Linlin Jia

Ph.D.

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Employment History

2023-2024.1 — **Postdoctoral researcher at the University of Bern, Switzerland**.
I work at the Pattern Recognition Group (PRG) on graph-based machine learning theory and its applications.

2021-2022 — **Postdoctoral researcher at INSA Rouen, Normandie Université, France**.
I work at the COBRA lab (Chimie Organique et Bioorganique - Réactivité et Analyse), applying graph machine learning methods to the Optimization of Polymers Using Sustainable SYnthesis (OCTOPUSSY). This is a collaborative work with the LITIS lab, Université Normandie, and the Centre for Sustainable and Circular Technologies, University of Bath.

2021 — **Study engineer at Université de Rouen, France**.

Education

2017-2021.7 — **Ph.D. in Computer Science, INSA Rouen, Normandie Université, France**.
I worked at the LITIS lab (Laboratoire d'informatique, de traitement de l'information et des systèmes) with the research subject: Machine learning and pattern recognition in chemoinformatics. Problematics addressed by my thesis consist of tackling open problems lying at the interface between graphs and machine learning methods, including applying graph kernels and graph edit distances within chemoinformatics and building new pre-image methods for graphs.

2014-2017 — **M.Sc. in Software Engineering, Xian Jiaotong University, China**.

2010-2014 — **B.S. in Information Engineering, Xian Jiaotong University, China**.

Research Interests

- **Machine learning on graphs (graph kernels, graph edit distances, GNNs, etc)**.
- **Graph machine learning in computational chemistry and chemoinformatics**.
- **Knowledge embedding in graphs**.
- **Generation and pre-image problems on graphs**.

Summary of Publications

Journals — **4** papers in international journals

Conferences — **3** papers in international conferences and workshops with proceedings

Preprints — **1** preprint paper

Patents — **1** patent

See the appendix for the full publication list.

Libraries

- `graphkit-learn`: A Python package on graph kernels, graph edit distances, and graph pre-image problem. [homepage]

Research Grants

Under Evaluation

- **Bridging Graph Spaces: Novel Algorithms and Their Applications**.
  Funding agency: Swiss National Science Foundation (SNSF)
  Starting date: -
  Duration in months: 24
  Budget requested: CHF 304,824 ($\approx$ USD 347,722)
  Description: I am the applicant for this grant.

Completed

2023 **Open Round 2023/2, Support for Young Academics**.
  Funding agency: Early Career Scientists Committee of the Faculty of Science at the University of Bern
  Starting date: November 1, 2023
  Duration in months: 2
  Budget approved: CHF 3,100 ($\approx$ USD 3,541)
  Description: This project invites a young academic for a short visit. I am the applicant for the grant and the host of the academic. We predict molecular energies using multi-scale machine learning methods and graph neural networks based on Interacting Quantum Atoms (IQA) scheme.

Projects

2023-2024 **Novel State-of-the-Art Graph Matching Algorithms**.
This project is funded by the Swiss National Science Foundation (SNSF). In the project, I work on the graph matching problem, develop novel graph matching algorithms, and explore their applications. I have published one conference article [C23].

2021-2023 **The project OCTOPUSSY and 2 other projects**.
OCTOPUSSY (Original Computational Techniques for the Optimization of Polymers Using Sustainable SYnthesis) was a collaborative project between the COBRA lab, the LITIS lab, Université Normandie and Centre for Sustainable, and Circular Technologies, University of Bath. I was one of the key contributors in the project, where I applied graph machine learning methods to the optimization of polymers. I was also a main participant of 2 other projects lying in the interdiscipline of machine learning and computational chemistry. I have submitted one journal article [PP23].

2018-2021 **The grant APi**.
The grant APi (Apprivoiser la Pré-image) is funded by the French national research agency (ANR) for research of the pre-image in machine learning for structured data. I worked on pattern recognition in discrete structured spaces. I have published three journal articles [J21, J22a, J22b], two workshop articles [W21a, W21b], and a library available online on GitHub (github.com/jajupmochi/graphkit-learn).

2014-2017 **Research on Service-oriented Programmable Control and Scheduling Scheme for Software Defined Network**.
I applied extreme learning machine to predict network mobility and published a patent about it [P1].

2014 **The Citi Financial Innovation Application Competition**.
We developed a multi-dimension dynamic credit evaluation system based on big data. I participated in the design and implementation of the system, including the database, the website, and the application on Android. We won the national third prize.

