Weitong Zhang

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GitHub: https://github.com/ZeroWeight
Homepage: https://zeroweight.github.io
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Professional Experience

University of North Carolina, Chapel Hill — Chapel Hill, NC, USA
Tenure-Track Assistant Professor, School of Data Science and Society — 2024–Current

Education

University of California, Los Angeles — Los Angeles, CA, USA
Ph.D. in Computer Science, Advisor: Quanquan Gu, GPA: 3.94 / 4.00 — 2019–2024

University of California, Los Angeles — Los Angeles, CA, USA
M.Sc. in Computer Science, Advisor: Quanquan Gu, GPA: 3.94 / 4.00 — 2019–2022

Tsinghua University — Beijing, China
B.E. in Automation, GPA: 3.86/4.00, Rank 6 / 150 — 2015–2019

Research Interest

My research is centered on machine learning, with particular interests in reinforcement learning. My research goal is to develop and understand the foundation of decision-making processes for complicated tasks such as LLM, agentic systems, and structural design. I am also interested in developing AI agents for scientific (chemistry, physics) tasks

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 Grants and External Support

- NVIDIA Academic Program, Scalable Energy Guided Graph Diffusion Model for Accelerated Drug Design
- Google Cloud Research Credit, Exact Energy Guided Generative Modeling for De-novo Drug Design

TEACHING

- **Instructor** at University of North Carolina at Chapel Hill   Spring 2025
  DATA 890: Special Topics: Decision Making and Reinforcement Learning
- **Teaching Assistant** at University of California, Los Angeles   Spring 2021, Fall 2021
  Introductory Digital Design Laboratory (CS M152A) (Course Website 21 Fall, Course Website 21 Spring)
- **Teaching Assistant** at University of California, Los Angeles   Winter 2022, Winter 2023
  Fundamentals of Artificial Intelligence (CS 161) (Course Website 22 Winter, Course Website 23 Winter)

PROFESSIONAL SERVICES

Conference Area Chair/Senior Program Committee

- International Conference on Machine Learning (ICML), 2025

Conference Reviewer / Program Committee

- International Conference on Learning Representations (ICLR), 2020, 2021, 2022, 2023, 2024, 2025
- Neural Information Processing Systems (NeurIPS), 2021, 2022, 2023, 2024
- International Conference on Machine Learning (ICML), 2021, 2022, 2023, 2024
- International Joint Conference on Artificial Intelligence (IJCAI), 2020, 2021, 2022, 2023, 2024
- International Conference on Artificial Intelligence and Statistics (AISTATS), 2022, 2023, 2024

Journal Reviewer

- Journal of Artificial Intelligence Research (JAIR)
- Transactions on Machine Learning Research (TMLR)
- PLOS ONE
- PLOS Global Public Health

INVITED TALKS

- Exact Energy Guidance in Diffusion Models and offline RL   2025-02-28
  Samsung AI seminar
- Exact Energy Guidance in Diffusion Models and offline RL   2024-12-05
  Department of Computer Science, Indiana University Bloomington
- Introduction to Reinforcement Learning: from Bayesian Optimization to Bandits   2024-08-29
  Prof. Chong Liu's Lab, Department of Chemistry, UCLA
- Uncertainty-Aware Unsupervised and Robust Reinforcement Learning   2024-08-23
  Prof. Pan Xu's Lab, Department of Biostatistics & Bioinformatics, Duke University
- Introduction to Graph Neural Networks and Diffusion Models   2024-06-07
  Prof. Chong Liu's Lab, Department of Chemistry, UCLA

PUBLICATIONS

* indicates equal contribution

[Sun+25]   Jingwen Sun, **Weitong Zhang**, Yuanzhou Chen, Benjamin B Hoar, Hongyuan Sheng, Jenny Y Yang, Quanquan Gu, and Chong Liu. "Inquiry into the Appropriate Data Preprocessing of Electrochemical Impedance Spectroscopy for Machine Learning". In: *The Journal of Physical Chemistry C* (2025).

[Wan+25]   Zhaoyang Wang, Weilei He, Zhiyuan Liang, Xuchao Zhang, Chetan Bansal, Ying Wei, **Weitong Zhang**, and Huaxiu Yao. "CREAM: Consistency Regularized Self-Rewarding Language Models". In: *International Conference on Learning Representations*. 2025.

[ZZG25]   Shiyuan Zhang, **Weitong Zhang**, and Quanquan Gu. "Energy-Weighted Flow Matching for Offline Reinforcement Learning". In: *International Conference on Learning Representations*. 2025.

[Zha+25]   Linxi Zhao, Yihe Deng, **Weitong Zhang**, and Quanquan Gu. "Mitigating Object Hallucination in Large Vision-Language Models via Image-Grounded Guidance". In: *Forty-second International Conference on Machine Learning (spotlight)*. 2025.

[Zho+25]   Yiyang Zhou, Zhaoyang Wang, Tianle Wang, Shangyu Xing, Peng Xia, Bo Li, Kaiyuan Zheng, Zijian Zhang, Zhaorun Chen, Wenhao Zheng, et al. "AnyPrefer: An Automatic Framework for Preference Data Synthesis". In: *International Conference on Learning Representations*. 2025.

[Hoa+24]   Benjamin B Hoar, **Weitong Zhang**, Yuanzhou Chen, Jingwen Sun, Hongyuan Sheng, Yucheng Zhang, Yisi Chen, Jenny Y Yang, Cyrille Costentin, Quanquan Gu, et al. "Redox-Detecting Deep Learning for Mechanism Discernment in Cyclic Voltammograms of Multiple Redox Events". In: *ACS electrochemistry* 1.1 (2024), pp. 52–62.

[Hua+24]   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: *Proceedings of the ACM on Web Conference 2024*. 2024, pp. 4607–4617.

[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.

[Zha+24a]   Junkai Zhang, **Weitong Zhang**, Dongruo Zhou, and Quanquan Gu. "Uncertainty-Aware Reward-Free Exploration with General Function Approximation". In: *Forty-first International Conference on Machine Learning*. 2024.

[Zha+24b]   **Weitong Zhang**, Zhiyuan Fan, Jiafan He, and Quanquan Gu. "Achieving Constant Regret in Linear Markov Decision Processes". In: *The Thirty-eighth Annual Conference on Neural Information Processing Systems*. 2024.

[Zhe+24]   Wenhao Zheng, Yixiao Chen, **Weitong Zhang**, Souvik Kundu, Yun Li, Zhengzhong Liu, Eric P Xing, Hongyi Wang, and Huaxiu Yao. "CITER: Collaborative Inference for Efficient Large Language Model Decoding with Token-Level Routing". In: *Adaptive Foundation Models: Evolving AI for Personalized and Efficient Learning*. 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).

[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 Adee, 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 Wolffram, 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, Nutcha 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.