

YANGTIAN ZHANG

Email: yangtian.zhang@yale.edu | Homepage: <https://zytzh.github.io/> | Github: <https://github.com/zytzh>

RESEARCH INTEREST

My research centers on **generative models**—particularly **diffusion and discrete diffusion models**—with a focus on how to apply them across diverse domains such as language, scientific discovery, and recommendation, and how to steer them toward desired objectives through techniques such as **reinforcement learning** and **distillation**.

EDUCATION

Shanghai Jiao Tong University

Bachelor of Engineering (B.Eng.) in Computer Science, Summa Cum Laude

Shanghai, China

Sept. 2018 – June 2022

- Member of **ACM Honors Class**, which is an elite CS program for top 5% talented students.

Yale University

Doctor of Philosophy (Ph.D.) student in Computer Science

New Haven, US

Sept. 2024 –

- Co-advised by **Prof. Rex Ying** and **Prof. David van Dijk**.
- Working on multi-modal foundation models and generative modeling techniques.

PUBLICATIONS

Variational Learning for Insertion-based Generation

[ICML Spotlight, top 2.2%]

Yangtian Zhang*, Zhe Wang*, Rex Ying, David van Dijk, Michalis Titsias, Jiaxin Shi (ICML 2026)

Learning Permutation Distributions via Reflected Diffusion on Ranks

Sizhuang He*, Yangtian Zhang*, Shiyang Zhang, David van Dijk (ICML 2026)

STRIDE: Post-Training LLMs to Reason and Refine Bio-Sequences via Edit Trajectories

Daiheng Zhang, Shiyang Zhang, Sizhuang He, Yangtian Zhang, Syed Asad Rizvi, David van Dijk (ICML 2026)

CoPersona: Collaborative Persona Graphs for Robust LLM Personalization

Yangtian Zhang*, Leyao Wang*, Hiren Madhu, Ngoc Bui, Walter Roznyatovskiy, Rex Ying (KDD 2026)

Non-Markovian Discrete Diffusion with Causal Language Models

Yangtian Zhang*, Sizhuang He*, Daniel Levine, Lawrence Zhao, David Zhang, Syed A Rizvi, Emanuele Zappala, Rex Ying, David van Dijk (NeurIPS 2025)

Flow Matching for Collaborative Filtering

Chengkai Liu*, Yangtian Zhang*, Jianling Wang, Rex Ying, James Caverlee (KDD 2025)

CaLMFlow: Volterra Flow Matching using Causal Language Models

Sizhuang He, Daniel Levine, Ivan Vrkic, Marco Francesco Bressana, David Zhang, Syed Asad Rizvi, Yangtian Zhang, Emanuele Zappala, David van Dijk

DiffPack: A Torsional Diffusion Model for Autoregressive Protein Side-Chain Packing

Yangtian Zhang*, Zuobai Zhang*, Bozitao Zhong, Sanchit Misra, Jian Tang (NeurIPS 2023)

E3Bind: An End-to-End Equivariant Network for Protein-Ligand Docking

Yangtian Zhang*, Huiyu Cai*, Chence Shi, Bozitao Zhong, Jian Tang (ICLR 2023)

PEER: A Comprehensive and Multi-Task Benchmark for Protein Sequence Understanding

Minghao Xu, Zuobai Zhang, Jiarui Lu, Zhaocheng Zhu, Yangtian Zhang, Ma Chang, Runcheng Liu, Jian Tang (NeurIPS 2022 Datasets and Benchmarks Track)

Torchdrug: A powerful and flexible machine learning platform for drug discovery

Zhaocheng Zhu, Chence Shi, Zuobai Zhang, Shengchao Liu, Minghao Xu, Xinyu Yuan, Yangtian Zhang, Junkun Chen, Huiyu Cai, Jiarui Lu, Chang Ma, Runcheng Liu, Louis-Pascal Xhonneux, Meng Qu, Jian Tang

A Survey on Diffusion Models for Recommender Systems

Jianghao Lin, Jiaqi Liu, Jiachen Zhu, Yunjia Xi, Chengkai Liu, Yangtian Zhang, Yong Yu, Weinan Zhang (CoRR 2024)

RESEARCH EXPERIENCE

- Meta Platforms, Inc.

