

## EDUCATION

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<b>University of California, Los Angeles</b> Ph.D. Candidate in Computer Science, Advisor: Quanquan Gu, GPA: 3.94 / 4.00	Los Angeles, CA, USA 2019–Current
<b>Tsinghua University</b> 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

**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

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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

- [Zha+24] 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).
- [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.
- [She+23b] Hongyuan Sheng, Jingwen Sun, Benjamin Hoar, **Weitong Zhang**, Danlei Xiang, Tianhua Tang, Avijit Hazra, et al. “Autonomous closed-loop mechanistic investigation of molecular electrochemistry via automation”. In: *ChemRxiv preprint* (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.
- [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.
- [Zha+23b] **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+23c] **Weitong Zhang**<sup>\*</sup>, Jiafan He<sup>\*</sup>, Dongruo Zhou, Amy Zhang, and Quanquan Gu. “Provably Efficient Representation Learning in Low-rank Markov Decision Processes”. In: *UAI*. 2023.
- [Zha+23d] **Weitong Zhang**<sup>\*</sup>, Xiaoyun Wang<sup>\*</sup>, 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* (2022).
- [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* (2021).
- [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*. Ed. by H. Larochelle, M. Ranzato, R. Hadsell, M. F. Balcan, and H. Lin. Vol. 33. Curran Associates, Inc., 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).
- [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+23] Velma Lopez, Estee Y Cramer, Robert Pagano, John M Drake, Eamon B O’Dea, Benjamin P Linas, Turgay Ayer, Jade Xiao, Madeline Adee, Jagpreet Chhatwal, et al. “Challenges of COVID-19 Case Forecasting in the US, 2020-2021”. In: *medRxiv* (2023), pp. 2023–05.
- [She+23a] 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.
- [Ray+20] Evan L Ray, Nutchawan 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).