

Yunchao (Lance) Liu

CONTACT INFORMATION	Office: 5154G Medical Research 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 <ul style="list-style-type: none">• Doctor of Philosophy (Ph.D.) student in Computer Science Aug 2018 – Present• Advisors: Dr. Jens Meiler, Dr. Tyler Derr• Cumulative GPA: 3.92 / 4.00	
	University of Texas at Dallas <ul style="list-style-type: none">• Master of Science (M.S.) in Computer Science May 2015• Cumulative GPA: 3.85 / 4.0	
	Beijing University of Posts and Telecommunications <ul style="list-style-type: none">• Bachelor of Science (B.S.) in Management Sep 2013	
RESEARCH EXPERIENCE	Meiler Lab , Vanderbilt University PhD Candidate, Computer Science Department Sep 2018 – Present <ul style="list-style-type: none">• 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 <ul style="list-style-type: none">• Advisor: Dr. Xiaolin Hu• Research Interests: Visual Saliency for Road Sign Detection	
PUBLICATIONS	Xueqi Cheng, Yu Wang, Yunchao Liu , Yuying Zhao, Charu C Aggarwal, Tyler Derr. Edge Classification on Graphs: New Directions in Topological Imbalance. Proceedings of the ACM 18th International Conference on Web Search and Data Mining (WSDM), 2025.	
	Yunchao Liu , Ha Dong, Xin Wang, Rocco Moretti, Yu Wang, Zhaoqian Su, Jiawei Gu, Bobby Bodenheimer, Charles Weaver, Jens Meiler, Tyler Derr. WelQrate: Defining the Gold Standard in Small Molecule Drug Discovery Benchmarking. Proceedings of the 38th Conference on Neural Information Processing Systems (NeurIPS), 2024.	
	Grace Zhang, Xiaohan Kuang, Yuhao Zhang, Yunchao Liu , Zhaoqian Su, Tom Zhang, Yinghao Wu. Machine-learning-based structural analysis of interactions between antibodies and antigens. BioSystems , 2024.	
	Yu Wang, Tong Zhao, Yuying Zhao, Yunchao Liu , Xueqi Cheng, Neil Shah, Tyler Derr. A Topological Perspective on Demystifying GNN-Based Link Prediction Performance. Proceedings of the 12th International Conference on Learning Representations (ICLR), 2024.	
	Yuying Zhao, Yu Wang, Yunchao Liu , Xueqi Cheng, Charu Aggarwal, Tyler Derr. Fairness and Diversity in Recommender Systems: A Survey. ACM Transactions on Intelligent Systems and Technology (TIST), 2024.	
	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. Proceedings 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. Proceedings of the 13th Annual ACM SIGGRAPH Conference on Motion, Interaction and Games (MIG), 2020.	
PREPRINTS	Yunchao Liu , Rocco Moretti, Yu Wang, Ha Dong, Bailu Yan, Bobby Bodenheimer, Tyler Derr and Jens Meiler. Advancements in Ligand-Based Virtual Screening through the Synergistic Integration of Graph Neural Networks and Expert-Crafted Descriptors bioRxiv, 2023.	

SERVICES**Journal Reviewer**

- PLOS Computational Biology 2024
- ACM Computing Surveys 2024
- Information Fusion 2024
- Big Data Research 2024
- International Journal of Electrical and Computer Engineering (IJECE) 2024
- Information Fusion 2023
- Journal of Computational Biophysics and Chemistry 2023
- ACM Transactions on Knowledge Discovery from Data (TKDD) 2023
- Big Data Research 2022

Conference Reviewer

- 46th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC) 2024
- 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
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HONORS & AWARDS	• 1st Place with DiffWater project @ AI Showcase at Vanderbilt University	Apr 2024
	• 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
TEACHING	• Guest Speaker @ DS 3891: Intro to Generative Artificial Intelligence Models	Mar 2024
	• RFDiffusion @ Rosetta Workshop	Dec 2023
MENTORING	Network and Data Science Lab , Vanderbilt University	2024 Fall
	• Xin (Allen) Wang, M.S. Computer Science, from Vanderbilt University	
	Data Science Institute , Vanderbilt University	2024 Fall
	• Hexuan (Hillbert) Fan, M.S. Data Science, from Vanderbilt University	
	Data Science Institute , Vanderbilt University	2024 Spring
	• LeyaoWang (Laura) Wang, B.S. Computer Science, from Vanderbilt University	
	Data Science Institute , Vanderbilt University	2023 Fall
	• Xiaohan Kuang, M.S. Data Science, from Vanderbilt University	
	• Yuhao Zhang, M.S. Data Science, from Vanderbilt University	
	Network and Data Science Lab , Vanderbilt University	2023 Summer
	• Meilin Guo, M.S. Computer Science, from Columbia University	
INVITED TALKS	Meiler Lab , Vanderbilt University	2023 Summer
	• Ha Dong, B.S. Neuroscience & Physics, from Amherst College	
	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	
POSTERS	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)	
	• Xiaobo Lin, Zhaoqian Su, <u>Yunchao Liu</u> , Jingxian Liu, Xiaohan Kuang, Jesse Spencer-Smith. SuperMetal: A Generative AI Framework for Rapid and Precise Metal Ion Location Prediction in Proteins <i>Machine Learning in Structural Biology (MLSB) @ NeurIPS</i> 2024.	
	• <u>Yunchao Liu</u> , 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 <i>Learning on Graphs Conference (LoG)</i> 2022.	
	• <u>Yunchao Liu</u> , 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 <i>Summer RosettaCon</i> 2022.	
REFERENCES	Available Upon Request	

[CV compiled on 2024-10-30]