

Taicheng Guo

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[Homepage](#)

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RESEARCH INTERESTS

My research interest broadly lies in large language models (LLM) and machine learning, in particular LLM-based Agents, LLM for Scientific Domains (Data Science, Natural Science, etc), LLM Interpretability, AI4Science and Recommender 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

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