Zhiqiang ZHONG

POSTDOCTORAL RESEARCHER · PH.D. IN COMPUTER SCIENCE

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"Down to earth while aiming high."

Research Interests

Graph Machine Learning, Knowledge-augmented Machine Learning, Drug Discovery, Social Networks Analysis, Knowledge Graph.

Education

Ph.D. in Computer Science	*Belval, Luxembourg*
UNIVERSITY OF LUXEMBOURG	*04.2018 - 04.2022*
Master in Finance	*Paris, France*
PARIS DAUPHINE UNIVERSITY (PARIS SCIENCES ET LETTRES UNIVERSITY, PSL)	*09.2016 - 12.2017*
Engineer Degree (Master) in Data Science	*Cergy, France*
EISTI	*09.2015 - 11.2017*
Bachelor in Mathematics	*Qingdao, China*
CHINA UNIVERSITY OF PETROLEUM	*09.2011 - 07.2015*

Employment

Postdoctoral Researcher	*Aarhus, Denmark*
AARHUS UNIVERSITY	*05.2022 - Now*
Doctoral Researcher	*Belval, Luxembourg*
UNIVERSITY OF LUXEMBOURG	*04.2018 - 04.2022*

Projects

Eurostars Eureka: AAVanguard *Aarhus, Denmark*
POSTDOCTORAL RESEARCHER *05.2022 - 05.2024*

- A new artificial intelligence platform for the creation of next-generation AAV capsids for Gene Therapy.
- Predicting protein properties and designing new proteins with desired properties; Investigating gene expression manners and operating genetic medicines.

FNR-COVID19: PandemicGR *Belval, Luxembourg*
MAIN CONTRIBUTOR *05.2020 - 11.2020*

- In-depth analysis of pandemic information dynamics, based on a dataset collected from Twitter users with locations labelled in Greater Region of Luxembourg.
- Publicly available at `https://satoss.uni.lu/projects/pandemicgr/`

FNR-Pride: SP2: Security and Privacy in Social Networks *Belval, Luxembourg*
DOCTORAL RESEARCHER *04.2018 - 04.2022*

- Studying security and privacy issues in social networks, including link prediction and attribute inference, by integrating techniques from different fields, such as graph machine learning and information security.

Service

PC Member: ICDE 2025, SocInfo 2020, AICONF 2023, SocialNLP @TheWeb 2021-2024.
Awarded Reviewer: KDD 2025.
Reviewer: KDD 2021-2025, ECML-PKDD 2020-2023, ICLR 2025, TheWebConf 2021-2024, WSDM 2023, TKDD, TKDE, Artif. Intell., DMKD, TMLR, Elsevier-Neurocomputing.

Awards

11.2024 *Supervisor* **of Runner-up MSc Thesis for the IT Speciale Prisen**, IDA IT - Driving IT 2024.   *Denmark*

Grants

EuroHPC AI and Data-Intensive Applications Access Call

ACCEPTED   *2024*

EuroHPC Benchmark Access Call

ACCEPTED   *2024*

Young International Academics (YIA) - Marie Sklodowska Curie Action (MSCA) Program   *Luxembourg*

ACCEPTED   *2024*

Publications

*: Equal contributions; ⋆: Corresponding author.

PEER-REVIEWED PUBLICATIONS

1. **Zhiqiang Zhong**, Davide Mottin. Exploring Graph Structure Comprehension Ability of Multimodal Large Language Models: Case Studies. *Learning on Graphs Conference (LoG)*. (2024).

2. **Zhiqiang Zhong**⋆, Davide Mottin. Efficiently Predicting Mutational Effect on Homologous Proteins by Evolution Encoding. *European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML-PKDD)*. (2024).

3. **Zhiqiang Zhong**, Kuangyu Zhou, Davide Mottin. Harnessing Large Language Models as Post-hoc Correctors. *The Annual Meeting of the Association for Computational Linguistics (ACL)*. (2024).

4. Yi Wei Cheng, **Zhiqiang Zhong**, Jun Pang, Cheng-Te Li. Hierarchical Bipartite Graph Convolutional Network for Recommendation. *IEEE Computational Intelligence Magazine (CIM)*. (2024).

5. Ninghan Chen, Xihui Chen, **Zhiqiang Zhong**, Jun Pang. Bridging Performance of X (formerly known as Twitter) Users: A Predictor of Subjective Well-Being During the Pandemic. *ACM Transactions on the Web*. (2024).

6. **Zhiqiang Zhong**, Yangqianzi Jiang, Davide Mottin. On the Robustness of Post-hoc GNN Explainers to Label Noise. *Learning on Graphs Conference (LoG)*. (2023).

7. Marc Christiansen*, Lea Villadsen*, **Zhiqiang Zhong**, Stefano Teso, Davide Mottin. How Faithful are Self-Explainable GNNs? *Learning on Graphs Conference (LoG)*. (2023).

8. **Zhiqiang Zhong**, Davide Mottin. Knowledge-augmented Graph Machine Learning for Drug Discovery: From Precision to Interpretability. *ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD)*. (2023).

9. Ninghan Chen, Xihui Chen, **Zhiqiang Zhong**, Jun Pang. A Tale of Two Roles: Exploring Topic-specific Susceptibility and Influence in Cascade Prediction. *Journal of Data Mining and Knowledge Discovery (DMKD) - Journal Track of ECML-PKDD*. (2023).

