

Cai Zhou

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First year PhD at MIT EECS.

Education Background

- **Massachusetts Institute of Technology** **Cambridge, MA**
PhD in EECS, CSAIL & LIDS 2024-2029
- **Tsinghua University** **Beijing**
Undergraduate in Department of Automation, Class of General Artificial Intelligence 2021-2024
GPA: 3.93/4.0, Ranking: Top 2%
- **Tsinghua University** **Beijing**
Undergraduate in Statistics, Joint Degree 2021-2024
- **Tsinghua University** **Beijing**
Undergraduate in School of Economy and Management 2020-2021

Research Interest

My research interest lies broadly in **theoretical and applied machine learning**. I aim to understand the foundations of machine learning, with a special focus on its probabilistic and geometric nature. I'm also interested in application areas including computer vision, natural language processing and computational biology.

Publications and Research Experience

Conference Papers

- On the Theoretical Expressive Power and Design Spaces of High Order Graph Transformers
Cai Zhou, Rose Yu, Yusu Wang
Twenty-seventh International Conference on Artificial Intelligence and Statistics (AISTATS, 2024)
TL;DR: Theoretically analyze the expressive power and approximation power of high order graph transformers; propose scalable and powerful high order graph transformers and simplicial transformers.
- Facilitating Graph Neural Networks with Random Walk on Simplicial Complexes
Cai Zhou, Xiyuan Wang, Muhan Zhang.
Thirty-seventh Conference on Neural Information Processing Systems (NeurIPS, 2023) [PDF]
TL;DR: Design positional and structural encodings for GNNs based on random walk on simplicial complexes, specifically EdgeRWSE and Hodge1Lap for 1-simplices (edge-level) that can provably improve expressive power and practical performance.
- From Relational Pooling to Subgraph GNNs: A Universal Framework for More Expressive Graph Neural Networks
Cai Zhou*, Xiyuan Wang*, Muhan Zhang.
Fortieth International Conference on Machine Learning (ICML, 2023) [PDF]
TL;DR: Propose k, l -WL algorithm (running k -WL on a graph with l labels) and theoretically establish a strict expressive power hierarchy; Incorporate a wide range of GNNs including relational pooling and subgraph GNNs.

Preprints

- Latent Graph Diffusion: A Unified Framework for Generation and Prediction on Graphs
Cai Zhou, Xiyuan Wang, Muhan Zhang.
Forty-first International Conference on Machine Learning (ICML, 2024), Under Review [PDF]
TL;DR: Propose Latent Graph Diffusion, a generative framework for both generation and prediction tasks utilizing latent graph diffusion with equivariant transformer. Derive theoretical guarantees for solving regression and classification tasks with diffusion models. Conduct both generation and prediction experiments for molecules.
- Locally Supervised Deep Learning by Maximizing Information Propagation
Yulin Wang, Zanlin Ni, Yifan Pu, **Cai Zhou**, Shiji Song, Gao Huang
International Journal of Computer Vision (IJCV), Under Review
TL;DR: Apply information theory to model locally supervised learning, propose InfoPro loss to alleviate information collapse in locally trained deep networks and verify the effectiveness in computer vision tasks.

Academic Services

- Reviewer for AISTATS 2024, NeurIPS 2024, ICLR 2025, AISTATS 2025
- Teaching Assistant for General Artificial Intelligence System Practice, 2023-Summer, Tsinghua University

Crucial Honors and Awards

Comprehensive Awards.....

- Outstanding Graduate by Beijing Ministry of Education and by Tsinghua University
- Outstanding Undergraduate Thesis by Beijing Ministry of Education and by Tsinghua University, 2024
- National Scholarship (Highest honor for undergraduates in China), 2023
- Comprehensive Excellence Award of Tsinghua University (Highest honor in THU and the Dept. Automation), 2023 & 2021
- Research and Innovation Excellence Award of Tsinghua University, 2022
- Academic Excellence Award of Tsinghua University, 2022
- Several prizes in national English speech contests and proficiency competitions.

Mathematics and Physics.....

- First prize of National Physics Competition for Undergraduates, 2021

Technical and General Skills

Technical Skills.....

- **Mathematics:** Calculus, Algebra, Discrete and Combinatorial Mathematics, Differential Geometry, Algebraic Topology, Complex Analysis, Fourier Analysis, Functional Analysis, Operation Research, etc.
- **Statistics:** Probability Theory, Statistical Inference, Stochastic Process, Multivariate Statistics and Regression, Computational Statistics, Time Series Analysis, Causal Inference, Bayesian Statistics, Biostatistics, etc.
- **Programming Skills:** Proficient in Python, Pytorch, PyG, DGL, C, C++, R, Linux, Latex, Markdown, Git, etc. Familiar with Tensorflow, Keras, C#, HTML, MATLAB, etc.

General Skills.....

Fluent in English; Good writing and presentation skills; Outstanding leadership and cooperation skills.