Yunchao (Lance) Liu

CONTACT INFORMATION

Office: 5154G Medical Rearch Building III
465 21st Ave S
Nashville, TN 37212
E-mail: yunchao.liu@vanderbilt.edu

Homepage: http://www.LiuYunchao.com
LinkedIn: http://www.linkedin.com/in/YunchaoLiu/
GitHub: https://github.com/LanceKnight
Google Scholar: http://scholar.google.com/citations?user=oFtlWfwAAAAJ&hl=en

EDUCATION

Vanderbilt University

- **Doctor of Philosophy (Ph.D.)** student in Computer Science — Aug 2018 – Present
- Advisors: Dr. Jens Meiler, Dr. Tyler Derr, Dr. Bobby Bodenheimer
- Cumulative GPA: 3.92 / 4.00

University of Texas at Dallas

- **Master of Science (M.S.)** in Computer Science — May 2015
- Cumulative GPA: 3.85 / 4.0

Beijing University of Posts and Telecommunications

- **Bachelor of Science (B.S.)** in Management — Sep 2013

RESEARCH EXPERIENCE

Meiler Lab, Vanderbilt University
PhD Candidate, Computer Science Department — Sep 2018 – Present

- Advisors: Dr. Jens Meiler, Dr. Tyler Derr, Dr. Bobby Bodenheimer
- Research Interests: AI for Drug Design, Topological/Geometric Deep Learning, Generative Models, Self-Supervised Learning, Small Molecules/Proteins

State Key Laboratory of Intelligent Technology and Systems, Tsinghua University
Research Assistant, Department of Computer Science and Technology — Jul 2012 – Mar 2013

- Advisor: Dr. Xiaolin Hu
- Research Interests: Visual Saliency for Road Sign Detection

PUBLICATIONS

Yunchao Liu, Yu Wang, Oanh Vu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler and Tyler Derr. Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery. Preceedings of the 37th Association for the Advancement of Artificial Intelligence (AAAI), 2023.

Yunchao Liu, Rocco Moretti, Bobby Bodenheimer and Jens Meiler. Foldit Drug Design Game Usability Study: Comparison of Citizen and Expert Scientists. Preceedings of the 13th Annual ACM SIGGRAPH Conference on Motion, Interaction and Games (MIG), 2020.

PREPRINTS

Yunchao Liu, Rocco Moretti, Yu Wang, Bobby Bodenheimer, Tyler Derr and Jens Meiler. Integrating Expert Knowledge with Deep Learning Improves QSAR Models for CADD Modeling bioRxiv, 2023.

Yu Wang, Tong Zhao, Yuying Zhao, **Yunchao Liu**, Xueqi Cheng, Neil Shah, Tyler Derr A Topological Perspective on Demystifying GNN-Based Link Prediction Performance arXiv, 2023.

Yuying Zhao, Yu Wang, **Yunchao Liu**, Xueqi Cheng, Charu Aggarwal, Tyler Derr Fairness and Diversity in Recommender Systems: A Survey arXiv, 2023.

HONORS & AWARDS

- Finalist of Vanderbilt THree Minute Thesis Competition — Nov 2023
- AAAI2023 student scholarship travel award — Dec 2022
- Reviewer Award @ ICML-AI4Science — Jun 2022
- Nvidia Hardware Grant (RTX A6000) — Mar 2022

SERVICES

Journel Reviewer

- Journal of Computational Biophysics and Chemistry 2023
- ACM Transactions on Knowledge Discovery from Data (TKDD) 2023
- Big Data Research 2022

