Ziqi Chen

EDUCATION

The Ohio State University, Columbus, US
PhD student — *Aug. 2019 - current*
Master student — *Aug. 2018 - May. 2019*
Department of Computer Science and Engineering

Wuhan University, Wuhan, China — *Sept. 2014 - Jun. 2018*
Bachelor of Engineering
School of Computer Science

RESEARCH INTERESTS

My current research primarily focuses on developing novel generative models or reinforcement learning algorithms for drug discovery, particularly in small molecule generation and biological sequence design.

PUBLICATION

The full list of my papers is available at Google Scholar. * below indicates equal contributions.

1. Ziqi Chen, Bo Peng, Srinivasan Parthasarathy, and Xia Ning. Shape-conditioned 3d molecule generation via equivariant diffusion models. *arXiv*, page arXiv:2308.11890, 2023
2. Ziqi Chen, Oluwatosin R. Ayinde, James R. Fuchs, Huan Sun, and Xia Ning. G2retro as a two-step graph generative models for retrosynthesis prediction. *Communications Chemistry*, 6(1), may 2023
3. Ziqi Chen*, Baoyi Zhang*, Hongyu Guo, Prashant Emani, Trevor Clancy, Chongming Jiang, Mark Gerstein, Xia Ning, Chao Cheng, and Martin Renqiang Min. Binding peptide generation for MHC class i proteins with deep reinforcement learning. *Bioinformatics*, 39(2), jan 2023
4. Ziqi Chen, Martin Renqiang Min, Hongyu Guo, Chao Cheng, Trevor Clancy, and Xia Ning. T-cell receptor optimization with reinforcement learning and mutation polices for precision immunotherapy. In *Research in Computational Molecular Biology. RECOMB 2023. Lecture Notes in Computer Science*, pages 174–191. Springer Nature Switzerland, 2023
5. Ziqi Chen, Martin Renqiang Min, Srinivasan Parthasarathy, and Xia Ning. A deep generative model for molecule optimization via one fragment modification. *Nature Machine Intelligence*, Dec 2021
6. Ziqi Chen*, Bo Peng*, Vassilis N. Ioannidis, Mufei Li, George Karypis, and Xia Ning. A knowledge graph of clinical trials (CTKG). *Scientific Reports*, 12(1), mar 2022
7. Ziqi Chen, Martin Renqiang Min, and Xia Ning. Ranking-based convolutional neural network models for peptide-MHC class I binding prediction. *Frontiers in molecular biosciences*, 8:128, May 2021

WORK EXPERIENCE

NEC Labs America, Princeton, US — *May. 2021 - Aug. 2021*
Research Intern

- Developed a framework PepPPO based on a reinforcement learning algorithm (i.e., Proximal Policy Optimization) to generate peptide sequences binding to any given MHC Class I proteins by mutating one amino acid at each step. This work is accepted by Bioinformatics.

- Developed a framework TCRPPO based on Proximal Policy Optimization to generate valid CDR3 sequence of β chain in T-cell Receptors binding to any given peptide sequences by mutating one amino acid at each step. This work is accepted by Research in Computational Molecular Biology 2023.

Meta Platforms, Menlo Park, US *May. 2022 - Aug. 2022*
Software Engineer Intern, Machine Learning

- Explored reinforcement learning algorithms to improve feed ranking in Facebook.
- Developed a deep Q-learning model to personalize re-ranking in feeds based on predictions from a multi-task learning framework. Results of A/B tests show that this model achieves promising improvements in user engagement metrics.
- Developed a model based on off-policy reinforcement learning algorithm for slate re-ranking.
- Built data pipelines for personalized feed re-ranking and slate ranking.

ACADEMIC ACHIEVEMENTS

Second-Class Scholarship of Wuhan University *2015, 2016 and 2017*

TECHNICAL STRENGTHS

Program Languages	Python, Shell Script, Java, SQL
Software & Tools	Pytorch, Numpy
OS	Linux, Windows