

PROFESSIONAL EXPERIENCE

University of North Carolina, Chapel Hill

Tenure-Track Assistant Professor, School of Data Science and Society

Chapel Hill, NC, USA

2024–Current

EDUCATION

University of California, Los Angeles

Ph.D. in Computer Science, Advisor: Quanquan Gu, GPA: 3.94 / 4.00

Los Angeles, CA, USA

2019–2024

University of California, Los Angeles

M.Sc. in Computer Science, Advisor: Quanquan Gu, GPA: 3.94 / 4.00

Los Angeles, CA, USA

2019–2022

Tsinghua University

B.E. in Automation, GPA: 3.86/4.00, Rank 6 / 150

Beijing, China

2015–2019

RESEARCH INTEREST

- **Reinforcement Learning:** Markov decision process, Sample efficiency, Representation Learning, Uncertainty in RL
- **AI for Science:** Molecule prediction/generation, Epidemic models, Multi-Modal Models (Diffusion Models, LLMs)

PROJECTS

Molecule Property Prediction using Large Language Model

- Research project during the 2023 internship in NVIDIA RAPIDS team, mentor Dr. Xiaoyun Wang, Dr. Joe Eaton
- Design multi-modal large language model (LLMs) predicting the molecule property given the structural information.
- Collect, clean and augment the molecule annotations using large language model
- Fuse the molecular graph information and SMILES information using Q-Formers
- Provide quantitative evaluation and superior performance on several downstream molecule property predictions tasks.
- Accepted by NeurIPS 2023 Workshop on New Frontiers of AI for Drug Discovery and Development

3D Structured Molecule Generation with Equivariant Diffusion Models

- Continue project after NVIDIA internship with Dr. Xiaoyun Wang et. al..
- Using equivariant diffusion models for position generation and discrete diffusion models for atom type generation.
- Introducing the atom neutralization method which improves the molecule stability from $\sim 90\% \rightarrow 95\%$
- Presented at [Nvidia GTC 2023: 3D Molecule Generation with the Equivariant Score-Based Diffusion Process](#)
- Accepted by ICML 2023 Workshop on Structured Probabilistic Inference & Generative Modeling

Molecule Property Prediction with 3D Structured Data and Graph Neural Networks

- Research project 2022 during the internship in NVIDIA RAPIDS team, mentor Dr. Xiaoyun Wang, Dr. Joe Eaton
- Using Contrastive Learning to learn the graph representation of 3D structured data with Equivariant Transformers
- Apply methods (Laplacian Embedding, Self-attention Pooling, Dropout, etc.) to improve the scalability of the GNNs
- Improve 50% by contrastive learning compared with baseline model (accuracy (MAE) 0.0156 \rightarrow 0.0144)

AI-based Categorization to Decipher Reaction Mechanisms from Cyclic Voltammetry

- Launched the project in August 2021 Predict the Cyclic Voltammetry mechanism using deep learning.
- Interdisciplinary project with Prof. Chong Liu in Dept. of Chem. at UCLA, supported by [NSF#2140762](#).
- Use deep neural networks (transformer, ResNet, etc.) with problem-specific data augmentation methods.
- Achieve $\geq 95\%$ accuracy on simulation data, and $\geq 80\%$ accuracy on real-world experimental data.
- Published at ACS Measurement Science Au, follow up with a more complex cyclic voltammetry detection task, supported by [NSF#2247426](#).

Combating COVID-19 using machine learning

<https://covid19.uclaml.org>

- Launched the project in March 2020 to (1) help people stay informed about the spread of coronavirus by creating data visualization of confirmed, dead, and hospitalized cases of COVID-19; and (2) provide guidance to policy makers and individuals by using a machine learning empowered epidemic model to forecast the spread of the epidemic.
- Applied Gradient Descent to the SuEIR model to simulate the spread of epidemic. Applied graph knowledge to gain information for the relationship between states and counties in the United States.
- Used in the official forecast by [US Centers for Disease Control and Prevention \(CDC\)](#), [California Department of Public Health \(CDPH\)](#), [The US COVID-19 Forecast Hub](#), [German and Polish COVID-19 Forecast Hub](#).
- Media coverage: [UCLA Newsroom](#), [FiveThirtyEight](#), [TPM](#), [POLITICO](#), [CBS News 8](#), [New Yorker](#).

