Yangtian ZHANG

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Research Interests

My interest lies in machine learning algorithm and its applications. I'm both interested in **graph representation learning** and **reinforcement learning**. I'm currently working on incorporating geometric information into graph neural network and its applications such as drug discovery.

Education

Shanghai Jiao Tong University (SJTU)

Sept.2018–Present

Bachelor Student in Computer Science

- Member of **ACM Honors Class**, which is an elite program for **top 5**% talented students in CS Department.
- GPA: **90.66 / 100**, Ranking: **5 / 31**

Experience

Mila, Université de Montréal

Mar.2021–Present

Undergraduate Researcher at Mila Lab, advised by Prof. Jian Tang

- Research Topic: **Geometric Deep Learning**, **Equivariant Networks**, **Reinforcement Learning**
- Focus on machine learning algorithms related to drug discovery. Investigate both geometric deep learning and reinforcement learning methods, as well as their applications in real situation of drug discovery such as protein-ligand docking and drug virtual screening.

»» TorchDrug Platform

- Participated in building a powerful platform designed for drug discovery, covering techniques from graph machine learning(graph neural networks, geometric deep learning & knowledge graphs), deep generative models, deep sequence model to reinforcement learning.
- Implemented deep learning models for large molecules such as protein and kinase.
- The platform has already gained 400+ stars in GitHub. See Project website here

»» Deep Learning for Protein-Ligand Docking & Large Scale Virtual Screening

- Proposed a novel scoring function based on geometric deep learning, which utilizes information from the sampled points on protein surface. The scoring function can be used for docking and virtual screening.
- Combined the scoring function with equivalent network EGNN to reduce the cost of data augmentation.
- The scoring function currently achieves superior results in docking compared with the previous ML-based model such as DeepDock.

Apex Data & Knowledge Management Lab, SJTU

Aug.2020–Present

Undergraduate Researcher at APEX Lab, advised by Prof. Weinan Zhang

- Research Topic: **Machine Learning**, **Imitation Learning**, **Reinforcement Learning**
- Focus on algorithms such as Generative Adversarial Imitation Learning(GAIL) and Behavior Clone(BC) for imitation learning task. Investigate their variants and their possible applications in real world.

»» Imitation Learning via Multi-Step Occupancy Measure Matching

- Analyzed the roll-out discrepancy and the sample complexity of Multi Step Generative Adversarial Imitation Learning (MS-GAIL) and revealed their trade-off.
- Proposed an auto curriculum version of T-setp Occupancy Measure matching algorithm, AutoGAIL, that chooses the appropriate sequence length for sample efficiency in an adaptive manner.
- The model achieves better sample efficiency in MuJoCo environments such as Hopper. See Paper Draft here.

Honors & Awards

Zhiyuan Honorary Scholarship **(Top 5% in SJTU)** 2018-2021
Excellent School-level Scholarship **(Top 2% in SJTU)** 2018-2021
Meritorious Winner in Mathematical Contest in Modeling **(Top 8%)** 2020
The First Prize in Chinese Physics Olympiad **(Top 1%)** 2017

Other Selected Projects

Anime Super-Resolution July.2019–Aug.2019

- Implemented an anime-specific Super Resolution model based on SRGAN. It trains a generative adversarial network(GAN) as a perceptual loss to match the fidelity expected at higher resolution. See Project here.

Adaptive Color Subtitle Render Oct.2020–Dec.2020

- Proposed a computation-efficient DP-based algorithm to adaptively change the video subtitle color, ensuring enough contrast with background and perceptual smoothness.
- Solved the common subtitle legibility problem by formulating subtitle legibility problem as a traditional planning problem. See Project here.

MX Complier Mar.2020–June.2020

- Developed a compiler from C-like language (Mx*) to assembly language (NASM).
- Implemented optimizations like constant replacement, function inline and loop unrolling. See Project here.

Pintos Mar.2020–June.2020

- Implemented a basic operating system Pintos for the 80 x 86 architecture based on Stanford Course CS140.
- Supported kernel threads, loading and running user programs, and a file system. See Project here.

Teaching Experience

- **Teaching Assistant**

CS158: Data Structures and Algorithms (Honors Class)	2020
MS125: Principle and Practice of Computer Algorithms (Honors Class)	2020
CS420: Machine Learning	2021

Skills

- **Programming Languages:** Python, C/C++, Java, MATLAB, Verilog-HDL
- **Deep Learning Packages:** PyTorch, TensorFlow, Keras
- **Languages:** English (fluent), Mandarin (native)