Yifan Lu

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EDUCATION

Hangzhou Dianzi University   *Sep 2021 - Expected Jun 2025*
BEng in Artificial Intelligence Security (Honours)   GPA: 3.87/5.00
Advisor: Prof. Pengfei Jiao

RESEARCH EXPERIENCE

Heterogeneous Graph Neural Network Explainer   *Nov 2023 – Sept 2024*
- Theoretically demonstrated the amplifying effect of noisy information in heterogeneous graph scenarios.
- Employed denoising variational inference to robustly capture graph information within the latent variable space, transforming the GNN explanation challenge into an optimization task by integrating the Graph Information Bottleneck principle, effectively addressing irregularities caused by structural noise.
- Proposed a novel graph explanation generator based on type attention, incorporating heterogeneous relation learning to effectively capture complex semantics during the generation of explanatory subgraphs.

ML-based Antibody Design and Optimization   *July 2024 – Sept 2024*
- Leveraged LLMs to design antibodies using bidirectional contextual information, and further employed a diffusion-based method to optimize both sequences and structures.
- The first work to co-design and optimize species-specific antibody sequences and structures while identifying optimal binding sites.

Research on Heterogeneous Graph Transformer   *June 2023 – Sept 2023*
- Studied the efficiency and context capturing capability of Heterogeneous Graph Transformers, proposing a contextual neighbor sampling method and a Transformer-based framework for heterogeneous graph learning.

Heterogeneous Graph Link Prediction   *Mar 2023 – June 2023*
- Proposed a novel mutual information-based method for heterogeneous graph link prediction, enhancing performance through self-supervised learning.

Heterogeneous Hypergraph Neural Network   *June 2022 – Feb 2023*
- Simultaneously considered low-order pairwise relations and high-order complex semantics on heterogeneous hypergraphs while incorporating structural information learning.

ACADEMIC

[1] **Yifan Lu**, Pengfei Jiao, Xuan Guo, Ziyun Zou, Yiwei Wang, Mengzhou Gao, Huaming Wu. Robust Heterogeneous Graph Neural Network Explainer with Graph Information Bottleneck, *under review*.

[2] **Yifan Lu**, Ziyun Zou, Pengfei Jiao, Zehao Liu, Mengzhou Gao. LLM-based Species-Specific Antibody Design and Optimization for Protein Structures, *under review*.

[3] Pengfei Jiao, **Yifan Lu**, Huan Liu, Xuan Guo, Xiao Wang. Heterogeneous Graph Transformer with Contextual Neighbor Sampling, *under review*.

[4] Ziyun Zou, Lian Shen, Yanhao Li, **Yifan Lu**, Juan Liu, Xiangrong Liu. RETAIN: Reliable Topology Augmentation for both Heterophily and Homophily Graphs, *under review*.

[5] Mengzhou Gao, Zehao Liu, **Yifan Lu**, Pengfei Jiao. Physical Process Guided Graph Neural Networks for Anomaly Detection in CPSs, *IJCAI'24 Workshop: Artificial Intelligence for Time Series Analysis, 2024*.

[6] **Yifan Lu**, Mengzhou Gao, Huan Liu, Zehao Liu, Wei Yu, Xiaoming Li, Pengfei Jiao. Neighborhood overlap-aware heterogeneous hypergraph neural network for link prediction, *Pattern Recognition, 2023, 144: 109818*.

[7] **Yifan Lu**, Zehao Liu, Mengzhou Gao, Pengfei Jiao. Heterogeneous Link Prediction via Mutual Information Maximization Between Node Pairs, *CAAI International Conference on Artificial Intelligence, 2023*.

WORK EXPERIENCE

MindRank   *Hangzhou, China*
Machine Learning Intern   *July 2024 – Sept 2024*
- Designed a diffusion model to optimize antibody sequences and structures, resulting in a tenfold improvement in the binding affinity between antibodies and antigens.
- Conducted research and reproduced key work on antibody affinity prediction, and applied large language models to explore innovative approaches for antibody generation in specific species.

SKILLS

Programming:	Python, C/C++, Linux, MATLAB, HTML
Languages:	Chinese, English
Soft Skills:	Self-Motivated, Organized, Teamwork, Analytical Thinking, Responsible