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 Hong Kong
  ◦ Supervisor: Prof. Xiaomeng LI, Co-Supervisor: Prof. Hao Wang (Rutgers University)

- **Australian National University** *Jul 2018 - Jun 2022*
Bachelor of Advanced Computing (Honours) Canberra, Australia
  ◦ Supervisor: Senior Prof. Amanda Barnard & Dr. Amanda Parker
  ◦ 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**, 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.

[2] 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.

[3] 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.

[4] 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.

[5] **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.

[6] 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.

[7] **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.

[8] **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.

[9] **Xinyue Xu** et al., "Concept-based unsupervised domain adaptation," *Under review*, 2025.

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, 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
   Email: eexmli@ust.hk
   Relationship: [Ph.D. Supervisor]

2. **Prof. Hao WANG**
   Assistant Professor, Department of Computer Science
   Rutgers University
   Email: hw488@cs.rutgers.edu
   Relationship: [Ph.D. Co-Supervisor]

3. **Prof. Lu MI**
   Assistant Professor, School of Computational Science and Engineering
   Georgia Institute of Technology
   Email: lmi7@gatech.edu
   Relationship: [Mentor and Collaborator]