SCHOLARSHIPS AND AWARDS

• UCLA Dissertation Year Fellowship	2023
• Doctoral Student Fellowships, Amazon Fellow	2021
• UCLA Summer Mentored Research Fellowship	2021
• Tsinghua University Excellent Undergraduate, Class of 2019	2019
• Qualcomm Scholarship	2017–2018
• Finalist in Mathematical Contests in Modeling (MCM)	2017
• China National Scholarship	2016
• Tsinghua Scholarship for Social Practicing	2016
• Tsinghua Scholarship for [Science and Technology Innovation, Academic Excellence]	2016–2019
• Tsinghua Outstanding Freshmen Scholarship	2015
• Golden Prize for Chinese Physics Olympiad (CPHO)	2014

RESEARCH EXPERIENCE

Research Internship NVIDIA Corporation, RAPIDS-cuGraph team	Santa Clara, CA, USA Summer 2023
Research Internship NVIDIA Corporation, RAPIDS-cuGraph team	Los Angeles, CA, USA Summer 2022
Doctoral Student Fellow Amazon Science Hub For Humanity and Artificial Intelligence at UCLA	Los Angeles, CA, USA Winter 2022 - Winter 2023
Research Assistant Statistical Machine Learning Lab, University of California, Los Angeles	Los Angeles, CA, USA Fall 2019 - Present

Research Assistant Institute for Artificial Intelligence, Tsinghua University	Beijing, China Fall 2018 - Summer 2019
Research Internship Liveness Computer Vision Group, Face++, Megvii Tech. Co. Ltd.	Beijing, China Fall 2019 - Winter 2019
Research Assistant Center for Visual Computing, University of California, San Diego	La Jolla, CA, USA Summer 2018
Research Assistant National Research Center for Information Science and Technology, Tsinghua University	Beijing, China Fall 2016 - Summer 2018

TEACHING

- **Teaching Assistant** at University of California, Los Angeles Spring 2021, Fall 2021
Introductory Digital Design Laboratory (CS M152A) ([Course Website 21F](#), [Course Website 21S](#))
- **Teaching Assistant** at University of California, Los Angeles Winter 2022, Winter 2023
Fundamentals of Artificial Intelligence (CS 161) ([Course Website 22W](#), [Course Website 23W](#))

PROFESSIONAL SERVICES

- Conference Reviewer 2019–Current
ICML[2020-2023], NeurIPS[2020-2023], AAAI[2020-2023], AISTATS[2020-2023], ICLR[2019-2022], IJCAI[2020-2023]
- Journal Reviewer 2019–Current
PLOS ONE, JAIR, TMLR

SKILLS

- **Programming:** **Fluent** in Python and MATLAB, **Basic** C++, Java, JS, HTML, etc..
- **Machine Learning:** **Fluent** PyTorch framework (Huggingface, PyTorch Geometric)
- **Miscellaneous:** *nix shell, website construction, git, L^AT_EX. CI/CD (This CV and my homepage is CI/CD'ed)

