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RESEARCH INTERESTS

My long-term research goal is to develop intelligent systems with more effective and efficient planning and reasoning abilities.

For technologies, my studies encompass Large language models (LLM), LLM-based Agents, Mixture-of-Experts (MoE), and Generative Models.

For practical applications, my studies encompass Scientific Domains, Bayesian Optimization, and Recommender Systems, which naturally require better planning and reasoning capabilities of the intelligent systems.

EDUCATION

University of Notre Dame IN, US

Ph.D. in Computer Science and Engineering Jan. 2023 – Present

Advisor: Prof. Xiangliang Zhang. GPA: 4.0/4.0

King Abdullah University of Science and Technology (KAUST) Thuwal, Saudi Arabia

M.S. in Computer Science Aug. 2021 – Dec. 2022

Advisor: Prof. Xiangliang Zhang. GPA: 3.89/4.0

Xidian University Xi'an, China

Bachelor in Software Engineering Aug. 2013 – Jul. 2017

GPA: 3.5/4.0

HONORS&AWARDS

KDD Cup Machine Learning Competition Track (**2nd place**). [\[Link\]](#) 2020

NeurIPS Optimization Challenge. (**2nd place, warm-start track**) [\[Link\]](#) 2020

Kaggle Arabic Sentiment Analysis. (**5th place**) [\[Link\]](#) 2021

IEEE Computer Society Global student challenge. (**1st place**) [\[Link\]](#) 2021

PUBLICATIONS

[1] [LLM Agent] **Large Language Model based Multi-Agents: A Survey of Progress and Challenges**

Taicheng Guo, Xiuying Chen, Yaqi Wang, Ruidi Chang, Shichao Pei, Nitesh V. Chawla, Olaf Wiest, Xiangliang Zhang

In IJCAI 2024

[2] [MoE+Generative Models] **Beyond the Typical: Advanced Prediction of Chemical Reactions by Capturing Multiple Electron Redistribution Patterns via Mixture-of-experts**

Taicheng Guo, Changsheng Ma, Xiuying Chen, Bozhao Nan, Kehan Guo, Shichao Pei, Nitesh V. Chawla, Olaf Wiest, Xiangliang Zhang

In Submission

[3] [LLM] **What can Large Language Models do in chemistry? A comprehensive benchmark on eight tasks**

Taicheng Guo, Kehan Guo, Bozhao Nan, Zhenwen Liang, Zhichun Guo, Nitesh V. Chawla, Olaf Wiest, Xiangliang Zhang

In NeurIPS 2023

[4] [Language Models + Recommendation] **Few-shot News Recommendation via Cross-lingual Transfer**

Taicheng Guo, Lu Yu, Basem Shihada, Xiangliang Zhang

In WWW 2023

[5] **Data Interpreter: An LLM Agent For Data Science**

Sirui Hong, Yizhang Lin, Bangbang Liu, Binhao Wu, Danyang Li, Jiaqi Chen, Jiayi Zhang, Jinlin Wang, Lingyao Zhang, Mingchen Zhuge, Taicheng Guo, Tuo Zhou, Wei Tao, Wenyi Wang, Xiangru Tang, Xiangtao Lu, Xinbing Liang, Yaying Fei, Yuheng Cheng, Zongze Xu, Chenglin Wu, Li Zhang, Min Yang, Xiawu Zheng

Preprint

[6] **A Property-Guided Diffusion Model for Generating Molecular Graphs**

Changsheng Ma, Taicheng Guo, Qiang Yang, Xiuying Chen, Xin Gao, Shangsong Liang, Nitesh Chawla, Xiangliang Zhang

In ICASSP 2024

[7] **SceMQA: A Scientific College Entrance Level Multimodal Question Answering Benchmark**

Zhenwen Liang, Kehan Guo, Gang Liu, Taicheng Guo, Yujun Zhou, Tianyu Yang, Jiajun Jiao, Renjie Pi, Jipeng Zhang, Xiangliang Zhang

Preprint

[8] **Rethinking Scientific Summarization Evaluation: Grounding Explainable Metrics on Facet-aware Benchmark**

Xiuying Chen, Tairan Wang, Qingqing Zhu, Taicheng Guo, Shen Gao, Zhiyong Lu, Xin Gao, Xiangliang Zhang

Preprint

[9] **Defending Jailbreak Prompts via In-Context Adversarial Game**

Yujun Zhou, Yufei Han, Haomin Zhuang, Taicheng Guo, Kehan Guo, Zhenwen Liang, Hongyan Bao, Xiangliang Zhang

Preprint

[10] **Data-Efficient, Chemistry-Aware Machine Learning Predictions of Diels-Alder Reaction Outcomes**

Angus Keto, Taicheng Guo, Morgan Underdue, Thijs Stuyver, Connor Coley, Xiangliang Zhang, Elizabeth Krenske, Olaf Wiest

Preprint

WORK&INTERN
EXPERIENCE

Amazon

Applied Scientist Intern

Jun. 2024 – Sep. 2024

Mohamed bin Zayed University of Artificial Intelligence: MBZUAI

Research Intern

Aug. 2022 – Oct. 2022

Mentors: Dr. Shangsong Liang

Tuyoo Games

Senior Machine Learning Engineer

Sep. 2018 – Aug. 2020

Led GameAI projects including AI player (Monte Carlo Tree Search, MinMax algorithm, etc) for poker games, game props recommendation systems, etc. Received the Employee of the Year award in 2019.

Qunar

Product Manager

Jul. 2017 – May. 2018

User Growth and Personalized flight ticket notification system design.

PROFESSIONAL
SERVICE

Reviewer: WWW, KDD, Nature Communications

Teaching Assistant: CSE 40625 Machine Learning, University of Notre Dame,
Fall 2023