Research Scientist Intern, advised by Dr. Fei Sha

May. 2026 – Menlo Park, USA

Conducting research on the **distillation of diffusion language models** for efficient generation.
- Google Deepmind

Student Researcher, advised by Dr. Jiaxin Shi and Dr. Michalis Titsias

June. 2025 – Dec. 2025
New York, USA

Investigated advanced **discrete diffusion** frameworks and discrete probabilistic modeling approaches.
Designed and implemented a **learning-to-order insertion model** within a variational inference framework, optimizing the non-differentiable insertion-order objective with an **RLOO policy-gradient estimator**. Resulting paper accepted as **ICML 2026 Spotlight (top 2.2%)**.
- Microsoft Research AI4Science

Research Intern, advised by Dr. Tao Qin

April. 2024 – July 2024
Beijing, China

Conducted research on multi-modal foundation model for AI-driven scientific discovery.
- Mila - Quebec AI Institute

Graduate Research Assistant, advised by Prof. Jian Tang

Sept. 2021 – April 2024
Montreal, Canada

Developed non-euclidean generative modelling with applications in protein science. See [paper](#) here
Developed geometric deep learning techniques to molecular docking. See [paper](#) here.
- APEX Lab, Shanghai Jiao Tong University

Undergraduate Research Assistant, advised by Prof. Yong Yu and Prof. Weinan Zhang

Sept. 2020 – June 2022
Shanghai, China

Conducted **reinforcement learning** research on **imitation learning**, designing a multi-step generative adversarial imitation learning (GAIL) framework that better trades off rollout discrepancy against sample complexity. See [paper](#) here.

SELECTED PROJECTS

- Hands-on-RL: A Comprehensive Chinese Tutorial for Reinforcement Learning

Contributed to the tutorial by authoring sections related to imitation learning, synthesizing complex RL concepts into accessible content, and implementing practical examples on Jupyter notebooks. See [project](#) here.
- TorchDrug: A Powerful and Flexible Machine Learning Platform for Drug Discovery

Played a pivotal role in the development of TorchDrug, a robust ML platform for drug discovery, assisting in supporting 6 tasks and implementing over 25 models, specializing in bioinformatics applications.
Over 1,300 stars and 40,000 downloads. See [project](#) here.
- TorchProtein: A Specialized Machine Learning Library for Protein Science

Played a pivotal role in the development of TorchProtein, a specialized extension of TorchDrug, focusing on implementing representation learning models for both protein sequences and structures. See [project](#) here.

HONORS & AWARDS

Irving T. Ho Memorial Scholarship (4 undergrads per year)	2021
Zhiyuan Honorary Scholarship (Top 5% in SJTU)	2018-2021
Shanghai Jiao Tong University Excellent Scholarship (Top 10% in SJTU)	2018-2021
Outstanding Graduate Student	2022
Meritorious Winner in Mathematical Contest in Modeling (Top 7%)	2020
First Prize, National Olympiad in Physics	2017

SERVICES

Academic Reviewer: NeurIPS (2023–2024), ICML (2023–2024), ICLR (2024), AAAI (2024)
Teaching Assistant | Shanghai Jiao Tong University: CS158 Data Structures and Algorithms (2020), MS125 Principle and Practice of Computer Algorithms (2020), CS420 Machine Learning (2021)

TECHNICAL SKILLS

Programming Languages: Python, C/C++, Java, MATLAB, Verilog-HDL
Deep Learning Packages: PyTorch, TensorFlow, Keras
Language: Mandarin Chinese(Native), English(Fluent)