Yinhua Piao

Personal Information

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Education

2025–Present **Postdoc in Bioinformatics Institute**
Seoul National University, Seoul, Korea.

2020–2025 **Ph.D in Computer Science and Engineering**
Seoul National University, Seoul, Korea.
Advisor: Prof. Sun Kim
Thesis: Subgraph-informed Hierarchical Learning in Clinical and Biomedical Domains. ***(Outstanding Doctoral Dissertation Award)***

2018–2020 **M.S. in Computer Science and Engineering**
Seoul National University, Seoul, Korea.
Advisor: Prof. Sun Kim
Thesis: Graph Convolutional Networks for Predictive Healthcare using Clinical Notes.

2014–2018 **B.S. in Software Engineering**
Jilin University, Changchun, China.

Honors, Awards & Scholarships

Feb. 2025 Outstanding Doctoral Dissertation Award, SNU.

Dec. 2024 Research Fair Best Poster Award, SNU.

Aug. 2024 Youlchon AI Star Scholarship.

Feb. 2024 Samsung HumanTech Paper Award.

Apr. 2022 AIIS Retreat Best Poster Award.

Feb. 2022 Samsung HumanTech Paper Award (Bronze Prize).

Feb. 2022 AAAI Student Scholar Scholarship.

Jun.20–Jan.22 SNU Global Scholarships II.

Selected Publications

1. Piao, Y., Lee, S., Lu, Y., and Kim, S. Improving out-of-distribution generalization in graphs via hierarchical semantic environments. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition* (2024)
2. *Kim, N., *Piao, Y., and Kim, S. Clinical note owns its hierarchy: Multi-level hypergraph neural networks for patient-level representation learning. In *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)* (Toronto, Canada, July 2023), A. Rogers, J. Boyd-Graber, and N. Okazaki, Eds., Association for Computational Linguistics, pp. 5559–5573
3. Piao, Y., Lee, S., Lee, D., and Kim, S. Sparse structure learning via graph neural networks for inductive document classification. In *Proceedings of the AAAI conference on artificial intelligence* (2022), vol. 36, pp. 11165–11173
4. *Shin, J., *Piao, Y., Bang, D., Kim, S., and Jo, K. Drpreter: Interpretable anticancer drug response prediction using knowledge-guided graph neural networks and transformer. *International Journal of Molecular Sciences 23*, 22 (2022), 13919

Publications

1. Kim, Y., Piao, Y., Lee, S., and Kim, S. Aligning molecules and fragments in a shared embedding space for RL-based molecule generation. In *ICLR 2025 Workshop on Machine Learning for Genomics Explorations* (2025)
2. Bang, D., Sung, I., Piao, Y., Lee, S., and Kim, S. Predicting drug-likeness via biomedical knowledge alignment and EM-like one-class boundary optimization. In *Forty-second International Conference on Machine Learning* (2025)
3. Lu, Y., Piao, Y., Lee, S., and Kim, S. Context-aware hierarchical fusion for drug relational learning. *IEEE/ACM Transactions on Computational Biology and Bioinformatics* (2025)
4. Ha, S., Kim, J. H., Piao, Y., and Kim, S. MV-CLAM: Multi-view molecular interpretation with cross-modal projection via language model. In *NeurIPS 2024 Workshop on AI for New Drug Modalities* (2024)
5. Cho, C., Lee, S., Bang, D., Piao, Y., and Kim, S. Chemap: predicting drug approval with chemical structures before clinical trial phase by leveraging multi-modal embedding space and knowledge distillation. *Scientific Reports 14*, 1 (2024), 23010
6. Lee, S., Park, J., Piao, Y., Lee, D., Lee, D., and Kim, S. Multi-layered knowledge graph neural network reveals pathway-level agreement of three breast cancer multi-gene assays. *Computational and Structural Biotechnology Journal* (2024)

