

# Yifan Lu

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## EDUCATION

Hangzhou Dianzi University

Bachelor of Engineering in Artificial Intelligence Security (Honors)

Advisor: Prof. Pengfei Jiao

Sep 2021 - Expected Jun 2025

GPA: 83.76/100

## ACADEMIC

1. **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.
2. **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.
3. 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.
4. **Yifan Lu**, Pengfei Jiao, Xuan Guo, Ziyun Zou, Yiwei Wang, Mengzhou Gao, Huaming Wu. Robust Heterogeneous Graph Neural Network Explainer with Graph Information Bottleneck, *Submitted to ICLR 2025*.
5. **Yifan Lu**, Ziyun Zou, Pengfei Jiao, Zehao Liu, Mengzhou Gao. LLM-based Species-Specific Antibody Design and Optimization for Protein Structures, *Submitted to ICASSP 2025*.
6. Pengfei Jiao, **Yifan Lu**, Huan Liu, Xuan Guo, Xiao Wang. Heterogeneous Graph Transformer with Contextual Neighbor Sampling, *Submitted to IEEE Transactions on Artificial Intelligence*.
7. Ziyun Zou, Lian Shen, Yanhao Li, **Yifan Lu**, Juan Liu, Xiangrong Liu. RETAIN: Reliable Topology Augmentation for both Heterophily and Homophily Graphs, *Submitted to ICASSP 2025*.

## RESEARCH EXPERIENCE

### Heterogeneous Graph Neural Network Explainer

Nov 2023 – Sept 2024

- **Amplification of Noisy Information:** Theoretical analysis revealed the amplifying effects of noisy information in heterogeneous graph scenarios, emphasizing its impact on GNN performance and explanation quality.
- **Latent Representation through Denoising Variational Inference:** 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.
- **Novel Explanation Generation Framework:** Proposed a type attention-based explanation generator that leverages heterogeneous relation learning to capture complex semantics. This framework facilitated the generation of explanatory subgraphs with improved coherence and explainability, advancing the state-of-the-art in heterogeneous GNN explanations.

### ML-based Antibody Design and Optimization

July 2024 – Sept 2024

- **Advanced Antibody Design:** Leveraged LLMs to design antibodies using bidirectional contextual information, enabling precise sequence generation.
- **Integrated Optimization Framework:** Employed a diffusion-based method to co-optimize antibody sequences and structures, achieving measurable improvements in binding affinity and specificity by 10.85%.
- **Species-Specific Innovations:** Pioneered a co-design approach for species-specific antibodies, identifying optimal binding sites and advancing the precision of therapeutic antibody development.

### Graph Neural Networks for Anomaly Detection

Dec 2023 – Apr 2024

- **Modeling Sensor States as Graphs:** Represented sensor state features in Cyber-Physical Systems as graph structures to effectively capture and model their relationships.
- **Improved Detection Accuracy:** Demonstrated significant improvements in detecting anomalies by leveraging the graph-based approach, contributing to more robust and reliable system monitoring.

## Research on Heterogeneous Graph Transformer

June 2023 – Sept 2023

- **Transformer-Based Framework:** Designed a Transformer-based learning framework tailored for heterogeneous graphs, enhancing representation learning performance and scalability in complex graph structures.
- **Improved Contextual Understanding:** Proposed a novel sampling strategy that can identify nodes playing a critical role in distinguishing classes and ensures that the sampled node sequences contain diverse heterogeneous semantics.

## Heterogeneous Graph Link Prediction

Mar 2023 – June 2023

- **Novel Link Prediction Method:** Developed a mutual information-based method for link prediction in heterogeneous graphs, leveraging self-supervised learning to improve performance.
- **Advancing Self-Supervised Techniques:** Demonstrated the potential of self-supervised learning in heterogeneous graph settings, contributing to more accurate and efficient graph link prediction frameworks.

## Heterogeneous Hypergraph Neural Network

June 2022 – Feb 2023

- **Unified Relation Modeling:** Integrated low-order pairwise relations and high-order complex semantics to accurately represent heterogeneous hypergraphs.
- **Structural Information Learning:** Incorporated structural information learning, enhancing the model's ability to capture intricate relationships within hypergraphs.

## WORK EXPERIENCE

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### MindRank | 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.

## SELECTED HONORS

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- **Gold Medal.** China International College Students' Innovation Competition 2024. Oct 2024
- **First Class Scholarship.** Hangzhou Dianzi University. Oct 2024
- **Champion.** Yunzhenxin Cup Mathematical Modeling Competition. June 2022

## SKILLS

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

## OTHER RELATED EXPERIENCE

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**Conference Reviewer:** The Thirteenth International Conference on Learning Representations (ICLR 2025)

**Conference Attendance:** Poster on The 33rd International Joint Conference on Artificial Intelligence (IJCAI 2024)

**Teaching Assistant:** Artificial Intelligence and Machine Learning, 2023