



#### DOCTORAL RESEARCH

# "Explaining and Designing the Message Passing Mechanism in Graph Neural Networks"

Research Significance: This research investigates the fundamental mechanisms in complex neural network computations by leveraging graph drawing strategies, randomness analysis, and reduced-order modeling strategies. These mechanisms are important as they govern the understanding, design, and application of artificial intelligence algorithms. The current popular explainability research theory can only provide limited insight into these mechanisms. In much of my research, I look to expose and exploit combinatorial, geometric, and random structures in machine learning problems to learn and verify various properties of deep learning models from the data and the algorithm framework to yield reduced-order models explainable and general. In short, this research is skeptical of the existing AI technology.

**Research Progress**: The progress of all my work is as follows (The contents of the doctoral dissertation are marked with an asterisk):

· Explaining and designing graph neural networks.

--\*Completion: 100% for explaining GNNs

--\*Completion: 100% for designing new GNN framework

-- Completion: 30% for distributed GNNs

· Explaining and optimizing of attention mechanism.

--\*Completion: 100% for graph attention-- Completion: 20% for Transformer attention

· Explaining and optimizing "X-Norm" (e.g., BatchNorm) (The theoretical part is verified and almost completed.)

-- Completion: 60%

What is Transformer? A perspective from graph generation and alignment.

-- Completion: 20%

### **PUBLICATIONS**

- I. Xue Li, "Retelling the Story of X-Normalization", (In writing).
- Xue Li and Yuanzhi Cheng, "Tired of Over-smoothing? Stress Graph Drawing Is All You Need!", IEEE TPAMI (In review).
- Xue Li and Yuanzhi Cheng, "Understanding the Message Passing in Graph Neural Networks via Power Iteration Clustering", Neural Networks, 140, pp. 130-135, 2021.
- 4. Xue Li and Yuanzhi Cheng, "Irregular Message Passing Networks", Knowledge-Based Systems, 257, 2022.
- 5. Xue Li, "Directed LPA: Propagating Labels in Directed Networks", Physics Letters A, 8(383), 732-737, 2019.
- 6. Xue Li, "Growth Curve based Label Propagation Algorithm for Community Detection", Physics Letters A, 21(383), 2481-2487, 2019.
- 7. Xue Li and Xindan Gao, "A Collaborative Filtering Recommendation Algorithm Based on Theme Mining", Chinese Mini-Micro Computer Systems, 39(04):664-667, 2018.

### **EDUCATION**

2019 – 2023 Doctor of Computer Science
 School of Computer Science and Technology
 Harbin Institute of Technology

 2015-2017 Master of Computer Science
 School of Computer Science and Technology
 Northeast Forestry University

2010 – 2015 **Bachelor of Computer Sciences**Network Engineering

Qingdao Technological University

#### **AWARDS**

2012 Outstanding Pilot Trainee
Hafei Aviation Industry Group Co., Ltd

2015 Faculty of Computer Science Master's Scholarship
Northeast Forestry University

2017 Outstanding Master's Thesis Award Northeast Forestry University

Youth Scientific Research Progress Award
Harbin Institute of University

## ACTIVITIES & SOCIETIES

PROJECT
Business Plan at Hafei Aviation Group
AR Aviation Tourism Project Design – 2018

CONFERENCES
Oral Presentation at the Annual NFU
Retelling the Story of GNN – 2020

POSTERS
Poster at the Meeting of Swarm Agents Club
Attention is Not Quite All You Need – 2021

#### OUTLOOK FOR FUTURE RESEARCH

I will complete my Ph.D. in Computer Science by September 2023. Now, I am applying for a teaching job or postdoctoral position. I began my studies (B.S.) at the Qingdao Technological University in Network Engineering and continued with a Masters's (M.S.) in Computer Science, studying recommendation systems and graph theory at the Northeast Forestry University (Summa Cum Laude). During 2017-2019, I worked as a helicopter pilot at the Aviation Industry Corporation of China, Ltd. (AVIC). We flew helicopters (AS-350B2) for forest protection, fire prevention, geological exploration, aerial photography, and other tasks. I also led an AR aviation tourism project in 2018. In this role, I spent time working as a prototype engineer, aeronautical system modeler, and flying data analyst. Currently, I am pursuing research at the intersection of interpretable artificial intelligence and complex network dynam-