Taicheng Guo

Updated March 9, 2024

Email: tguo2@nd.edu **Homepage** **Google Scholar**

RESEARCH INTERESTS

My long-term research goal is to develop intelligent systems with human-like planning and reasoning abilities. The central theme of my current research is to improve these capabilities from diversity, uncertainty-aware, learning from feedback, scalability, and step-by-step perspectives.

For technologies, my studies encompass LLM, LLM-based Agents, LLM Interpretability, Generative Models, and Mixture-of-experts.

For practical applications, my studies encompass Scientific Domains, Bayesian Optimization, and Recommender Systems, all of 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] **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 Submission

[2] **Modeling non-uniform uncertainty in Reaction Prediction via Boosting and Dropout**
Taicheng Guo, Changsheng Ma, Xiuying Chen, Bozhao Nan, Kehan Guo, Shichao Pei, Nitesh V. Chawla, Olaf Wiest, Xiangliang Zhang
In Submission

[3] **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] **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

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