

EDUCATION

Tsinghua University <i>Master of Science, Data Science and Information Technology, GPA: 3.93/4 (Major 4/4)</i> <i>Supervisors: Prof. Wenwu Zhu and Prof. Yang Li</i> <i>Main Courses: Machine Learning(4.0); Fundamentals of Digital Image and Video Processing(4.0)</i>	Beijing, China <i>Sep. 2022 - Jun. 2025</i>
Minzu University of China <i>Bachelor of Science, Statistics, GPA: 4.43/5 (94.3/100), Rank 1st</i> <i>Main Courses: Mathematical Analysis(99); Advanced Algebra(92); Probability Theory(97); Applied Mathematical Statistics(99); Data Structure(94); Principle Operational Research; Applied Stochastic Processing</i>	Beijing, China <i>Sep. 2018 - Jun. 2022</i>

RESEARCH INTERESTS

Machine Learning, especially in Large Language Models, Causal Inference and Graph Neural Networks.

PUBLICATIONS

1. Peiwen Li, Xin Wang, Zeyang Zhang, Linxin Xiao, Yang Li, Wenwu Zhu.
CaLMol: Disentangled Causal Graph LLM for Molecular Relational Learning. *In Submission.*

2. Peiwen Li, Xin Wang, Zeyang Zhang, Yijian Qin, Ziwei Zhang, Jialong Wang, Yang Li, Wenwu Zhu.
Causal-Aware Graph Neural Architecture Search under Distribution Shifts. *In Submission.* *arXiv:* [link](#)

3. Peiwen Li, Menghua Wu. **Learning to Refine Domain Knowledge for Biological Network Inference.**
The 38th NeurIPS 2024 Workshop on AI for New Drug Modalities (AIDrugX). [link](#)

4. Peiwen Li, Xin Wang, Zeyang Zhang, Yuan Meng, Fang Shen, Yue Li, Jialong Wang, Yang Li, Wenwu Zhu.
RealTCD: Temporal Causal Discovery from Interventional Data with Large Language Model.
The 33rd ACM International Conference on Information and Knowledge Management (ACM CIKM), 2024. [link](#)

5. Peiwen Li, Yuan Meng, Xin Wang, Fang Shen, Yue Li, Jialong Wang, and Wenwu Zhu.
Causal Discovery in Temporal Domain from Interventional Data.
The 32nd ACM International Conference on Information and Knowledge Management (ACM CIKM), 2023. [link](#)

EXPERIENCE

Regina Barzilay Group, MIT CSAIL <i>Research Intern. Work with Menghua Wu.</i>	Remote <i>May 2024 - Now</i>
Learning to Refine Domain Knowledge for Biological Network Inference Propose an amortized inference algorithm for refining domain knowledge towards biological network inference.	
Multimedia and Network Big Data Lab, Tsinghua University <i>Research Student. Advisors: Prof. Wenwu Zhu and Prof. Xin Wang.</i>	Beijing, China <i>Nov. 2021 - Now</i>
CaLMol: Disentangled Causal Graph LLM for Molecular Relational Learning Propose CaLMol, capable of exploiting causal molecular relationships to predict interactions for new drugs.	
Causal-Aware Graph Neural Architecture Search under Distribution Shifts Propose superior approach CARNAS, which can unveil and utilize the causal graph-architecture relationship to customize neural architecture and address distribution shifts during the architecture search process.	
RealTCD: Temporal Causal Discovery from Interventional Data with Large Language Model Propose the efficient RealTCD, a framework able to leverage domain knowledge through LLMs to discover temporal causal relationships without interventional targets, which is especially applicable in industrial scenarios.	
Causal Discovery in Temporal Domain from Interventional Data Propose novel TECDI, the first attempt to employ interventional data for real-world temporal causal discovery.	
Explainability in Graph Neural Architecture Search by Decorrelated Subgraph Reweighting <i>Undergraduate Thesis</i> Design a framework e-GraphNAS to analyze why a certain architecture is obtained by a GraphNAS algorithm.	
Alibaba Cloud, Alibaba Group <i>Research Intern. Alibaba Innovative Research Program.</i>	Hangzhou, China <i>May 2023 - Dec. 2023</i>
Anomaly Detection based on GNN and Causal Discovery, and applications in AIOps of data center.	

MISC

Skills: Coding: C, Python, R, Matlab, SPSS, SAS, L^AT_EX. **Academic Service:** Conference Reviewer: KDD(2024)

AWARDS

• Comprehensive Excellence Scholarship, Tsinghua University

• Outstanding Graduate Award of Beijing (4%)

• Merit Student of Beijing (1%)

• Meritorious Winner in Interdisciplinary Contest In Modeling

• Second Prize in National Mathematics Competition for Undergraduate Students (Beijing)

2023,2024

2022

2021

2020

2019,2020