Conference Reviewer

- New Frontiers of AI for Drug Discovery and Development (AI4D3) @ Conference on Neural Information Processing Systems (NeurIPS) 2023
- AI4Science @ Conference on Neural Information Processing Systems (NeurIPS) 2023
- Generative AI and Biology (GenBio) @ Conference on Neural Information Processing Systems (NeurIPS) 2023
- Structured Probabilistic Inference & Generative Modeling (SPIGM) @ International Conference on Machine Learning (ICML) 2023
- SIAM International Conference on Data Mining (SDM) 2023
- Machine Learning on Graphs @ ACM International Conference on Web Search and Data Mining (WSDM) 2023
- AI4Science @ International Conference on Machine Learning (ICML) 2023
- ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) 2023
- Association for the Advancement of Artificial Intelligence (AAAI) 2023
- ACM International Conference on Web Search and Data Mining (WSDM) 2023
- Machine Learning on Graphs @ International Conference on Data Mining (ICDM) 2022
- AI4Science @ Conference on Neural Information Processing Systems (NeurIPS) 2022
- AI4Science @ International Conference on Machine Learning (ICML) 2022
- Deep Generative Models for Highly Structured Data (DGM4HSD) @ International Conference on Learning Representations (ICLR) 2022
- Conference on Neural Information Processing Systems (NeurIPS) 2022
- Machine Learning on Graphs (MLoG) @ ACM International Conference on Web Search and Data Mining (WSDM) 2022
- ACM The Web Conference (TheWebConf) 2022
- International Conference on Learning Representations (ICLR) 2022
- ACM International Conference on Web Search and Data Mining (WSDM) 2022
- ACM International Conference on Information and Knowledge Management (CIKM) 2021
- ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) 2021
- AI4Science @ Conference on Neural Information Processing Systems (NeurIPS) 2021

Chairship

- Publicity Chair at Machine Learning on Graphs (MLoG) Workshop at ICDM'23 2023
- Publicity Chair at Machine Learning on Graphs (MLoG) Workshop at WSDM'23 2023

Program Committee

- Graph Techniques for Adversarial Activity Analytics (GTA3) @ IEEE Big Data Conference 2023
- Graph Techniques for Adversarial Activity Analytics (GTA3) @ IEEE Big Data Conference 2022

Volunteering

- Volunteer at New Frontiers of AI for Drug Discovery and Development (AI4D3) @ NeurIPS 2023
- Session Chair at Association for the Advancement of Artificial Intelligence (AAAI) 2023
- Volunteer at Association for the Advancement of Artificial Intelligence (AAAI) 2023
- Volunteer at International Conference on Learning Representations (ICLR) 2022
- Session Manager at ACM International Conference on Web Search and Data Mining (WSDM) 2022

MENTORING

Data Science Institute, Vanderbilt University

- Xiaohan Kuang, M.S. Computer Science, from Vanderbilt University 2023 Fall
- Yuhao Zhang, M.S. Computer Science, from Vanderbilt University 2023 Fall

Network and Data Science Lab, Vanderbilt University

- Meilin Guo, M.S. Computer Science, from Columbia University 2023 Summer

Meiler Lab, Vanderbilt University

- Ha Dong, B.S. Neuroscience & Physics, from Amherst College 2023 Summer

---

INVITED TALKS

Molecular-Kernel Graph Neural Network for Drug Discovery — Jun 2023
- Max Planck Institute for Mathematics in the Sciences
- Leipzig, Germany

Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery. — Mar 2023
- Molecular Modeling & Drug Discovery Talks (Organized by Mila & Valence Discovery)
- Virtual Event

Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery. — Feb 2023
- The 37th AAAI conference on artificial intelligence
- Walter E. Washington Convention Center, Washington, DC, USA

Foldit Drug Design Game Usability Study: Comparison of Citizen and Expert Scientists — Oct 2020
- ACM SIGGRAPH Conference on Motion, Interaction and Games (MIG)
- Zucker Family Graduate Education Center (virtual due to COVID-19)

PRESENTATIONS & POSTERS

Yunchao Liu, Yu Wang, Oanh Vu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler and Tyler Derr. Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery *Learning on Graphs Conference (LoG)*, Poster 2022.

Yunchao Liu, Yu Wang, Oanh Vu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler and Tyler Derr. Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery *Summer RosettaCon*, Poster 2022.

Yunchao Liu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler. Foldit Drug Design Game Usability Study: Comparison of Citizen and Expert Scientists, *ACM SIGGRAPH Conference on Motion, Interaction and Games (MIG)*, Presentation, 2020.

REFERENCES

Available Upon Request