)*, 2024.
16. Hyosoon Jang, Minsu Kim, and **Sungsoo Ahn**, Learning energy decompositions for partial inference in GFlowNets, In *International Conference on Learning Representations (ICLR)*, 2024, oral presentation (86/7304 = 1.18% accept rate).
17. Yunhui Jang, Seul Lee, and **Sungsoo Ahn**, A simple and scalable representation for graph generation, In *International Conference on Learning Representations (ICLR)*, 2024.
18. Yunhui Jang, Dongwoo Kim, and **Sungsoo Ahn**, Hierarchical graph generation with K2 trees, In *International Conference on Learning Representations (ICLR)*, 2024.
19. Minsu Kim, Taeyoung Yun, Emmanuel Bengio, Dinghuai Zhang, Yoshua Bengio, **Sungsoo Ahn**, and Jinkyoo Park, Local search GFlowNets, In *International Conference on Learning Representations (ICLR)*, 2024, spotlight presentation (366/7304 = 5.0% accept rate).
20. Hyosoon Jang, Seonghyun Park, Sangwoo Mo, and **Sungsoo Ahn**, Diffusion probabilistic models for structured node classification, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2023.
21. Minsu Kim, Federico Berto, **Sungsoo Ahn**, and Jinkyoo Park, Bootstrapped training of score-conditioned generator for offline design of biological sequences, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2023.
22. Hyuna Cho, Minjae Jeong, Sooyeon Jeon, **Sungsoo Ahn**, and Wonhwa Kim, Multi-resolution spectral coherence for graph generation with score-based diffusion, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2023.
23. Sungbin Shin, Yohan Jo, **Sungsoo Ahn**, and Namhoon Lee, A closer look at the intervention procedure of concept bottleneck models, *International Conference on Machine Learning (ICML)*, 2023.
24. Junsu Kim, Younggyo Seo, **Sungsoo Ahn**, Kyunghwan Son, and Jinwoo Shin, Imitating graph-based planning with goal-conditioned policies, In *International Conference on Learning Representations (ICLR)*, 2023.

25. Nayeong Kim, Sehyun Hwang, **Sungsoo Ahn**, Jaesik Park, and Suha Kwak, Learning debiased classifier with biased committee, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2022.
26. Kyunghwan Son, Junsu Kim, **Sungsoo Ahn**, Roben Delos Reyes, Yung Yi, and Jinwoo Shin, Disentangling sources of risk for distributional multi-agent reinforcement learning, *International Conference on Machine Learning (ICML)*, 2022.
27. Jaehyung Kim, Dongyeop Kang, **Sungsoo Ahn**, and Jinwoo Shin, What makes better augmentation strategies? Augment difficult but not too different, In *International Conference on Learning Representations (ICLR)*, 2022.
28. **Sungsoo Ahn**, Binghong Chen, Tianzhe Wang, and Le Song, Spanning tree-based graph generation for molecules, In *International Conference on Learning Representations (ICLR)*, 2022, spotlight presentation (174/3422 = 5.2% accept rate).
29. Sihyun Yu, **Sungsoo Ahn**, Le Song, and Jinwoo Shin, RoMA: Robust model adaptation for offline model-based optimization, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2021.
30. Junsu Kim, **Sungsoo Ahn**, Hankook Lee, and Jinwoo Shin, Self-improved retrosynthetic planning, In *International Conference on Machine Learning (ICML)*, 2021.
31. Hankook Lee, **Sungsoo Ahn**, Seung Woo Seo, You Young Song, Sung Ju Hwang, Eunho Yang, and Jinwoo Shin, RetCL: A selection-based approach for retrosynthesis via contrastive learning, In *International Joint Conference on Artificial Intelligence (IJCAI)*, 2021.
32. Jaeho Lee, Sejun Park, Sangwoo Mo, **Sungsoo Ahn**, and Jinwoo Shin, Layer-adaptive sparsity for the magnitude-based pruning, In *International Conference on Learning Representations (ICLR)*, 2021.
33. **Sungsoo Ahn**, Junsu Kim, Hankook Lee, and Jinwoo Shin, Guiding deep molecular optimization with genetic exploration, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2020.
34. **Sungsoo Ahn**, Younggyo Seo, and Jinwoo Shin, Learning what to defer for maximum independent sets, *International Conference on Machine Learning (ICML)*, 2020.
35. Junhyun Nam, Hyuntak Cha, **Sungsoo Ahn**, Jaeho Lee, and Jinwoo Shin, Learning from failure: De-biasing classifier from biased classifier, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2020.
36. **Sungsoo Ahn**, Shell Xu Hu, Andreas Damianou, Neil D Lawrence, and Zhenwen Dai, Variational information distillation for knowledge transfer, In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, 2019.
37. **Sungsoo Ahn**, Michael Chertkov, and Jinwoo Shin, Bucket renormalization for approximate inference, In *International Conference on Machine Learning (ICML)*, 2018.
38. **Sungsoo Ahn**, Michael Chertkov, Jinwoo Shin, and Adrian Weller, Gauged mini-bucket elimination for approximate inference, In *International Conference on Artificial Intelligence*

