Zhenyu Lei

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Research Interests

My primary research interests lie at solving real-world challenges with **LLMs** (distillation, agents, RL, model editing), **AI for science** (AI for neural science, AI for chemistry), and **data mining** (graph machine learning, spatial-temporal models).

Education

University of Virginia, Charlottesville, VA, USA   2023.8-present
Ph.D. in ECE
Advisor: Jundong Li

Xi'an Jiaotong University, Xi'an, Shaanxi, China   2019.8-2023.6
B.S. in Physics
GPA:89.46/100 (3.82/4.3) (**Transcript**)
Advisor: Minnan Luo

Publications (* equal contribution)

[19] **Reforming the Mechanism: Editing Reasoning Patterns in LLMs with Circuit Reshaping**
Zhenyu Lei, Qiong Wu, Jianxiong Dong, Yinhan He, Emily Dodwell, Yushun Dong, Jundong Li
In submission

[19] **Editing Multimodal Molecule Language Models**
Zhenyu Lei, Patrick Soga, Yaochen Zhu, Yinhan He, Yushun Dong, Jundong Li
In submission

[18] **Learning from Diverse Reasoning Paths with Routing and Collaboration**
Zhenyu Lei, Zhen Tan, Song Wang, Yaochen Zhu, Zihan Chen, Yushun Dong, Jundong Li
EMNLP 2025

[17] **From Cross-Task Examples to In-Task Prompts: A Graph-Based Pseudo-Labeling Framework for In-context Learning**
Zihan Chen, Song Wang, Xingbo Fu, Chengshuai Shi, **Zhenyu Lei**, Cong Shen, Jundong Li
EMNLP 2025

[16] **A survey of scaling in large language model reasoning**
Zihan Chen, Song Wang, Zhen Tan, Xingbo Fu, **Zhenyu Lei**, Peng Wang, Huan Liu, Cong Shen, Jundong Li
Arxiv

[15] **Fairness-Aware Graph Learning: A Benchmark**
Yushun Dong, Song Wang, **Zhenyu Lei**, Zaiyi Zheng, Jing Ma, Chen Chen, Jundong Li
KDD 2025

[14] **Graph Prompting for Graph Learning Models: Recent Advances and Future Directions**
Xingbo Fu, Zehong Wang, Zihan Chen, Jiazheng Li, Yaochen Zhu, **Zhenyu Lei**, Cong Shen, Yanfang Ye, Chuxu Zhang, Jundong Li
KDD 2025

[13] **Energy-Based Models for Predicting Mutational Effects on Proteins**

Patrick Soga, **Zhenyu Lei**, Yinhan He, Camille Bilodeau, Jundong Li
KDD 2025

[12] **Harnessing Large Language Models for Disaster Management: A Survey**
Zhenyu Lei, Yushun Dong, Weiyu Li, Rong Ding, Qi Wang, Jundong Li
ACL 2025

[11] **BrainMAP: Learning Multiple Activation Pathways in Brain Networks**
Song Wang*, **Zhenyu Lei***, Zhen Tan, Jiaqi Ding, Xinyu Zhao, Yushun Dong, Guorong Wu, Tianlong Chen, Chen Chen, Aiying Zhang, Jundong Li
AAAI'25 (Oral)

[10] **ST-FiT: Inductive Spatial-Temporal Forecasting with Limited Training Data**
Zhenyu Lei, Yushun Dong, Jundong Li, Chen Chen
AAAI'25 (Oral)

[9] **Deep Interactions for Multimodal Molecular Property Prediction**
Patrick Soga, **Zhenyu Lei**, Camille Bilodeau, and Jundong Li
PAKDD'25

[8] **Idea: A flexible framework of certified unlearning for graph neural networks**
Yushun Dong, Binchi Zhang, **Zhenyu Lei**, Na Zou, Jundong Li
KDD'24

[7] **PyGDebias: A Python Library for Debiasing in Graph Learning**
Yushun Dong, **Zhenyu Lei**, Zaiyi Zheng, Song Wang, Jing Ma, Alex Jing Huang, Chen Chen, Jundong Li
WWW'24

[6] **LMBot: Distilling Graph Knowledge into Language Model for Graph-less Deployment in Twitter Bot Detection**
Zijian Cai, Zhaoxuan Tan, **Zhenyu Lei**, Hongrui Wang, Zifeng Zhu, Qinghua Zheng, Minnan Luo
WSDM'24

[5] **HOFA: Twitter Bot Detection with Homophily-Oriented Augmentation and Frequency Adaptive Attention**
Sen Ye, Zhaoxuan Tan, **Zhenyu Lei**, Ruijie He, Hongrui Wang, Qinghua Zheng, Minnan Luo
arXiv'23

[4] **TwiBot-22: Towards graph-based Twitter bot detection**
Shangbin Feng, Zhaoxuan Tan, Herun Wan, Ningnan Wang, Zilong Chen, Binchi Zhang, Qinghua Zheng, Wenqian Zhang, **Zhenyu Lei**, Shujie Yang, Xinshun Feng, Qingyue Zhang, Hongrui Wang, Yuhan Liu, Yuyang Bai, Heng Wang, Zijian Cai, Yanbo Wang, Lijing Zheng, Zihan Ma, Jundong Li, Minnan Luo
NeurIPS'23

[3] **KALM: Knowledge-Aware Integration of Local, Document, and Global Contexts for Long Document Understanding**
Shangbin Feng, Zhaoxuan Tan, Wenqian Zhang, **Zhenyu Lei**, Yulia Tsvetkov
ACL'23

[2] **BIC: Twitter Bot Detection with Text-Graph Interaction and Semantic Consistency**
Zhenyu Lei*, Herun Wan*, Wenqian Zhang, Shangbin Feng, Jundong Li, Qinghua Zheng, Minnan Luo
ACL'23

[1] **KCD: Knowledge Walks and Textual Cues Enhanced Political Perspective Detection in News Media**

Wenqian Zhang, Shangbin Feng, Zilong Chen, **Zhenyu Lei**, Jundong Li, Minnan Luo
NAACL'22

Honors and Awards

UVA Presidential Fellowship in Collaborative Neuroscience	2025
UVA Precision Health Initiative Trainee Travel Stipend	2025
UVA Engineering Academic Commitment to Excellence (ACE) Fellowship	2024
Scholarship for Outstanding Sichuan Students	2021
Provincial First Prize, CUMCM	2020
Dean's List, Xi'an Jiao Tong University	2020, 2021

Services

Reviewer for CIKM	2025
Reviewer for COLM	from 2024
Reviewer for KDD	from 2024
Reviewer for ACL Rolling Review	from 2023, Dec
Reviewer for NeurIPS	from 2023

Mentorship

Sen Ye → first author in 1*WSDM 2024 submission, PhD student @ Peking University

Zijian Cai → first author in 1*WSDM, MS student @ The Institute of Automation, CAS

Teaching

Teaching Assistant of Convex Optimization, University of Virginia	2025 Fall
Teaching Assistant of CS 3501 Foundation of Data Analysis, University of Virginia	2024 Spring

Skills

- Programming Skills: Python, PyTorch, MATLAB, C/C++, bash, HTML/CSS, LaTeX

- Language Skills: Mandarin (native), English (TOEFL 101: R 29, L 29, S 22, W 21)