10. **Zhiqiang Zhong**, Cheng-Te Li, Jun Pang. Hierarchical Message-Passing Graph Neural Networks. *Journal of Data Mining and Knowledge Discovery (DMKD) - Journal Track of ECML-PKDD*. (2023).

11. **Zhiqiang Zhong**, Guadalupe Gonzalez, Daniele Grattarola, Jun Pang. Unsupervised Network Embedding Beyond Homophily. *Transactions on Machine Learning Research (TMLR)*. (2022).

12. **Zhiqiang Zhong**, Cheng-Te Li, Jun Pang. Multi-grained Semantics-aware Graph Neural Networks. *IEEE Transactions on Knowledge and Data Engineering (TKDE)*. (2022).

13. **Zhiqiang Zhong**, Sergey Ivanov, Jun Pang. Simplifying Node Classification on Heterophilous Graphs with Compatible Label Propagation. *Transactions on Machine Learning Research (TMLR)*. (2022).

14. Ninghan Chen, Xihui Chen, **Zhiqiang Zhong**, Jun Pang. The Burden of Being a Bridge: Analysing Subjective Well-being of Multilingual Users during the COVID-19 Pandemic. *European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML-PKDD)*. (2022).

15. **Zhiqiang Zhong**, Cheng-Te Li, Jun Pang. Personalised Meta-path Generation for Heterogeneous Graph Neural Networks. *Journal of Data Mining and Knowledge Discovery (DMKD) - Journal Track of ECML-PKDD*. (2022).

16. Ninghan Chen, Xihui Chen, **Zhiqiang Zhong**, Jun Pang. Exploring Spillover Effects for COVID-19 Cascade Prediction. *Journal of Entropy*. (2022).

17. Ninghan Chen, Xihui Chen, **Zhiqiang Zhong**, Jun Pang. From #Jobsearch to #Mask: Improving COVID-19 Cascade Prediction with Spillover Effects. *In Proceedings of the International Conference on Advances in Social Network Analysis and Mining (ASONAM)*. (2021).

18. Ninghan Chen, **Zhiqiang Zhong**, Jun Pang. An Exploratory Study of COVID-19 Information on Twitter in the Greater Region. *Journal of Big Data and Cognitive Computing*. (2020).

19. **Zhiqiang Zhong**, Yang Zhang, Jun Pang. NeuLP: An End-to-end Deep-learning Model for Link Prediction. *In Proceedings of the International Conference on Web Information Systems Engineering (WISE)*. (2020).

20. **Zhiqiang Zhong**, Yang Zhang, Jun Pang. A Graph-based Approach to Explore Relationship between Hashtags and Images. *In Proceedings of the International Conference on Web Information Systems Engineering (WISE)*. (2019).

PUBLIC DATASETS

1. Ninghan Chen, Xihui Chen, **Zhiqiang Zhong**, Jun Pang. GR-EGO COVID-19 TWITTER DATASET. *IEEE DataPort. (2022)*.

PAPERS SUBMITTED/UNDER REVISION

1. **Zhiqiang Zhong**⋆⋆, Simon Sataa-Yu Larsen*, Haoyu Guo*, Tao Tang*, Kuangyu Zhou, Davide Mottin. Automatic Annotation Augmentation Boosts Translation between Molecules and Natural Language.

2. **Zhiqiang Zhong**, Kuangyu Zhou, Davide Mottin. Benchmarking Large Language Models for Molecule Prediction Tasks.

3. **Zhiqiang Zhong**⋆, Anastasia Barkova, Davide Mottin. Knowledge-augmented Graph Machine Learning for Drug Discovery: A Survey.

Teaching

Guest Lecture for Data Mining Msc. Students

AARHUS UNIVERSITY   *05.2024*

• Lecture title: Leveraging Large Language Models for Molecule Prediction Tasks

Msc. and Bsc. Thesis Advisor

AARHUS UNIVERSITY   *02.2024-06.2024*

• Towards Robust Post-hoc Graph Neural Network Explainers.
• Cross-Domain Pre-Training of Graph Neural Networks for Spatial-Temporal Data.
• Large Language Model-augmented Synthetic Graph Generation. (**Runner-up for the IT-speciale prisen from IDA IT**)
• Large Language Model augmented pre-training of Graph Neural Networks.

Msc. Research Project Supervisor

AARHUS UNIVERSITY AND RICE UNIVERSITY   *05.2023-08.2023*

• Evaluation of Post-hoc Graph Neural Network Explainers.

Guest Lecture for Data Science Msc. Students

AALBORG UNIVERSITY   *04.2023*

• Lecture title: Knowledge-augmented Graph Machine Learning for Drug Discovery.

Msc. Thesis Advisor

AARHUS UNIVERSITY   *02.2023-06.2023*

• Evaluation and implementation of Self-Explainable GNN models
• Ship Classification with Graph Neural Networks

Msc. Thesis Advisor

AARHUS UNIVERSITY   *10.2022-03.2023*

• Anti-money Laundering in Mobile Money using Data Mining Techniques

Guest Lecture for Data Mining Msc. Students

AARHUS UNIVERSITY   *05.2022*

• Lecture title: Hierarchical Message-passing Graph Neural Networks

Msc. Thesis Advisor

UNIVERSITY OF LUXEMBOURG   *02.2021-08.2021*

• Comparison of Graph Neural Networks in Euclidean and Hyperbolic Space

Teaching Assistant for Distributed Systems

UNIVERSITY OF LUXEMBOURG

09.2019 - 02.2022

Teaching Assistant for Introduction to IT Security

UNIVERSITY OF LUXEMBOURG

09.2018-02.2019