Yingfang Yuan

I am a Research Fellow (Postdoc) working with Professors Wei Pang and Lynne Baillie in the School of Mathematical and Computer Sciences at Heriot-Watt University. My research interests include inter/multi-disciplinary AI, metascientific AI, and deep learning, with a particular focus on graph neural networks. Additionally, I have entrepreneurial experience, leveraging AI techniques to address real-world problems.

PERSONAL DETAILS

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EDUCATION

- Feb 2020 - June 2024, **Funded PhD in Computer Science**, the School of Mathematical and Computer Sciences, **Heriot-Watt University**, UK (transfer from Aberdeen University).
  Thesis title: Fast Hyperparameter Optimisation of Graph Neural Network for Molecular Property Prediction.

- Oct 2018 - Dec 2019, **Funded PhD in Computer Science**, the School of Natural and Computing Sciences, **Aberdeen University**, UK (transfer to Heriot-Watt University).

- Sep 2016 - Nov 2017, **MSc in Big Data and High-Performance Computing (2:1)**, Department Of Computer Science, **Liverpool University**, UK.
  Thesis title: Musikalisches Würfelspiel and Data Visualisation (Grade: 71).

- Sep 2013 - Sep 2014, **Visiting student**, Department of Computer Science, **Chaoyang University of Technology**, Taiwan.

- Sep 2012 - Sep 2015, **Diploma in Software Engineering (Grade: 81.74)**, Department of Computer Science, **Chengdu Neusoft University**, Sichuan, China.

EMPLOYMENT HISTORY

- April 2022 - April 2025, **Research Associate (Full-time Postdoc)**, EPSRC-funded project PRIME, **Heriot-Watt University**. Undertaking a range of data mining and machine learning approaches on public and project datasets to identify harms arising from discriminatory processes in digital services used by minority ethnic individuals, with the aim of promoting fairness.

  - We proposed a generic approach to quantify cross-sectoral discrepancies in user experience between different groups of individuals using latent class analysis.
  - We proposed the use of Graph Neural Networks to model geodemographic data in order to support the decision-making processes of policymakers and stakeholders.
  - We have developed PRIME Technical Toolkit (`https://primetoolkit.co.uk/`).
  - This project is shortlisted for Principal's Research Impact and Engagement Awards at Heriot-Watt: Influence.
  - 3 posters, see `https://www.primecommunities.online/posters`.
  - 1 published paper and 4 papers under review.

GRANT

- **Principle Investigator** - "Graph Neural Networks for Recommendation System with Fairness and Safety", EPSRC IAA, Total Value: £8,690.72, April 2023- June 2023.

AWARD

- Principal's Research Impact and Engagement Awards (Sustainable Futures), Project: Circular Chemical Economy (UKRI funded), Heriot-Watt University, 2024.

- The PRIME project work was awarded "Best Presentation", 10th International Conference on Signal Processing, Title: Quantifying Discrepancies in Online User Experiences and Modelling Geodemographic Data with Graph Neural Networks: Some Results from the PRIME Project, 2024.

RESEARCH METRIC

- h-index: 6, i10-index: 4

- Total number of publications: 10; Total number of papers under review: 6.

SELECTED PUBLICATIONS

* means equal authorship

1. Song, J.*, **Yuan, Y.*,** Chang, K., Xu, B., Xuan, J. and Pang, W., 2024, Exploring public attention in the circular economy through topic modelling with twin hyperparameter optimisation. *Energy and AI*, 100433.

2. **Yuan, Y.**, Wang, W., Li, X. and Pang, W., 2024, Evolving Molecular Graph Neural Networks with Hierarchical Evaluation Strategy. In *Proceedings of the Genetic and Evolutionary Computation Conference* (pp. 1417-1425).

3. Song, J.*, **Yuan, Y*.** and Pang, W., 2024, July. SAIS: A Novel Bio-Inspired Artificial Immune System Based on Symbiotic Paradigm. In *Proceedings of the Genetic and Evolutionary Computation Conference Companion* (pp. 2115-2118).

4. **Yuan, Y.***, Yang, Z.*, Xu, Y.*, Zhan, S., Bai, H. and Chen, K., 2023. FACE: Evaluating Natural Language Generation with Fourier Analysis of Cross-Entropy. *Thirty-seventh Conference on Neural Information Processing Systems (NeurIPS 2023)*.

5. Wang, W., Moreau, N.G., **Yuan, Y.**, Race, P.R. and Pang, W., 2019. Towards machine learning approaches for predicting the self-healing efficiency of materials. *Computational Materials Science, 168*, pp.180-187.

