

# Yifei Wang

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## WORKING EXPERIENCE

**Massachusetts Institute of Technology (MIT)**, Cambridge, MA, USA

- Postdoc, Computer Science and Artificial Intelligence Laboratory (CSAIL)
  - Domain: Machine Learning, Self-supervised Learning, Foundation Models
  - Advisor: Prof. Stefanie Jegelka

Dec 2023 – Present

## EDUCATION

**Peking University**, Beijing, China

- Ph.D. in Applied Mathematics, School of Mathematical Sciences
  - Thesis: Self-supervised Contrastive Learning: Theory and Method
  - Advisors: Prof. Yisen Wang, Prof. Zhouchen Lin, Prof. Jiansheng Yang

Sep 2017 – Jul 2023

**Peking University**, Beijing, China

- B.S. in Data Science, School of Mathematical Sciences
- B.A. in Philosophy (double degree), Department of Philosophy

Sep 2013 – Jul 2017

Sep 2014 – Jul 2017

## AWARDS & SCHOLARSHIPS

- Best Paper Award, ICML 2024 ICL Workshop 2024
- Outstanding Ph.D. Dissertation Runner-Up Award, CAAI 2024  
Awarded by Chinese Association for Artificial Intelligence (CAAI), the leading AI academic organization in China.
- Excellent Graduate of Beijing Municipality, Top 0.1%, Beijing 2023  
Awarded for outstanding graduates among all Beijing universities.
- National Scholarship (twice), Top 0.1% nation-wide, China 2021, 2022
- President Scholarship, Top 1% university-wide, Peking University 2022
- Baidu Scholarship Nomination Award, Top 20 worldwide, Baidu Inc. 2022
- Silver Best Paper Award, ICML 2021 AML Workshop 2021
- Best Machine Learning Paper Award (1/685), ECML-PKDD 2021

## ROLES & RESPONSIBILITIES

- Area Chair, ICLR 2024, ICLR 2025 2024, 2025
- Organizer, NeurIPS 2024 Workshop on Red Teaming GenAI 2024
- Organizer, MIT ML Tea Seminar 2024
- Reviewer, NeurIPS, ICML, AISTATS, AAAI, LoG, ECML-PKDD, CVPR, ICCV, ACL 2021 – 2024

## RESEARCH INTERESTS

Machine Learning, Self-supervised Learning, Foundation Models, AI Safety, Interpretability

## PUBLICATIONS

37 peer-reviewed publications. 25 as (co-)first author. \* denotes shared first authorship.

### REFEREED CONFERENCE AND JOURNAL PAPERS

- [37] **Yifei Wang\***, Yuyang Wu\*, Zeming Wei, Stefanie Jegelka, Yisen Wang, A Theoretical Understanding of Self-Correction through In-context Alignment, in *Proceedings of the 38th Conference on Neural Information Processing Systems (NeurIPS 2024)*. **Best Paper Award at ICML 2024 ICL Workshop.**
- [36] **Yifei Wang\***, Kaiwen Hu\*, Sharut Gupta, Ziyu Ye, Yisen Wang, Stefanie Jegelka, Understanding the Role of Equivariance in Self-supervised Learning, in *Proceedings of the 38th Conference on Neural Information Processing Systems (NeurIPS 2024)*.
- [35] Sharut Gupta\*, Chenyu Wang\*, **Yifei Wang\***, Tommi Jaakkola, Stefanie Jegelka, In-Context Symmetries: Self-Supervised Learning through Contextual World Models, in *Proceedings of the 38th Conference on Neural Information Processing Systems (NeurIPS 2024)*. **Oral Presentation (top 4) at NeurIPS 2024 SSL Workshop.**
- [34] Xinyi Wu, Amir Ajorlou, **Yifei Wang**, Stefanie Jegelka, Ali Jadbabaie, On the Role of Attention Masks and LayerNorm in Transformers, in *Proceedings of the 38th Conference on Neural Information Processing Systems (NeurIPS 2024)*.

