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
- Course: Linear Programming, Digital Speech Processing, Neural Network and Deep Learning, Reinforcement Learning

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*

- Built an RLHF-based LLM, **Molo** by integrating reinforcement learning on top of Mistral and LLaMA-7B LLMs with property-driven feedback to enable ligand optimization beyond the limits of supervised approaches.
- 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.
- Manuscript in preparation for submission to ICLR 2026.

Keystrokes Prediction from Electromyography Signals Jan 2025 - 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.
- **Published Paper**:"Learning Graph Representation for Predicting Student Mental Wellbeing in Robot Assisted Journal Writing Context" on ACII 2024.

Technical Skills

Developer Tools: Python, MATLAB, HTML/CSS, Javascript, Shell
Frameworks: Pytorch, Tensorflow, Scikit-learn, Pandas, Node.js
Languages: Mandarin(native), English(fluent), French(novel)