

## PROFESSIONAL EXPERIENCE

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### University of North Carolina, Chapel Hill

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

Chapel Hill, NC, USA

2024–Current

## EDUCATION

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### 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

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- **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

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### 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

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• 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

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

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

## TEACHING

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- **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

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- 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

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- **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<sup>A</sup>T<sub>E</sub>X. CI/CD (This CV and my homepage is CI/CD'ed)

## PUBLICATIONS

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\* 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.