- [33] George Ma\*, **Yifei Wang\***, Derek Lim, Stefanie Jegelka, Yisen Wang, A Canonization Perspective on Invariant and Equivariant Learning, in *Proceedings of the 38th Conference on Neural Information Processing Systems (NeurIPS 2024)*.
- [32] Qixun Wang, **Yifei Wang**, Yisen Wang, Xianghua Ying, Dissecting the Failure of Invariant Learning on Graphs, in *Proceedings of the 38th Conference on Neural Information Processing Systems (NeurIPS 2024)*.
- [31] Lin Li, **Yifei Wang**, Chawin Sitawarin, Michael W. Spratling, OODRobustBench: A Benchmark and Large-scale Analysis of Adversarial Robustness under Distribution Shift, in *Proceedings of the 41st International Conference on Machine Learning (ICML 2024)*, 2024.
- [30] Yihao Zhang, Hangzhou He, Jingyu Zhu, Huanran Chen, **Yifei Wang**, Zeming Wei, On the Duality Between Sharpness-Aware Minimization and Adversarial Training, in *Proceedings of the 41st International Conference on Machine Learning (ICML 2024)*, 2024.
- [29] Qi Zhang, Tianqi Du, Haotian Huang, **Yifei Wang**, Yisen Wang, Look Ahead or Look Around? A Theoretical Comparison Between Autoregressive and Masked Pretraining, in *Proceedings of the 41st International Conference on Machine Learning (ICML 2024)*, 2024.
- [28] **Yifei Wang\***, Qi Zhang\*, Yaoyu Guo, Yisen Wang, Non-negative Contrastive Learning, in *Proceedings of the 12th International Conference on Learning Representations (ICLR 2024)*, 2024.
- [27] **Yifei Wang\***, Jizhe Zhang\*, Yisen Wang, Do Generated Data Always Help Contrastive Learning?, in *Proceedings of the 12th International Conference on Learning Representations (ICLR 2024)*, 2024.
- [26] Tianqi Du\*, **Yifei Wang\***, Yisen Wang, On the Role of Discrete Tokenization in Visual Representation Learning, in *Proceedings of the 12th International Conference on Learning Representations (ICLR 2024)*, 2024.
- [25] Xiaojun Guo\*, **Yifei Wang\***, Zeming Wei, Yisen Wang, Architecture Matters: Uncovering Implicit Mechanisms in Graph Contrastive Learning, in *Proceedings of the 37th Conference on Neural Information Processing Systems (NeurIPS 2023)*, 2023.
- [24] Qi Zhang\*, **Yifei Wang\***, Yisen Wang, Tri-contrastive Learning: Identifiable Representation Learning with Automatic Discovery of Feature Importance, in *Proceedings of the 37th Conference on Neural Information Processing Systems (NeurIPS 2023)*, 2023.
- [23] **Yifei Wang\***, Liangchen Li\*, Yisen Wang, Balance, Imbalance, and Rebalance: Understanding Robust Overfitting from a Minimax Game Perspective, in *Proceedings of the 37th Conference on Neural Information Processing Systems (NeurIPS 2023)*, 2023.
- [22] Ang Li\*, **Yifei Wang\***, Yisen Wang, Adversarial Examples Are Not Real Features, in *Proceedings of the 37th Conference on Neural Information Processing Systems (NeurIPS 2023)*, 2023.
- [21] George Ma\*, **Yifei Wang\***, Yisen Wang, Laplacian Canonization: A Minimalist Approach to Sign and Basis Invariant Spectral Embedding, in *Proceedings of the 37th Conference on Neural Information Processing Systems (NeurIPS 2023)*, 2023.
- [20] Qi Zhang\*, **Yifei Wang\***, Yisen Wang, On the Generalization of Multi-modal Contrastive Learning, in *Proceedings of the 40th International Conference on Machine Learning (ICML 2023)*, 2023.
- [19] Jingyi Cui\*, Weiran Huang\*, **Yifei Wang\***, Yisen Wang, Rethinking Weak Supervision in Helping Contrastive Representation Learning, in *Proceedings of the 40th International Conference on Machine Learning (ICML 2023)*, 2023.
- [18] Zeming Wei, **Yifei Wang**, Yiwen Guo, Yisen Wang, CFA: Class-wise Calibrated Fair Adversarial Training, in *Proceedings of the IEEE / CVF Computer Vision and Pattern Recognition Conference (CVPR 2023)*, 2023.
- [17] Qi Chen, **Yifei Wang**, Zhengyang Geng, Yisen Wang, Jiansheng Yang, Zhouchen Lin, Equilibrium Image Denoising with Implicit Differentiation, *IEEE Transactions on Image Processing (TIP)*, 32, 1868-1881, 2023.
- [16] **Yifei Wang\***, Qi Zhang\*, Tianqi Du, Jiansheng Yang, Zhouchen Lin, Yisen Wang, A Message Passing Perspective on Learning Dynamics of Contrastive Learning, in *Proceedings of the 11th International Conference on Learning Representations (ICLR 2023)*, 2023.
- [15] Zhijian Zhuo\*, **Yifei Wang\***, Yisen Wang, Towards a Unified Theoretical Understanding of Non-contrastive Learning via Rank Differential Mechanism, in *Proceedings of the 11th International Conference on Learning Representations (ICLR 2023)*, 2023.