and Statistics (AISTATS), 2018.

39. **Sungsoo Ahn**, Michael Chertkov, and Jinwoo Shin, Gauging variational inference, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2017.

40. **Sungsoo Ahn**, Michael Chertkov, and Jinwoo Shin, Synthesis of MCMC and belief propagation, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2016, oral presentation (46/2500 = 1.8% accept rate), first NeurIPS oral from a South Korean Instituition.

41. **Sungsoo Ahn**, Sejun Park, Michael Chertkov, and Jinwoo Shin, Minimum weight perfect matching via blossom belief propagation, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2015, spotlight presentation (82/1838 = 4.5% accept rate).

Journal

1. Nayoung Kim, Minsu Kim, **Sungsoo Ahn**, Jinkyoo Park, Decoupled Sequence and Structure Generation for Realistic Antibody Design, In *Transactions of Machine Learning Research (TMLR)*, 2024.

2. Seonghyun Park, Narae Ryu, Gahee Kim, Dongyeop Woo, Se-Young Yun, and **Sungsoo Ahn**, Non-backtracking graph neural networks, In *Transactions of Machine Learning Research (TMLR)*, 2024.

3. Seojin Kim, Jaehyun Nam, Junsu Kim, Hankook Lee, Sungsoo Ahn, Jinwoo Shin, Fragment-based Multi-view Molecular Contrastive Learning, In *Transactions of Machine Learning Research (TMLR)*, 2024.

4. **Sungsoo Ahn**, Michael Chertkov, and Jinwoo Shin, Bucket renormalization for approximate inference, In *Journal of Statistical Mechanics: Theory and Experiment*, 12(12), 124015, 2019.

5. **Sungsoo Ahn**, Michael Chertkov, and Jinwoo Shin, Gauging variational inference, In *Journal of Statistical Mechanics: Theory and Experiment*, 12(12), 124022, 2019.

6. **Sungsoo Ahn**, Michael Chertkov, Andrew E Gelfand, Sejun Park, and Jinwoo Shin, Maximum weight matching using odd-sized cycles: Max-product belief propagation and half-integrality, In *IEEE Transactions on Information Theory*, 64(3), 1471–1480, 2018.

Workshop

1. Seonghyun Park, Kiyoung Seong, Soojung Yang, Rafael Gomez-Bombarelli, **Sungsoo Ahn**, Learning Collective Variables from Time-lagged Generation, In *International Conference of Machine Learning (ICML)*, *GenBio Workshop*, 2025.

2. Seonghwan Seo, Minsu Kim, Tony Shen, Martin Ester, Jinkyoo Park, **Sungsoo Ahn**, Woo Youn Kim, Generative flows on synthetic pathway for drug design, In *Neural Information Processing Systems (NeurIPS)*, *AIDrugX Workshop*, 2024.

3. Nayoung Kim, Seongsu Kim, Minsu Kim, Jinkyoo Park, **Sungsoo Ahn**, MOFFlow: Flow matching for structure prediction of metal-organic frameworks, In *Neural Information Processing Systems (NeurIPS)*, *AIDrugX Workshop*, 2024.

