

Cai Zhou

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An undergraduate majoring in Automation and AI, minoring in statistics. A passionate, persistent perfectionist and a continual learner. Understand the world through theory, change the world with science and technology.

Education Background

- **Tsinghua University** **Beijing**
Undergraduate in School of Economy and Management 2020-2021
- **Tsinghua University** **Beijing**
Undergraduate in Department of Automation, Class of General Artificial Intelligence 2021-2024
- **Tsinghua University** **Beijing**
Undergraduate in Statistics, Minor degree 2021-2024
- **GPA: 3.93/4.0, Ranking: Top 2%**

Research Interest

My research interest lies broadly in **theoretical and applied machine learning**, with a focus on **graph learning**. Currently, I aim to understand the foundation of machine learning (information theory, optimization, statistical inference) and graph learning (theoretical expressive power, representation and generation, scalability). I'm also experienced in application areas including **Computer Vision**, **Natural Language Processing** and **Computational Biology**.

Centered at machine learning and graph learning, my long term research goal is to empower science and AI with learning across various subfields including vision, language and structured data. Concretely, I will be dedicated to the following topics: (1) **multi-modal foundation models**, or more broadly, AI systems that can perceive and reason like human; (2) **AI4science**, especially for molecule generation, drug discovery and healthcare.

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) [PDF]
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.

Ongoing Projects.....

- Project: Theoretical Analysis of LLMs' Emergent Ability
Peking University *School of Artificial Intelligence* Advisors: Profs. *Songchun Zhu & Muhan Zhang*
Use random graph theories to theoretically analyze the emergent ability of LLMs.
- Project: Bayesian Sequential Learning for Frequentist Continual Learning
Princeton University *Theoretical Machine Learning Group* Advisor: Prof. *Jason Lee*
Theoretically formulate continual learning and establish connections with sequential learning (bandits and RL).

Academic Services

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

Crucial Honors and Awards

Comprehensive Awards.....

- 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
- S prize of Mathematical Contest In Modeling (MCM), 2021

Technical and General 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.