

Xinyue XU

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EDUCATION

- **Hong Kong University of Science and Technology** Sep 2022 - Present
Doctor of Philosophy in Electronic and Computer Engineering
◦ Supervisor: Prof. Xiaomeng Li Hong Kong
- **Australian National University** Jul 2018 - Jun 2022
Bachelor of Advanced Computing (Honours)
◦ Supervisor: Senior Prof. Amanda Barnard & Dr. Amanda Parker Canberra, Australia
◦ Specialisations: Intelligent Systems

RESEARCH EXPERIENCE

- **ANU Computational Science Group** Jun 2021 - Jun 2022
Honours Student Supervisor: Senior Prof. Amanda Barnard & Dr. Amanda Parker
- **MIT CSAL Computational Connectomics Group** Sep 2021 - May 2022
Research Internship Advisor: Prof. Lu Mi & Prof. Hao Wang
- **National University of Singapore** Jan 2021 - Mar 2021
Research Internship Advisor: Dr. Gang Guo

PUBLICATIONS AND MANUSCRIPTS

*=EQUALLY CONTRIBUTED CO-FIRST AUTHORS

- [1] **Xinyue Xu***, Yueying Hu*, Hui Tang, Yi Qin, Lu Mi, Hao Wang, and Xiaomeng Li, "Concept-based unsupervised domain adaptation," *The 42st International Conference on Machine Learning (ICML)*, 2025.
- [2] **Xinyue Xu**, Yi Qin, Lu Mi, Hao Wang, and Xiaomeng Li, "Energy-based concept bottleneck models: Unifying prediction, concept intervention, and probabilistic interpretations," *International Conference on Learning Representations (ICLR)*, 2024.
- [3] Yi Qin, **Xinyue Xu**, Hao Wang, and Xiaomeng Li, "Energy-based conceptual diffusion model," *The 38th Conference on Neural Information Processing Systems (NeurIPS) Safe Generative AI Workshop*, 2024.
- [4] Chen Zhao, Kai Wang, Qianji Jiao, **Xinyue Xu**, et al., "Machine learning models for evaluating biological reactivity within molecular fingerprints of dissolved organic matter over time," *Geophysical Research Letters (GRL)*, 2024.
- [5] Chen Zhao*, **Xinyue Xu***, et al., "Exploring the complexities of dissolved organic matter photochemistry from the molecular level by using machine learning approaches," *Environmental Science & Technology (EST)*, 2023.
- [6] **Xinyue Xu***, Yuhan Hsi*, Haonan Wang, and Xiaomeng Li, "Dynamic data augmentation via monte-carlo tree search for prostate mri segmentation," in *International Conference on Neural Information Processing*. Springer, 2023, pp. 272–282.
- [7] Zhongren Chen*, **Xinyue Xu***, Shengyi Jiang, Hao Wang, and Lu Mi, "Subgraph frequency distribution estimation using graph neural networks," *ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD) Workshop on Deep Learning on Graphs*, 2022.
- [8] **Xinyue Xu** and Xiaolu Zheng, "Hybrid model for network anomaly detection with gradient boosting decision trees and tabtransformer," in *ICASSP 2021 - 2021 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, 2021, pp. 8538–8542.
- [9] **Xinyue Xu**, Xiang Ding, Zhenyue Qin, and Yang Liu, "Classification Models for Medical Data with Interpretative Rules," in *International Conference on Neural Information Processing*, 2021, pp. 227–239.

HONORS AND AWARDS

- Hong Kong PhD Fellowship, 2022 - 2026
- HKPFS Conference Travel Allowance, 2023 - 2024
- HKUST RedBird PhD Award, 2022 - 2023
- HKUST Academic Excellence Awards (Continuing Students), 2023 - 2024

TEACHING EXPERIENCE

- **Hong Kong University of Science and Technology**

Feb 2023 – Dec 2023

Teaching Assistant

Instructors: Prof. Bertram Shi & Prof. Ross Murch

ELEC 1200 A System View of Communications: from Signals to Packets

- **Shanghai Jiao Tong University Summer School**

Dec 2019 – Jan 2020

Teaching Assistant

Instructors: Prof. Xiaojun Zhu & Prof. Xiangdong An

Statistics of Stochastic Process & Algorithms and Analysis

RESEARCH INTERESTS

Interpretable ML: Concept-based models, Rule-based explanations, Counterfactual explanations

Large Language Models: Mechanistic Interpretability, Multimodal LLM

AI for Science: Healthcare, Environmental Science, Material Science

ADDITIONAL INFORMATION

Skills: Python (PyTorch, TensorFlow), SQL, Java, Haskell, C++, ARMv7, Ada, HTML/CSS

Services: ICONIP 2023 - 2024 Program Committee Member, ICONIP 2025 Reviewer, ICLR 2025 Reviewer

Memberships: IEEE Graduate Student Member, Asia Pacific Neural Network Society Member, Australian Computer Society Associate Member

REFERENCES

1. **Prof. Xiaomeng LI**

Assistant Professor, Department of Electronic and Computer Engineering

Hong Kong University of Science and Technology

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2. **Prof. Hao WANG**

Assistant Professor, Department of Computer Science

Rutgers University

Email: hw488@cs.rutgers.edu

3. **Prof. Lu MI**

Assistant Professor, School of Computational Science and Engineering

Georgia Institute of Technology

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