Zhichun Guo

Ph.D. Candidate
Department of Computer Science and Engineering
University of Notre Dame

Phone: +1(574)335-9815
Email: zguo5@nd.edu
Homepage: https://zguo.io/

Research Interests

Graph Learning: enhance the effectiveness and efficiency of graph neural networks on various real-world applications
AI for Chemistry: transform chemistry dilemmas into AI problems and propose AI methods to deal with them
Trustworthy AI: enhance the fairness and explainability of AI models

Education

University of Notre Dame, Notre Dame, IN, US   Jan 2020 – *Present*
Ph.D. in Computer Science and Engineering
Advisor: Prof. Nitesh V. Chawla
Committee members: Dr. Wei Wang (UCLA), Dr. Neil Shah (Snap Inc.), Dr. Meng Jiang (ND), Dr. Xiangliang Zhang (ND)

University of Notre Dame, Notre Dame, IN, US   Aug 2019 – Jan 2020
Master in Computer Science and Engineering
Advisor: Prof. Chaoli Wang

Fudan University, Shanghai, China   Aug 2014 – Jul 2019
B.S. in Computer Science and Technology
Advisor: Prof. Yang Chen

Professional Experience

Snap Inc., Seattle, Washington, US   June 2023 - Sept 2023
Research Intern
Worked on efficient and effective link prediction
Mentors: Dr. Neil Shah and Dr. Tong Zhao

Snap Inc., Seattle, Washington, US   June 2022 - Nov 2022
Research Intern
Worked on accelerating link prediction for inference
Mentors: Dr. Neil Shah and Dr. Tong Zhao

University of Notre Dame, Notre Dame, IN, US   April 2018 - Aug 2018
Research Assistant
Worked on interactive visualization to evaluate researchers' scholarly performance
Advisor: Prof. Chaoli Wang

Chinese Academy of Sciences, Beijing, China   Jul 2017 - Sep 2017
Research Assistant
Worked on visual analysis of human mobility in cities
Advisor: Prof. Lei Shi

Honors and Awards

Snap Research Fellowship	2022
IEEE VIS Inclusivity & Diversity Scholarship	2022
Hui-Chun Chin and Tsung-Dao Lee Chinese Undergrad Research Endowment	2017
First Prize Scholarship for Outstanding Students	2017
EMC Scholarship for Outstanding Students	2016
NSF Center for Computer Assisted Synthesis Travel Award	2023
IJCAI Travel Grant	2023
SDM Student Travel Award	2023
AAAI Student Scholarship	2023
The Web Conference Scholarship	2021
SIGIR Student Travel Grant	2020

PUBLICATIONS

Selected Peer-Reviewed Publications

Full list of my publications shown on Google Scholar.

[NeurIPS'23] **What Indeed Can GPT 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
Conference on Neural Information Processing Systems Datasets and Benchmarks Track, 2023

[ICML'23] **Linkless Link Prediction via Relational Distillation**
Zhichun Guo, William Shiao, Shichang Zhang, Yozen Liu, Nitesh V. Chawla, Neil Shah, Tong Zhao
International Conference on Machine Learning, 2023

[IJCAI'23] **Graph-based Molecular Representation Learning**
Zhichun Guo, Kehan Guo, Bozhao Nan, Yijun Tian, Roshni G. Iyer, Yihong Ma, Olaf Wiest, Xiangliang Zhang, Wei Wang, Chuxu Zhang, Nitesh V. Chawla
International Joint Conference on Artificial Intelligence Survey Track, 2023

[ICLR'23] **Link Prediction with Non-Contrastive Learning**
William Shiao, **Zhichun Guo**, Tong Zhao, Evangelos E. Papalexakis, Yozen Liu, Neil Shah
International Conference on Learning Representations, 2023

[ICLR'23] **Learning MLPs on Graphs: A Unified View of Effectiveness, Robustness, and Efficiency**
Yijun Tian, Chuxu Zhang, **Zhichun Guo**, Xiangliang Zhang, Nitesh V. Chawla
International Conference on Learning Representations, 2023

[AAAI'23] **Boosting Graph Neural Networks via Adaptive Knowledge Distillation**
Zhichun Guo, Chunhui Zhang, Yujie Fan, Yijun Tian, Chuxu Zhang, Nitesh V. Chawla
AAAI Conference on Artificial Intelligence, 2023

[TVCG'22] **SD^2: Slicing and Dicing Scholarly Data for Interactive Evaluation of Academic Performance**
Zhichun Guo, Jun Tao, Siming Chen, Nitesh V. Chawla, Chaoli Wang
IEEE Transactions on Visualization and Computer Graphics, IF:5.23, 2022

[LoG'22] **FakeEdge: Alleviate Dataset Shift in Link Prediction**
Kaiwen Dong, Yijun Tian, **Zhichun Guo**, Yang Yang, Nitesh V. Chawla
Learning on Graphs Conference, 2022