6. **Yuan, Y.**, Wang, W. and Pang, W., 2021, July. Which hyperparameters to optimise? an investigation of evolutionary hyperparameter optimisation in graph neural network for molecular property prediction. In *Proceedings of the Genetic and Evolutionary Computation Conference Companion* (pp. 1403-1404).

7. **Yuan, Y.**, Wang, W. and Pang, W., 2021, June. A systematic comparison study on hyperparameter optimisation of graph neural networks for molecular property prediction. In *Proceedings of the Genetic and Evolutionary Computation Conference* (pp. 386-394).

8. **Yuan, Y.**, Wang, W. and Pang, W., 2021, June. A genetic algorithm with tree-structured mutation for hyperparameter optimisation of graph neural networks. In *2021 IEEE Congress on Evolutionary Computation* (pp. 482-489). IEEE.

ACADEMIC SERVICE

- Oct 2022 - Now, Funding Reviewer ∼ REPHRAIN, National Research Centre on Privacy, Harm Reduction and Adversarial Influence Online, UKRI.

- Journal Reviewer ∼ Information Science; IEEE Transactions on Emerging Topics in Computational Intelligence; Complex & Intelligent Systems; Journal of Heuristics; Applied Artificial Intelligence; Information Processing and Management.

- Conference Reviewer ∼ ICLR; AAAI; LOG; ICME; IJCNN; ICCV; ACAIT.

TEACHING AND SUPERVISION EXPERIENCE

- Course Developer ∼ F91DM Data Mining and Machine Learning & F91AI Artificial Intelligence (First UK Coursera MSc Online Course), Heriot-Watt University, Oct 2024 - Now.

- Teaching ∼ F90AM Advanced Machine Learning (3 Lectures), Heriot-Watt University, Feb 2025 - Feb 2025.

- Supervisor/Co-supervisor ∼ Undergraduate, Postgraduate, and PhD students, Heriot-Watt University, 2023 - Now.

- Guest Lecturer ∼ Exploring Graph Neural Networks: Techniques and Applications, Heriot-Watt University, Oct 2024.

- Guest Lecturer ∼ Graph Neural Networks: Methods, Applications, and Challenges, Heriot Watt University, Oct 2023.

- Teaching Assistant ∼ F20ML Statistical Machine Learning, Heriot-Watt University.

- Teaching Assistant ∼ F20BC/F21BC Bioinspired Computation, Heriot-Watt University.

- Teaching Assistant ∼ CS551G Data Mining and Visualisation, Aberdeen University.

- Data Science Coach ∼ Data Lab Innovation Week 2020.

ADMINISTRATIVE EXPERIENCE

- Vice President ∼ Chinese Students and Scholars Association, Heriot-Watt University, Sep 2023 - Now.

- Technical Director ∼ Digital Currency Society, University of Liverpool, Nov 2017 - Sep 2018.

PROJECT EXPERIENCE

- **Researcher** ∼ EPSRC 'Digital Circular Chemical Economy', Feb 2023 - April 2025.
  - The project focuses on a radical change to chemical manufacturing with a view to effective step changes in environmental sustainability and in circularity of materials.
  - We conducted multi-objective optimisation for topic modelling to explore public attention related to the circular economy.
  - We used latent class analysis to explore the attitudes of various groups toward environment-friendly detergent products.

- **Research Programmer** (part-time) ∼ NERC 'Explainable Artificial Intelligence approaches to understand and communicate spatial and temporal patterns of toxic chemicals', Feb 2022 - March 2022.
  - I successfully identified the most crucial factors affecting soil toxicity by using an Explainable AI (XAI) approach.

- **Research Assistant** (part-time) ∼ EPSRC 'Manufacturing Immortality', June 2021 - July 2021.
  - I contributed to the development of self-healing materials by applying machine learning approaches to predict molecular properties.

- **Research Assistant** (part-time) ∼ EPSRC 'Low Carbon Jet Fuel', Nov 2020 - Dec 2020.
  - I applied topic modeling approaches to analyse relevant texts, determining the attitudes and actions of stakeholders.

SKILLS

Languages: English (professional), Chinese (native)
Programming Skills: Python (advanced), C (intermediate), Java(intermediate), HTML+CSS (intermediate), Markdown(advanced), LaTeX(advanced)
Operation System: Windows (advanced), Linux(advanced)

ACADEMIC REFEREE

1. Prof. Wei Pang, MACS, Heriot-Watt University, w.pang@hw.ac.uk.

2. Dr. John Woodward, Head of Computer Science, Loughborough University, j.woodward@lboro.ac.uk.