Rui Gao

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EDUCATION & SCHOLARSHIP

University of California, Los Angeles

Sep 2024 - June 2026(Expected)

Master of Science, Electrical and Computer Engineering

Los Angeles, CA

• GPA: 4.0/4.0

Fudan University

Sep 2020 - Jul 2024

Bachelor of Engineering, Biomedical Engineering, School of Information Science and Engineering

Shanghai, CN

- GPA: 3.89/4.0, Ranking: 1/259
- Distinguished Graduate Students(1%)

RESEARCH & PROJECT EXPERIENCE

RLHF-inspired Large Language Model for Ligand Optimization

Jun 2025 - Present

Advisor: Prof Xiang Anthony Chen, Dr. Youngseung Jeon, University of California, Los Angeles Research Assistant

- Pioneered Molo, an RLHF-inspired ligand optimization model built on Mistral and LLaMA-7B, introducing property-driven reinforcement learning feedback to molecular design.
- Established a base ligand generator by performing **supervised fine-tuning (SFT)** and **LoRA adaptation** on existing molecule datasets, then designed **property-specific reward functions** to guide reinforcement learning toward pharmacologically relevant molecules.
- Demonstrated that Molo outperforms supervised and RL-only model baselines with higher success rates, improved property profiles, and stronger zero-shot generalization across in- and out-of-distribution tasks, showcasing the potential of scalable foundation models for real-world drug discovery.
- Manuscript in preparation for submission to ICLR 2026.

Keystrokes Prediction from Electromyography Signals

 $\mathrm{Jan}\ 2025\ \text{-}\ \mathrm{March}\ 2025$

Advisor: Prof. Jonathan Kao, University of California, Los Angeles M247 Neural Networks and Deep Learning

- Applied various neural network techniques and conducted comparative experiments including GRU,
 Bi-directional LSTM, and Attention-based architectures for modeling multi-channel EMG signals.
- Designed a customized **Conformer-based model** adapted to EMG signal characteristics, improved the original CTC loss, and achieved a **12.47% CER**(character error rate) on the validation set, outperforming the 18.94% baseline model TDSConv.

Applying RL Algorithms for Robust Autonomous Driving in MetaDrive

Sep 2024 - Dec 2024

Advisor: Prof. Bolei Zhou, University of California, Los Angeles

260 Reinforcement Learning

- Implemented and compared multiple reinforcement learning (RL) algorithms, including **TD3**, **SAC**, and **PPO**, in the **MetaDrive Safety Environment** to evaluate their **robustness** under **dynamic traffic and obstacle-rich scenarios**.
- Achieved 92.47% route completion in the test environment using PPO with entropy regularization, clip range tuning and learning rate decay, significantly outperforming the 52% baseline.

Multimodal Graph Neural Networks for Depression Prediction

Jul 2023 - Feb 2024

Advisor: Prof. Hatice Gunes, Dr. Batuhan Sayis, Cambridge University

Research Intern

- Conducted a four-week study involving 20-42 participants to study changes in depression based on interactions with both a robot-assisted system(participants interacting with a robot) and a voice-assisted system.
- Collected and processed experiment data using **Scikit-Learn** and **Numpy**, including questionnaire data (mental health questionnaires, e.g. Panas or PHQ9) and physiological data (experimental ECG and EDA).
- Developed and implemented a **temporal multimodal graph neural network** with **Pytorch** based on the Gratis model (a general graph representation learning framework) to predict participants' depression changes; wrote the final code.

PUBLICATIONS

[1]: Sayis, B., Gao, R., Song, S., Gunes, H. (2024). Learning Graph Representation for Predicting Student Mental Wellbeing in Robot Assisted Journal Writing Context. ACHW 2024

TECHNICIAN SKILLS

Developer Tools: Python, MATLAB, HTML/CSS, Javascript, Shell **Languages**: Mandarin (native), English (fluent), French (basic)