Research Experience

Nov 2023	**ACPR 2023**.
	○ An oral presentation on paper [C23].
Jan 2021	**S+SSPR Workshops 2020**.
	○ Two video presentations on papers [W21a] and [W21b]. [video1] [video2] [link]
Sep 2020	**2020 online CSC-Seminar in DE. and Fr**.
	○ Presenting a work: *A graph pre-image method based on graph edit distances*. [slides] [award]
2018	**Machine Learning Summer School 2018 Madrid**.
	○ 54-hour courses.
	○ A Machine Learning in the Industry session.
	○ Presenting a poster at the poster session. [poster]
2016	**Summer Program at the National University of Singapore**.
	○ Main courses: Biometrics in Depth, Computational Thinking and Community Detection in Large Graphs. I learned basic algorithms concerning pattern recognition, image processing, big data, community detection, and graph theory, and finished a project that used a cluster method to find out the relationships between a specific disease and possible micro RNAs.
	○ I received A's for both courses.

Teaching Activities

2022	Unofficially co-supervising a bachelor's thesis from the Renmin University of China.

Honors and Awards

2022	Associated member of the LITIS lab.
2017-2021	Scholarship of China Scholarship Council (CSC) for Ph.D. candidate for 42 months. Funding approved: EUR 54,600 ($\approx$ USD 63,882).
2015-2016	Honor of Outstanding Graduate Student.
2014	The National Third Prize of the Citi Financial Innovation Application Competition.
2012	The Second Prize of Chinese Mathematical Contest in Modeling.
2011-2013	"Siyuan" Scholarship of Xi'an Jiaotong University.

Skills

Programming	**Strong programming ability with Python, C++, Cython, and MATLAB**.
Interdiscipline	**Experience with chemistry softwares such as Gaussian, RDKit, DeepChem**.
Languages	**Fluent in Chinese and English, French on B2 level**.
	○ English test TOEFL IBT in October 2016, I scored 103 out of 120.
	○ French test TCF in June 2017, I scored 400 out of 600.
	○ Worked as a translator and proofreader volunteer in the Khan Academy simplified Chinese translation team from 2020 to 2023, and translated/proofread more than 100,000 words. [intro]
Hobbies	**Dancing, Hiking**.

Publications

[PP23] **Linlin Jia**, Éric Brémond, Larissa Zaida, Benoit Gaüzère, Vincent Tognetti, and Laurent Joubert. **Predicting Redox Potentials by Graph-Based Machine Learning Methods**. ChemRxiv. 2023. [doi] (Submitted to Journal of Computational Chemistry.)

[C23] **Linlin Jia**, Xiao Ning, Benoit Gaüzère, Paul Honeine, and Kaspar Riesen. **Bridging Distinct Spaces in Graph-based Machine Learning**. Asian Conference on Pattern Recognition (ACPR), 2023. [pdf] [code]

[J23] Xiao Ning, **Linlin Jia**, Yongyue Wei, Xi-An Li, and Feng Chen. **Epi-DNNs: Epidemiological Priors Informed Deep Neural Networks For Modeling COVID-19 Dynamics**. Computers in biology and medicine. 2023. [doi]

[J22b] **Linlin Jia**, Vincent Tognetti, Laurent Joubert, Benoit Gaüzère and Paul Honeine. **A Study on the Stability of Graph Edit Distance Heuristics**. Electronics, 2022. [preprint] [doi]

[J22a] **Linlin Jia**, Benoit Gaüzère, and Paul Honeine. **Graph Kernels Based on Linear Patterns: Theoretical and Experimental Comparisons**. Expert Systems with Applications, 2021. [preprint] [code] [doi]

[J21] **Linlin Jia**, Benoit Gaüzère, and Paul Honeine. **graphkit-learn: A Python Library for Graph Kernels Based on Linear Patterns**. Pattern Recognition Letters, 2021. [preprint] [code] [doi]

[W21b] **Linlin Jia**, Benoit Gaüzère, and Paul Honeine. **A Graph Pre-image Method Based on Graph Edit Distances**. Proceedings of IAPR Joint International Workshops on Statistical techniques in Pattern Recognition (SPR 2020) and Structural and Syntactic Pattern Recognition (SSPR 2020). 2021. [preprint] [video] [slides]

[W21a] **Linlin Jia**, Benoit Gaüzère, Florian Yger and Paul Honeine. **A Metric Learning Approach to Graph Edit Costs for Regression**. Proceedings of IAPR Joint International Workshops on Statistical techniques in Pattern Recognition (SPR 2020) and Structural and Syntactic Pattern Recognition (SSPR 2020). 2021. [preprint] [video] [slides]

[P16] Qu Hua, Zhao Jihong, Wu Jinkang, **Jia Linlin**, etc., **A Kind of Name Data Network Mobility Switching Method Predicted Using ELM**: China, CN106376041B[P]. [patent]