WEIKAI LI

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EDUCATION

UCLA, Los Angeles, California (Ph.D. in Computer Science)   09/2023 – present
- GPA: 4.00/4.00
- Advisor: I am fortunate to be advised by Prof. Yizhou Sun. I also closely work under Prof. Jason Cong's guidance.
- Research areas: Graph Neural Network (GNN), AI for Electronic Design Automation (EDA), Large Language Models (LLMs)' interpretability.

Tsinghua University, Beijing, China (B.Eng in Computer Science and Technology)   08/2019 – 06/2023
- GPA: 3.92/4.00 (ranking: 10/195)
- Outstanding Undergraduate Graduate of Tsinghua University (top 10%)
- Advisors: I was fortunate to be advised by Prof. Jie Tang, Prof. Yuxiao Dong, and Prof. Juanzi Li.
- Research areas: Graph Neural Network (GNN), Large language models (LLMs)' in-context learning.

RESEARCH EXPERIENCES

Graduate Student Researcher at UCLA   09/2023 – present
Advised by Prof. Yizhou Sun; also closely work under Prof. Jason Cong's guidance
- **AI for EDA's generalizable model design**: I enhanced the domain generalizability of graph neural networks (GNNs) in the high-level synthesis (HLS) prediction task by designing a hierarchical mixture-of-experts (MoE) structure; I also designed a two-stage training strategy to stabilize its training.
- **Compositional HLS prediction model** (ongoing): I am designing a compositional HLS prediction model to enhance its performance and domain generalizability.
- **LLMs' interpretability** (ongoing): I am interpreting the internal mechanisms of LLM post-training.

Undergraduate Student Researcher at Tsinghua University   01/2023 – 07/2023
Advised by Prof. Juanzi Li
- **LLM's in-context learning**: I analyzed the limitations of LLM's in-context learning on the event relation extraction task, and we demonstrated the importance of finetuning for specification-heavy tasks.

Undergraduate Student Research Intern at UCLA   07/2022 – 12/2022
Advised by Prof. Yizhou Sun
- **GNN's approximation**: I designed an efficient approximation method to calculate the influence of removing a node on a GNN model's prediction, leading to faster detection of influential nodes.

Undergraduate Student Researcher at Tsinghua University   08/2021 – 07/2022
Advised by Prof. Jie Tang and Prof. Yuxiao Dong
- **GNN benchmark**: We discovered the phenomenon of over-tuning hyper-parameters in GNN model evaluation, and we proposed a new benchmark to avoid this problem and improve evaluation stability.
- **GNN model design**: I used the mixture-of-experts (MoE) structure to increase GNN's parameter size and improve its performance on complex datasets.

PUBLICATIONS

[1] Hongzhe Du*, **Weikai Li***, Min Cai, Karim Saraipour, Zimin Zhang, Himabindu Lakkaraju, Yizhou Sun, and Shichang Zhang. "How Post-Training Reshapes LLMs: A Mechanistic View on Knowledge, Truthfulness, Refusal, and Confidence." Arxiv preprint 2025. (Outstanding Paper Award at the New England NLP workshop)

[2] **Weikai Li**, Ding Wang, Zijian Ding, Atefeh Sohrabizadeh, Zongyue Qin, Jason Cong, and Yizhou Sun. "Hierarchical Mixture of Experts: Generalizable Learning for High-Level Synthesis." AAAI 2025.

[3] Zijian Ding, Atefeh Sohrabizadeh, **Weikai Li**, Zongyue Qin, Yizhou Sun, and Jason Cong. "Efficient Task Transfer for HLS DSE." ICCAD 2024.

[4] Yunsheng Bai, Atefeh Sohrabizadeh, Zijian Ding, Rongjian Liang, **Weikai Li**, Ding Wang, Haoxing Ren, Yizhou Sun, and Jason Cong. "Learning to Compare Hardware Designs for High-Level Synthesis." MLCAD 2024.

[5] **Weikai Li**, Zhiping Xiao, Xiao Luo, and Yizhou Sun. "Fast Inference of Removal-Based Node Influence." WWW 2024.

[6] Jifan Yu*, Xiaozhi Wang*, Shangqing Tu, Shulin Cao, Daniel Zhang-Li, Xin Lv, Hao Peng, Zijun Yao, Xiaohan Zhang, Hanming Li, Chunyang Li, Zheyuan Zhang, Yushi Bai, Yantao Liu, Amy Xin, Nianyi Lin, Kaifeng Yun, Linlu Gong, Jianhui Chen, Zhili Wu, Yunjia Qi, **Weikai Li**, Yong Guan, Kaisheng Zeng, Ji Qi, Hailong Jin, Jinxin Liu, Yu Gu, Yuan Yao, Ning Ding, Lei Hou, Zhiyuan Liu, Bin Xu, Jie Tang, and Juanzi Li. "KoLA: Carefully Benchmarking World Knowledge of Large Language Models." ICLR 2024.

[7] Hao Peng*, Xiaozhi Wang*, Jianhui Chen*, **Weikai Li**, Yunjia Qi, Zimu Wang, Zhili Wu, Kaisheng Zeng, Bin Xu, Lei Hou, and Juanzi Li. "When does In-context Learning Fall Short and Why? A Study on Specification-Heavy Tasks." ArXiv preprint 2023.

[8] Ziang Li*, Ming Ding*, **Weikai Li**, Zihan Wang, Ziyu Zeng, Yukuo Cen, and Jie Tang. "Rethinking the Setting of Semi-supervised Learning on Graphs." IJCAI 2022.

(*Equal contribution)

SELECTED AWARDS AND HONORS

- NSF Student Travel Award (The Web Conference 2024)   2024
- Outstanding Undergraduate Graduate of Tsinghua University (top 10%)   2023
- Comprehensive Excellence Scholarship for junior year (top 10%)   2022
- Comprehensive Excellence Scholarship for sophomore year (top 10%)   2021
- Academic Excellence Scholarship for freshman year   2020
- Runner-up in Tsinghua Innovation Competition, industry and technology track, freshman group 2019
- First Prize in the National High School Mathematics League   2018

ACADEMIC SERVICES

- Conference reviewer: ICLR 2024, ICML 2024, ACMMM 2024, NeurIPS 2024, LoG 2024, AAAI 2025, ICLR 2025, WWW 2025, ICML 2025, ICCV 2025, NeurIPS 2025
- Journal reviewer: IEEE TBD 2024, PLOS ONE 2024
- Conference volunteer: NSF AI for EDA Workshop 2024

TEACHING EXPERIENCE

- 2024 fall, 2025 winter, and 2025 spring: TA of CS 31 (Introduction to Computer Science I), UCLA
- 2024 summer: TA of CS 97 (Introduction to Data Science), UCLA summer school for high school students

SKILLS AND INTERESTS

Coding skills
- Programming languages: C, C++, Python, Java
- Hardware description languages: VHDL, Verilog
- Others: MatLab, JavaScript

Language skills
- Native in Chinese (mandarin), and proficient in English

Interests
- I love badminton, singing, traveling, and enjoying beautiful landscapes.
- I have organized some department-level sports events.
- I have been a member of Tsinghua University's choir and UCLA's choir.