- [14] Rundong Luo\*, **Yifei Wang\***, Yisen Wang, Rethinking the Effect of Data Augmentation in Adversarial Contrastive Learning, in *Proceedings of the 11th International Conference on Learning Representations (ICLR 2023)*, 2023.
- [13] Xiaojun Guo\*, **Yifei Wang\***, Tianqi Du\*, Yisen Wang, ContraNorm: A Contrastive Learning Perspective on Oversmoothing and Beyond, in *Proceedings of the 11th International Conference on Learning Representations (ICLR 2023)*, 2023.
- [12] Mingjie Li, **Yifei Wang**, Yisen Wang, Zhouchen Lin, Unbiased Stochastic Proximal Solver for Graph Neural Networks with Equilibrium States, in *Proceedings of the 11th International Conference on Learning Representations (ICLR 2023)*, 2023.
- [11] Shiji Xin, **Yifei Wang**, Jingtong Su, Yisen Wang, On the Connection between Invariant Learning and Adversarial Training for OOD Generalization, in *Proceedings of the 37th AAAI Conference on Artificial Intelligence (AAAI 2023)*. **Oral Presentation**.
- [10] Qi Zhang\*, **Yifei Wang\***, Yisen Wang, How Mask Matters: Towards Theoretical Understandings of Masked Autoencoders, in *Proceedings of the 36th Conference on Neural Information Processing Systems (NeurIPS 2022)*. **Spotlight Presentation**.
- [9] Qixun Wang\*, **Yifei Wang\***, Hong Zhu, Yisen Wang, Improving Out-of-distribution Robustness by Adversarial Training with Structured Priors, in *Proceedings of the 36th Conference on Neural Information Processing Systems (NeurIPS 2022)*. **Spotlight Presentation**.
- [8] Yichuan Mo, Dongxian Wu, **Yifei Wang**, Yiwen Guo, Yisen Wang, When Adversarial Training Meets Vision Transformers: Recipes from Training to Architecture, in *Proceedings of the 36th Conference on Neural Information Processing Systems (NeurIPS 2022)*. **Spotlight Presentation**.
- [7] Qi Chen, **Yifei Wang**, Yisen Wang, Zhouchen Lin, Optimization-induced Graph Implicit Nonlinear Diffusion, in *Proceedings of the 39th International Conference on Machine Learning (ICML 2022)*.
- [6] Mingjie Li, Xiaojun Guo, **Yifei Wang**, Yisen Wang, Zhouchen Lin, G<sup>2</sup>CN: Graph Gaussian Convolution Networks with Concentrated Graph Filters, in *Proceedings of the 39th International Conference on Machine Learning (ICML 2022)*.
- [5] **Yifei Wang\***, Qi Zhang\*, Yisen Wang, Jiansheng Yang, Zhouchen Lin, Chaos is a Ladder: A New Theoretical Understanding of Contrastive Learning via Augmentation Overlap, in *Proceedings of the 10th International Conference on Learning Representations (ICLR 2022)*.
- [4] **Yifei Wang**, Yisen Wang, Jiansheng Yang, Zhouchen Lin, A Unified Contrastive Energy-based Model for Understanding the Generative Ability of Adversarial Training, in *Proceedings of the 10th International Conference on Learning Representations (ICLR 2022)*. **Silver Best Paper at ICML 2021 AML Workshop**.
- [3] **Yifei Wang**, Zhengyang Geng, Feng Jiang, Chuming Li, Yisen Wang, Jiansheng Yang, Zhouchen Lin, Residual Relaxation for Multi-view Representation Learning, in *Proceedings of the 35th Conference on Neural Information Processing Systems (NeurIPS 2021)*.
- [2] **Yifei Wang**, Yisen Wang, Jiansheng Yang, Zhouchen Lin, Dissecting the Diffusion Process in Linear Graph Convolutional Networks, in *Proceedings of the 35th Conference on Neural Information Processing Systems (NeurIPS 2021)*.
- [1] **Yifei Wang**, Yisen Wang, Jiansheng Yang, Zhouchen Lin, Reparameterized Sampling for Generative Adversarial Networks, in *Proceedings of the European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML-PKDD 2021)*. **Best Machine Learning Paper Award (1/685)**, invited to *Machine Learning*.