4. Yunhui Jang, Jaehyung Kim, **Sungsoo Ahn**, Chain-of-thoughts for molecular understanding, In *Neural Information Processing Systems (NeurIPS)*, *AIDrugX Workshop*, 2024.
5. Kiyoung Seong, Seonghyun Park, Seonghwan Kim, Woo Youn Kim, Sungsoo Ahn, Transition path sampling with improved off-policy training of diffusion path samplers, In *International Conference of Machine Learning (ICML)*, *SPIGM Workshop*, 2024.
6. Seonghyun Park, Narae Ryu, Gahee Kim, Dongyeop Woo, Se-Young Yun, and **Sungsoo Ahn**, Non-backtracking graph neural networks, In *Conference on Neural Information Processing Systems (NeurIPS)*, *GLFrontiers Workshop*, 2023, oral presentation.
7. Yunhui Jang, Dongwoo Kim, and **Sungsoo Ahn**, A simple and scalable representation for graph generation, In *Conference on Neural Information Processing Systems (NeurIPS)*, *GLFrontiers Workshop*, 2023.
8. Hyeonah Kim, Minsu Kim, **Sungsoo Ahn**, and Jinkyoo Park, Symmetric exploration in combinatorial optimization is free! *International Conference on Machine Learning (ICML)*, *Workshop on Sampling and Optimization in Discrete Space*, 2023.
9. Nayeong Kim, Juwon Kang, **Sungsoo Ahn**, Jungseul Ok, and Suha Kwak, Removing multiple biases through the lens of multi-task learning, *International Conference on Machine Learning (ICML)*, *Workshop on Spurious Correlations, Invariance and Stability*, 2023.
10. Jaeseung Heo, Seungbeom Lee, **Sungsoo Ahn**, and Dongwoo Kim, EPIC: Graph augmentation with edit path interpolation via learnable cost, *International Conference on Machine Learning (ICML)*, *Workshop on Data-centric Machine Learning Research*, 2023.
11. Minsu Kim, Federico Berto, **Sungsoo Ahn**, and Jinkyoo Park, Bootstrapped training of score-conditioned generator for offline design of biological sequences, *International Conference on Machine Learning (ICML)*, *Workshop on Structured Probabilistic Inference and Generative Modeling*, 2023.
12. Yunhui Jang, Dongwoo Kim, and **Sungsoo Ahn**, Hierarchical graph generation with k2 trees, *International Conference on Machine Learning (ICML)*, *Workshop on Structured Probabilistic Inference and Generative Modeling*, 2023.
13. Hyosoon Jang, Seonghyun Park, Sangwoo Mo, and **Sungsoo Ahn**, Diffusion probabilistic models for structured node classification, *International Conference on Machine Learning (ICML)*, *Workshop on Structured Probabilistic Inference and Generative Modeling*, 2023.
14. Seojin Kim, Jaehyun Nam, Junsu Kim, Hankook Lee, **Sungsoo Ahn**, and Jinwoo Shin, Contrastive learning of molecular representation with fragmented views, In *International Conference on Learning Representations (ICLR)*, *Machine Learning for Materials Workshop*, 2023.
15. Nayeong Kim, Sehyun Hwang, **Sungsoo Ahn**, Jaesik Park, and Suha Kwak, Learning debiased classifier with biased committee, *International Conference on Machine Learning (ICML)*, *Workshop on Spurious Correlations, Invariance, and Stability*, 2022.
16. Jiye Kim, Seungbeom Lee, Dongwoo Kim, **Sungsoo Ahn**, and Jaesik Park, Substructure-atom cross attention for molecular representation learning, In *Conference on Neural Information Processing Systems (NeurIPS)*, *Workshop on AI for Science*, 2022.

17. Sungbin Shin, Yohan Jo, **Sungsoo Ahn**, and Namhoon Lee, A closer look at the intervention procedure of concept bottleneck models, In *Conference on Neural Information Processing Systems (NeurIPS)*, *Workshop on Trustworthy and Socially Responsible Machine Learning (TSRML)*, 2022.
18. Sihyun Yu, Sangwoo Mo, **Sungsoo Ahn**, Jinwoo Shin, Visual abstract reasoning via logic-guided generation, *International Conference on Machine Learning (ICML)*, *Workshop on Self-Supervised Learning for Reasoning and Perception*, 2021, oral presentation.
19. Hankook Lee, **Sungsoo Ahn**, Seung Woo Seo, You Young Song, Sung Ju Hwang, Eunho Yang, and Jinwoo Shin, RetCL: A selection-based approach for retrosynthesis via contrastive learning, In *Conference on Neural Information Processing Systems (NeurIPS)*, *Workshop on Machine Learning for Molecules*, 2020.
20. **Sungsoo Ahn**, Shell Xu Hu, Andreas Damianou, Neil D Lawrence, and Zhenwen Dai, Variational mutual information distillation for transfer learning, In *Conference on Neural Information Processing Systems (NeurIPS)*, *Workshop on Continual Learning, 2018*.

