YANGTIAN ZHANG

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RESEARCH INTEREST

My primary research interests lie within the domain of Generative AI, Graph Neural Networks, and more recently, Multi-Modal Foundation Models. I'm deeply passionate about developing innovative AI solutions for real-world applications and scientific problems.

EDUCATION

Shanghai Jiao Tong University — Shanghai, China
Bachelor of Engineering (B.Eng.) in Computer Science, Summa Cum Laude — *Sept. 2018 – June 2022*

- Member of **ACM Honors Class**, which is an elite CS program for top 5% talented students.
- GPA: **90.79 / 100**

Yale University — New Haven, US
Doctor of Philosophy (Ph.D.) student in Computer Science — *Sept. 2024 –*

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

PUBLICATIONS

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 (In Submission)*

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 (In Submission)*

A Survey on Diffusion Models for Recommender Systems
Jianghao Lin, Jiaqi Liu, Jiachen Zhu, Yunjia Xi, Chengkai Liu, Yangtian Zhang, Yong Yu, Weinan Zhang (In Submission)

Imitation Learning via Multi-Step Occupancy Measure Matching
*Minghuan Liu, Hangyu Wang, Minkai Xu, **Yangtian Zhang**, Zhengbang Zhu, Weinan Zhang (Preprint)*

RESEARCH EXPERIENCE

Microsoft Research AI4Science — April. 2024 – July 2024
*Research Intern, advised by **Dr. Tao Qin*** — *Beijing, China*

- Conducted research on multi-modal foundation model for AI-driven scentific discovery.

Mila - Quebec AI Institute — Sept. 2021 – April 2024
*Graduate Research Assistant, advised by **Prof. Jian Tang*** — *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 Sept. 2020 – June 2022
*Undergraduate Research Assistant, advised by **Prof. Weinan Zhang*** *Shanghai, China*

- Designed a Multi-Step Generative Adversarial Imitation Learning framework. See paper here.

Selected Projects

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.

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.

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

- Neural Information Processing Systems (NeurIPS) 2023-2024
- International Conference on Machine Learning (ICML) 2023-2024
- International Conference on Learning Representations (ICLR) 2024
- Association for the Advancement of Artificial Intelligence (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)