#### WORKSHOP PAPERS

- [4] Ziyu Ye, Jiacheng Chen, Jonathan Light, **Yifei Wang**, Jiankai Sun, Mac Schwager, Philip Torr, Guohao Li, Yuxin Chen, Kaiyu Yang, Yisong Yue, Ziniu Hu. Reasoning in Reasoning: A Hierarchical Framework for Better and Faster Neural Theorem Proving. **NeurIPS 2024 Workshop** on Mathematical Reasoning and AI.
- [3] Hanqi Yan, Yulan He, **Yifei Wang** (corresponding author). The Multi-faceted Monosemanticity in Multimodal Representations. **NeurIPS 2024 Workshop** on Responsibly Building the Next Generation of Multimodal Foundational Models.
- [2] Lizhe Fang\*, **Yifei Wang\***, Khashayar Gatmiry, Lei Fang, Yisen Wang. Rethinking Invariance in In-context Learning. **ICML 2024 Workshop** on Theoretical Foundations of Foundation Models (TF2M).

- [1] Jingyi Cui\*, Weiran Huang\*, **Yifei Wang**, Yisen Wang. AggNCE: Asymptotically Identifiable Contrastive Learning. **NeurIPS 2022 Workshop** on Self-supervised Learning. **Oral Presentation.**

#### PREPRINT

- [4] Lizhe Fang\*, **Yifei Wang\***, Zhaoyang Liu, Chenheng Zhang, Stefanie Jegelka, Jinyang Gao, Bolin Ding, Yisen Wang. What is Wrong with Perplexity for Long-context Language Modeling? arXiv:2410.23771 (2024).
- [3] Qi Zhang\*, **Yifei Wang\***, Jingyi Cui, Xiang Pan, Qi Lei, Stefanie Jegelka, Yisen Wang. Beyond Interpretability: The Gains of Feature Monosemanticity on Model Robustness. arXiv preprint arXiv:2410.21331 (2024).
- [2] Qixun Wang, **Yifei Wang**, Yisen Wang, Xianghua Ying. Can In-context Learning Really Generalize to Out-of-distribution Tasks? arXiv preprint arXiv:2410.09695 (2024).
- [1] Zeming Wei, **Yifei Wang**, Ang Li, Yichuan Mo, Yisen Wang . Jailbreak and guard aligned language models with only few in-context demonstrations. arXiv preprint arXiv:2310.06387 (2023). **Cited over 150 times and featured in Anthropic’s research blog.**

#### INVITED TALKS

- A Principled Path to Safe Foundation Models, MIT ML Tea Seminar Oct 2024
- Building Safe Foundation Models from Principled Understanding, New York University Sep 2024
- Reimagining Self-supervised Learning with Context, Princeton University Aug 2024
- Non-negative Contrastive Learning, Cohere AI Jun 2024
- Self-supervised Learning of Identifiable Features, TU Munich May 2024
- Non-negative Contrastive Learning, MIT LIDS Tea Seminar Apr 2024
- Understanding and Applying Self-supervised Learning via Graph, Deep Potential 2023
- Towards Theoretical Foundations of Self-Supervised Learning, KAIST 2022
- Towards Truly Unlearnable Examples for Data Privacy, Chinese Academy of Science 2022
- Reparameterized Sampling for GANs, Beijing Academy of Artificial Intelligence (BAAI) 2021
- Reparameterized Sampling for GANs, Plenary Talk at ECML-PKDD 2021 2021

#### TEACHING EXPERIENCE

- Guest Lecturer, CSCI 3370: Deep Learning, Boston College Fall 2024  
Instructor: Prof Yuan Yuan
- Teaching Assistant, Introduction to AI (Trustworthy ML Class) Fall 2022  
Instructor: Prof Yisen Wang
- Teaching Assistant, Advanced Topics in Machine Learning Fall 2022  
Instructor: Prof Yisen Wang
- Teaching Assistant, Advanced Mathematics Spring 2021  
Instructor: Prof Chao Wang
- Teaching Assistant, Optimization Methods in Machine Learning Fall 2019  
Instructor: Prof Zhouchen Lin
- Teaching Assistant and Co-instructor, Machine Learning Fall 2017  
Instructor: Prof Tong Lin. I **instructed two-week classes** on Support Vector Machine.