PUBLICATIONS

* indicates equal contribution

- [She+24] Hongyuan Sheng, Jingwen Sun, Oliver Rodríguez, Benjamin B Hoar, **Weitong Zhang**, Danlei Xiang, Tianhua Tang, Avijit Hazra, Daniel S Min, Abigail G Doyle, et al. “Autonomous closed-loop mechanistic investigation of molecular electrochemistry via automation”. In: *Nature Communications* 15.1 (2024), p. 2781.
- [Sun+24] Jingwen Sun, **Weitong Zhang**, Yuanzhou Chen, Benjamin Hoar, Hongyuan Sheng, Jenny Yang, Cyrille Costentin, Quanquan Gu, and Chong Liu. “What is the appropriate data representation of electrochemical impedance spectroscopy in machine-learning analysis?” In: (2024).
- [Zha+24a] Junkai Zhang, **Weitong Zhang**, Dongruo Zhou, and Quanquan Gu. “Uncertainty-Aware Reward-Free Exploration with General Function Approximation”. In: *arXiv preprint arXiv:2406.16255* (2024).
- [Zha+24b] **Weitong Zhang**, Zhiyuan Fan, Jiafan He, and Quanquan Gu. “Settling Constant Regrets in Linear Markov Decision Processes”. In: *arXiv preprint arXiv:2404.10745* (2024).

- [Zha+24c] Linxi Zhao, Yihe Deng, **Weitong Zhang**, and Quanquan Gu. “Mitigating Object Hallucination in Large Vision-Language Models via Classifier-Free Guidance”. In: *arXiv preprint arXiv:2402.08680* (2024).
- [Den+23] Yihe Deng, **Weitong Zhang**, Zixiang Chen, and Quanquan Gu. “Rephrase and respond: Let large language models ask better questions for themselves”. In: *arXiv preprint arXiv:2311.04205* (2023).
- [Hoa+23] Benjamin Hoar, **Weitong Zhang**, Yuanzhou Chen, Jingwen Sun, Hongyuan Sheng, Yucheng Zhang, Jenny Yang, Cyrille Costentin, Quanquan Gu, and Chong Liu. “Object-detecting deep learning for mechanism discernment in multi-redox cyclic voltammograms”. In: (2023).
- [Hua+23] Zijie Huang, Jeehyun Hwang, Junkai Zhang, Jinwoo Baik, **Weitong Zhang**, Dominik Wodarz, Yizhou Sun, Quanquan Gu, and Wei Wang. “Causal Graph ODE: Continuous Treatment Effect Modeling in Multi-agent Dynamical Systems”. In: *The Symbiosis of Deep Learning and Differential Equations III*. 2023.
- [Ji+23] Kaixuan Ji, Qingyue Zhao, Jiafan He, **Weitong Zhang**, and Quanquan Gu. “Horizon-free Reinforcement Learning in Adversarial Linear Mixture MDPs”. In: *The Twelfth International Conference on Learning Representations*. 2023.
- [ZZG23] Junkai Zhang, **Weitong Zhang**, and Quanquan Gu. “Optimal horizon-free reward-free exploration for linear mixture mdps”. In: *International Conference on Machine Learning*. PMLR. 2023, pp. 41902–41930.
- [Zha+23a] **Weitong Zhang**, Jiafan He, Zhiyuan Fan, and Quanquan Gu. “On the interplay between misspecification and sub-optimality gap in linear contextual bandits”. In: *International Conference on Machine Learning*. PMLR. 2023, pp. 41111–41132.
- [Zha+23b] **Weitong Zhang**, Jiafan He, Dongruo Zhou, Q Gu, and A Zhang. “Provably efficient representation selection in low-rank Markov decision processes: from online to offline RL”. In: *Uncertainty in Artificial Intelligence*. PMLR. 2023, pp. 2488–2497.
- [Zha+23c] **Weitong Zhang**, Xiaoyun Wang, Weili Nie, Joe Eaton, Brad Rees, and Quanquan Gu. “MoleculeGPT: Instruction Following Large Language Models for Molecular Property Prediction”. In: *NeurIPS 2023 Workshop on New Frontiers of AI for Drug Discovery and Development*. 2023.
- [Zha+23d] **Weitong Zhang**, Xiaoyun Wang, Justin Smith, Joe Eaton, Brad Rees, and Quanquan Gu. “Diffmol: 3d structured molecule generation with discrete denoising diffusion probabilistic models”. In: *ICML 2023 Workshop on Structured Probabilistic Inference & Generative Modeling*. 2023.
- [Hoa+22] Benjamin B Hoar, **Weitong Zhang**, Shuangning Xu, Rana Deeba, Cyrille Costentin, Quanquan Gu, and Chong Liu. “Electrochemical mechanistic analysis from cyclic voltammograms based on deep learning”. In: *ACS Measurement Science Au* 2.6 (2022), pp. 595–604.
- [Jia+21] Yiling Jia, **Weitong Zhang**, Dongruo Zhou, Quanquan Gu, and Hongning Wang. “Learning Neural Contextual Bandits through Perturbed Rewards”. In: *International Conference on Learning Representations*. 2021.
- [ZZG21] **Weitong Zhang**, Dongruo Zhou, and Quanquan Gu. “Reward-free model-based reinforcement learning with linear function approximation”. In: *Advances in Neural Information Processing Systems* 34 (2021), pp. 1582–1593.
- [Wu+20] Yue Frank Wu, **Weitong Zhang**, Pan Xu, and Quanquan Gu. “A finite-time analysis of two time-scale actor-critic methods”. In: *Advances in Neural Information Processing Systems* 33 (2020), pp. 17617–17628.
- [Zha+20] **Weitong Zhang**, Dongruo Zhou, Lihong Li, and Quanquan Gu. “Neural Thompson Sampling”. In: *International Conference on Learning Representations*. 2020.