7. Lu, Y., Piao, Y., and Kim, S. Enhancing drug-drug interaction prediction with context-aware architecture. In *The Second Tiny Papers Track at ICLR 2024*
8. Piao, Y., Lee, S., Lu, Y., and Kim, S. Improving out-of-distribution generalization in graphs via hierarchical semantic environments. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition* (2024)
9. *Kim, N., *Piao, Y., and Kim, S. Clinical note owns its hierarchy: Multi-level hypergraph neural networks for patient-level representation learning. In *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)* (Toronto, Canada, July 2023), A. Rogers, J. Boyd-Graber, and N. Okazaki, Eds., Association for Computational Linguistics, pp. 5559–5573
10. Yi, J., Lee, S., Lim, S., Cho, C., Piao, Y., Yeo, M., Kim, D., Kim, S., and Lee, S. Exploring chemical space for lead identification by propagating on chemical similarity network. *Computational and Structural Biotechnology Journal 21* (2023), 4187–4195
11. Piao, Y., Lee, S., Lee, D., and Kim, S. Sparse structure learning via graph neural networks for inductive document classification. In *Proceedings of the AAAI conference on artificial intelligence* (2022), vol. 36, pp. 11165–11173
12. *Shin, J., *Piao, Y., Bang, D., Kim, S., and Jo, K. Drpreter: Interpretable anticancer drug response prediction using knowledge-guided graph neural networks and transformer. *International Journal of Molecular Sciences 23*, 22 (2022), 13919
13. Lim, S., Lee, S., Piao, Y., Choi, M., Bang, D., Gu, J., and Kim, S. On modeling and utilizing chemical compound information with deep learning technologies: A task-oriented approach. *Computational and Structural Biotechnology Journal 20* (2022), 4288–4304
14. Lee, S., Lee, D., Piao, Y., and Kim, S. Spgp: Structure prototype guided graph pooling. In *NeurIPS 2022 Workshop: New Frontiers in Graph Learning* (2022)
15. Bae, J. H., Shin, Y., Piao, Y., Lim, J. H., and Kim, S. Mo1641: Confidence estimation in clinical decision support system for determination of colonoscopy surveillance interval. *Gastroenterology 162*, 7 (2022), S–839
16. Kim, S., Bae, S., Piao, Y., and Jo, K. Graph convolutional network for drug response prediction using gene expression data. *Mathematics 9*, 7 (2021), 772
17. Piao, Y. Graph convolutional networks for predictive healthcare using clinical notes, 2020

Preprints

1. Yijingxiu Lu, Yinhua Piao, M. S., and Kim, S. Improving reaction yield prediction with chemical role and reaction center aware representation learning. *Under Submission* (2025)
2. Lee, S., Piao, Y., Lee, D., and Kim, S. Multi-task informed learnable prototypes on few shot learning for molecular property prediction. *Under submission* (2023)
3. Kim, S., Kim, N., Piao, Y., and Kim, S. Grapht5: Unified molecular graph-language modeling via multi-modal cross-token attention. *Under submission* (2023)

Community Service

2022-2025	(Proceedings) AAAI, IJCAI, NeurIPS, CVPR, KDD, ACML, ICCV, ACL.
2022-2025	(Journal) Npj Systems Biology and Applications, BMC Bioinformatics, Pattern Analysis and Applications, Scientific Reports, Transactions on Knowledge Discovery from Data, BMC Biology, BMC Medical Informatics and Decision Making, Journal of Biomedical Informatics, Computational and Structural Biotechnology Journal.

Presentations

Jan. 2025	**Invited Talk**, Improving out-of-distribution generalization in graphs via hierarchical semantic environments. *AI/Computing Frontier School in Seoul National University*
Dec. 2023	**Invited Talk**, Multi-level Hypergraph Neural Networks for Patient-level Representation Learning. *ModuleCon, ModuleLab in Ewha Womans University*
Dec. 2023	**Invited Talk**, Sparse Structure learning via GNNs for Document Classification. *ModuleCon, ModuleLab in Ewha Womans University*
Nov. 2022&2023	**Tutorial** Self-supervised Learning on Molecule Graphs. *AI-BIO Researcher Training Course, AIIS in Seoul National University*
Sep. 2022	**Invited Talk**, Sparse Structure learning via GNNs for Document Classification. *CSE Fun Lunch Seminars in Seoul National University*
Apr. 2022	**Invited Talk**, Sparse Structure learning via GNNs for Document Classification *AI Retreat, AIIS in Seoul National University*

Teaching

Spring 2025	**Teaching Assistant**, Machine Learning on Bioinformatics.
Fall 2024	**Head Teaching Assistant**, Algorithms.
Spring 2024	**Head Teaching Assistant**, Machine Learning on Bioinformatics.
Fall 2023	**Teaching Assistant**, Algorithms.
Spring 2023	**Teaching Assistant**, Machine Learning on Bioinformatics.
Fall 2022	**Teaching Assistant**, Algorithms.
Spring 2022	**Teaching Assistant**, Machine Learning on Bioinformatics..
Fall 2020	**Teaching Assistant**, Algorithms.

Supervision

2024-2025	**Junha Kim** Master Student, SNU. On the process of molecule generation using subgraph mining.
2023-2024	**Sumin Ha & Jun Hyeong Kim**, Master Student, SNU. Resulting paper are presented at NeurIPS AIdrugX Workshop 2024.
2023	**Sangyeup Kim**, Master Student, SNU. Resulting paper is under submission (with Nayeon Kim).
2022-2023	**Nayeon Kim**, Master Student, SNU. Resulting paper got a oral presentation (top 0.7%) at ACL 2023.
2021-2022	**Jihye Shin**, Master Student, SNU. Resulting paper got accepted by IJMS 2022.

Languages

Chinese and Korean: Native
English: Fluent

May 10, 2025