[LoG'22] **Flashlight: Scalable Link Prediction with Effective Decoders**
Yiwei Wang, Bryan Hooi, Yozen Liu, Tong Zhao, **Zhichun Guo**, Neil Shah
Learning on Graphs Conference, 2022

[IJCAI'22] **RecipeRec: a heterogeneous graph learning model for recipe recommendation**
Yijun Tian, Chuxu Zhang, **Zhichun Guo**, Chao Huang, Ronald Metoyer, Nitesh V Chawla
International Joint Conference on Artificial Intelligence, 2022

[WWW'21] **Few-Shot Graph Learning for Molecular Property Prediction**
Zhichun Guo, Chuxu Zhang, Wenhao Yu, John Herr, Olaf Wiest, Meng Jiang, Nitesh V. Chawla
The Web Conference, 2021

[CIKM'20] **GraSeq: Graph and Sequence Fusion Learning for Molecular Property Prediction**
Zhichun Guo, Wenhao Yu, Chuxu Zhang, Meng Jiang, Nitesh V. Chawla
ACM International Conference on Information and Knowledge Management, 2020

Preprints and Under Submissions

[Preprint] **Node Duplication Improves Cold-start Link Prediction**
Zhichun Guo, Tong Zhao, Yozen Liu, Kaiwen Dong, William Shiao, Neil Shah, Nitesh V Chawla
Under Submission, 2023

[Preprint] **Pure Message Passing Can Estimate Common Neighbor for Link Prediction**
Kaiwen Dong, **Zhichun Guo**, Nitesh V Chawla
Under Submission, https://arxiv.org/pdf/2309.00976.pdf, 2023

[Preprint] **How Does Message Passing Improve Collaborative Filtering?**
Mingxuan Ju, William Shiao, **Zhichun Guo**, Yanfang Ye, Yozen Liu, Neil Shah, Tong Zhao
Under Submission, 2023

Talks and Presentations

AI for Drug Discovery	**University of Notre Dame**, AI & Society, *Course Panel Discussion*, 2023
Linkless Link Prediction via Relational Distillation	**Learning on Graphs Seminar**, *Invited Talk*, 2023
Graph-based Molecular Representation Learning	**IJCAI**, *Conference Presentation*, 2023
Linkless Link Prediction via Relational Distillation	**ICML**, *Conference Presentation*, 2023
Generalizing GNNs for Multi-applications with Effective Training Strategies	**SDM**, *Doctoral Forum Presentation*, 2023
Boosting Graph Neural Networks via Adaptive Knowledge Distillation	**AAAI**, *Conference Presentation*, 2023
Slicing and Dicing Scholarly Data for Interactive Evaluation of Academic Performance	**IEEE VIS**, *Conference Presentation*, 2022
Knowledge Distillation	**Brandeis University**, Prof. Chuxu Zhang's Group, *Invited Talk*, 2022
Few-Shot Graph Learning for Molecular Property Prediction	**WWW**, *Conference Presentation*, 2021
GraSeq: Graph and Sequence Fusion Learning for Molecular Property Prediction	**CIKM**, *Conference Presentation*, 2020

Teaching Experience

NSF Center for Computer Assisted Synthesis Training Videos   2021

- Role: Lecturer

- Lectures:

    - Training Procedure of Graph Neural Networks for Reaction Prediction

    - Deep Learning Based Molecular Representations

    - Transfer Learning, Meta-Learning, and Meta-Transfer Learning

    - String-based Representation of Molecules: SMILES, SMARTS and SELFIES

CSE 20312 Data Structures (Undergraduate Level)   Spring 2020

- Role: Teaching Assistant

- Duties: Review assignments, Q&A during office hours, Grade

Professional Services

Organizer

Learning on Graphs Conference (**LoG**) Meetup	2023

Conference PC/Reviewer

International Conference on Learning Representations (**ICLR**)	2024
AAAI Conference on Artificial Intelligence (**AAAI**)	2024, 2023
SIAM International Conference on Data Mining (**SDM**)	2024
Learning on Graphs Conference (**LoG**)	2023
Neural Information Processing Systems (**NeurIPS**)	2023
SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD**)	2023, 2022
International Joint Conference on Artificial Intelligence (**IJCAI**)	2023
IEEE International Conference on Data Mining (**ICDM**)	2022
IEEE Visualization Conference (**VIS**)	2021

Journal Invited Reviewer

IEEE Transactions on Knowledge and Data Engineering (**TKDE**)	2023
ACM Transactions on Knowledge Discovery from Data (**TKDD**)	2023, 2022
IEEE Transactions on Big Data	2023
Digital Discovery	2023
IEEE Transactions on Neural Networks and Learning System (**TNNLS**)	2022
Data Mining and Knowledge Discovery (**DAMI**)	2023, 2022
Bioinformatics	2022
Neurocomputing	2023, 2022
Visual Informatics	2023, 2022
Journal of Social Computing	2022
Journal of Big Data	2022, 2021
Journal of Artificial Intelligence Research	2021