- [Zou+20] Difan Zou, Lingxiao Wang, Pan Xu, Jinghui Chen, **Weitong Zhang**, and Quanquan Gu. “Epidemic model guided machine learning for COVID-19 forecasts in the United States”. In: *MedRxiv* (2020), pp. 2020–05.
- [Liu+18] Shuai Liu, **Weitong Zhang**, Xiaojun Wu, Shuo Feng, Xin Pei, and Danya Yao. “A simulation system and speed guidance algorithms for intersection traffic control using connected vehicle technology”. In: *Tsinghua Science and Technology* 24.2 (2018), pp. 160–170.

Publications as group authors

- [Lop+24] Velma K Lopez, Estee Y Cramer, Robert Pagano, John M Drake, Eamon B O’Dea, Madeline Adey, Turgay Ayer, Jagpreet Chhatwal, Ozden O Dalgic, Mary A Ladd, et al. “Challenges of COVID-19 Case Forecasting in the US, 2020–2021”. In: *PLoS computational biology* 20.5 (2024), e1011200.
- [She+23] Katriona Shea, Rebecca K Borchering, William JM Probert, Emily Howerton, Tiffany L Bogich, Shou-Li Li, Willem G van Panhuis, Cecile Viboud, Ricardo Aguás, Artur A Belov, et al. “Multiple models for outbreak decision support in the face of uncertainty”. In: *Proceedings of the National Academy of Sciences* 120.18 (2023), e2207537120.
- [Cra+22] Estee Y Cramer, Evan L Ray, Velma K Lopez, Johannes Bracher, Andrea Brennen, Alvaro J Castro Rivadeneira, Aaron Gerding, Tilmann Gneiting, Katie H House, Yuxin Huang, et al. “Evaluation of individual and ensemble probabilistic forecasts of COVID-19 mortality in the United States”. In: *Proceedings of the National Academy of Sciences* 119.15 (2022), e2113561119.
- [Bra+21] Johannes Bracher, Daniel Wolfram, Jannik Deuschel, Konstantin Görgen, Jakob L Ketterer, Alexander Ullrich, Sam Abbott, Maria Vittoria Barbarossa, Dimitris Bertsimas, Sangeeta Bhatia, et al. “A pre-registered short-term forecasting study of COVID-19 in Germany and Poland during the second wave”. In: *Nature communications* 12.1 (2021), p. 5173.
- [Ray+20] Evan L Ray, Nutch Wattanachit, Jarad Niemi, Abdul Hannan Kanji, Katie House, Estee Y Cramer, Johannes Bracher, Andrew Zheng, Teresa K Yamana, Xinyue Xiong, et al. “Ensemble forecasts of coronavirus disease 2019 (COVID-19) in the US”. In: *MedRxiv* (2020), pp. 2020–08.