Academic Services

Area Chair

1. Conference on Neural Information Processing Systems (NeurIPS) 2022 – 2025
2. International Conference on Machine Learning (ICML) 2022 – 2025
3. International Conference on Learning Representations (ICLR) 2024 – 2025
4. International Conference on Artificial Intelligence and Statistics (AISTATS) 2022 – 2024
5. Association for the Advancement of Artificial Intelligence (AAAI) 2024
6. Transactions of Machine Learning Research (TMLR) 2024 – 2025

Workflow Chair

1. International Conference on Machine Learning (ICML) 2022

Reviewer

1. Conference on Neural Information Processing Systems (NeurIPS) 2018 – 2021
2. International Conference on Machine Learning (ICML) 2019 – 2021
3. International Conference on Learning Representations (ICLR) 2019 – 2024
4. International Conference on Artificial Intelligence and Statistics (AISTATS) 2019 – 2021

Talks

1. Foundation Models for Material Discovery July. 2025
   Korea Institute of Material Science (KIMS), Changwon, South Korea

2. Generative Models for Molecular Discovery July. 2025
   Seoul National University, Seoul, South Korea
3. A Generative Model for Metal Organic Frameworks July. 2025
   KAIST-MILA Annual Workshop, Montreal, Canada
4. Machine Learning for Transition Path Sampling July. 2025
   Korean In silico bio Design and Discovery Society (KIDDS), Daejeon, South Korea
5. Generative Models for Molecular Discovery May. 2025
   LG AI Research, Seoul, South Korea
6. Optimization methods for material science Dec. 2024
   POSCO Holdings, Seoul, South Korea
7. Structure- and energy-based machine learning for molecules Dec. 2024
   KAIST-MILA Prefrontal AI Workshop, Montreal, Canada
8. Amortizing intractable inference for molecular discovery Nov. 2024
   Physics Informed Machine Learning Workshop, New Mexico, United States
9. Opportunities and challenges in deep graph generative models Nov. 2023
   AI Korea, Seoul, South Korea
10. Machine learning for drug discovery Oct. 2023
    Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea
11. Graph structured prediction and graph generation with deep learning Jun. 2023
    Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea
12. Deep neural networks for graph optimization Nov. 2022
    University of Arizona, Arizona, United States
13. Geometric deep learning for drug discovery Aug. 2022
    Korean Artificial Intelligence Association (KAIA), Jeju, South Korea
14. Machine learning for drug discovery Jun. 2022
    Centre for Frontier AI Research, Singapore
15. Elimination techniques in probabilistic graphical models Jun. 2021
    Skolkovo Institute of Science and Technology (Skoltech), Moscow, Russia
16. Guiding deep molecular optimization with genetic exploration Dec. 2020
    Samsung Advanced Institute of Technology (SAIT), Suwon, South Korea
17. Scaling deep reinforcement learning to Large combinatorial problems Feb. 2020
    Pohang University of Science and Technology (POSTECH), Pohang, South Korea
18. Bucket renormalization for approximate inference Jul. 2018
    University of Oxford, Oxford, England
19. Mini-bucket renormalization Feb. 2018
    Physics Informed Machine Learning Workshop, Santa Fe, New Mexico, United States

20. Gauge transformation of graphical models Jul. 2017
Los Alamos National Laboratory (LANL), New Mexico, United States
21. Optimizing gauge transformation for inference in graphical model Feb. 2017
Banff Workshop, Alberta, Canada
22. Synthesis of MCMC and belief propagation Jul. 2016
Los Alamos National Laboratory (LANL), New Mexico, United States
23. Minimum weight perfect matching via blossom belief propagation Nov. 2015
Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea

Courses

1. Geometric deep learning (AI810) Spring 2025
Korea Advanced Institute of Science and Technology (KAIST)
2. Introduction to artificial intelligence (CSED105). Fall 2024
Pohang University of Science and Technology (POSTECH)
3. Machine learning for graphs (CSED/AIGS703I) Spring 2024
Pohang University of Science and Technology (POSTECH)
4. Introduction to artificial intelligence (CSED105). Fall 2023
Pohang University of Science and Technology (POSTECH)
5. Probabilistic graphical models (CSED/AIGS524) Spring 2023
Pohang University of Science and Technology (POSTECH)
6. Introduction to machine learning (CSED490B) Fall 2022
Pohang University of Science and Technology (POSTECH)
7. Probabilistic graphical models (CSED/AIGS524) Spring 2022
Pohang University of Science and Technology (POSTECH)

Awards

1. NVIDIA Academic Grant Program Award Spring 2025