KANGYU ZHENG

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Education

Rensselaer Polytechnic Institute   Sep. 2024 – Now
Ph.D in Computer Science   *Troy, NY*

The Ohio State University   Sep. 2021 – Jun. 2024
Master of Science in Computer Science   *Columbus, Ohio*

University of Minnesota   Sep. 2018 – Jun. 2021
Bachelor of Science in Computer Science   *Minneapolis, Minnesota*

Research Experience

Developing evaluation benchmark for drug discovery   Oct. 2023 - May. 2024
Advised by Dr. Tianfan Fu

- Develop fair evaluation benchmarks for different types of structure-based drug discovery algorithms.
- Found that models based on genetic algorithms perform better than those based on generative models, with related papers accepted as poster on ICML 2024 AI for Science Workshop

Designing quantum machine learning model for drug property   Oct. 2024 - Present
Advised by Dr. Zhiding Liang and Dr. Tianfan Fu

- Using quantum circuit search method to find robust QML circuits for ADMET task

Work Experience

The Ohio State University   Sep. 2021 – Dec. 2023
Teaching Assistant   *Columbus, Ohio*

- Assisted in teaching, with duties including grading homework and lab assignments, as well as conducting office hours.
- Participated in courses including Modeling and Problem Solving with Excel and Access and Artificial Intelligence I.
- Involved in answering Excel and Access queries and writing Python programs to demonstrate artificial intelligence concepts, such as MLP (Multilayer Perceptron), k-NN (k-Nearest Neighbors), and SVM (Support Vector Machine).

Tencent   May. 2024 – Aug. 2024
Applied research Intern   *Shenzhen, China*

- Collaborate with other team members to develop an auto-driving system for a developing game. Using PPO algorithm and tested on CARLA

Publications

1. **Zheng, K.**, Fu, T., Liang, Z. (2025). QCS-ADME: Quantum Circuit Search for Drug Property Prediction with Imbalanced Data and Regression Adaptation

2. **Zheng, K.**, Lu, Y., Zhang, Z., Wan, Z., Ma, Y., Zitnik, M., and Fu, T. (2024). Structure-based drug design benchmark: Do 3d methods really dominate?

3. Liu, C., Wan, Z., Wang, Y., Shen, H., Wang, H., **Zheng, K.**, Zhang, M., and Arcucci, R. (2024). Benchmarking and boosting radiology report generation for 3d high-resolution medical images.

Research Interest and Technical Skills

Research Interest: AI for science/quantum, Quantum computing
Languages and Framework: Rust, C/C++, Python, Java, MATLAB, OCaml, Pytorch, Qiskit, Pennylane