Yingfang Yuan

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I am a Research Fellow (Postdoctoral Researcher) in the BCML Lab, School of Mathematical and Computer Sciences, Heriot-Watt University, working with Prof. Wei Pang.

Research Interests

Fields: Machine Learning; Deep Learning; Artificial Intelligence.
Topics: Agentic AI; Multi-Agent Systems; Graph Neural Networks; AutoML; Inter/Multi-disciplinary AI.

Education

- **Heriot-Watt University** *Feb. 2020 - Jun. 2024*
  (Funded) PhD in Computer Science, viva successfully defended in 2023 Edinburgh, UK
  - **Thesis**: Fast Hyperparameter Optimisation of Graph Neural Network for Molecular Property Prediction.
    Supervisor: Prof. Wei Pang; Prof. Mike Chantler; Prof. George M. Coghill
- **University of Aberdeen** *Oct. 2018 - Dec. 2020*
  (Funded) PhD in Computer Science (Transfer to Heriot-Watt University) Aberdeen, UK
- **University of Liverpool** *Sep. 2016 - Nov. 2017*
  MSc in Big Data and High-Performance Computing Liverpool, UK
- **Chaoyang University of Technology** *Sep. 2013 - Sep. 2014*
  Visiting Student Taiwan, China
- **Chengdu Neusoft University** *Sep. 2012 - Jun. 2015*
  Diploma in Software Engineering Sichuan, China

Experience

- **Heriot-Watt University** *Edinburgh, UK*
  Research Fellow (Postdoc, starting during the PhD writing-up year) Apr. 2022 – Present
  - PRIME (Protecting Minority Ethnic Communities Online) is a UKRI-funded 3-year project (2022-2025, ∼£3.34M).
  - The project aims to improve understanding of Minority Ethnic (ME) communities' online experiences, particularly in accessing key services related to health, social housing, and energy.
  - Proposed a generic approach using latent class analysis to quantify cross-sectoral discrepancies in user experience across groups.
  - Applied graph neural networks to model geodemographic data and support decision-making for policymakers and stakeholders.
  - Developed the PRIME Technical Toolkit (primetoolkit.co.uk).

Selected Publications

∗ means corresponding author, † means equal contribution

[1]] Yang, Z., Xu, D., Pang, W. and **Yuan, Y***., 2025. Script: Graph-Structured and Query-Conditioned Semantic Token Pruning for Multimodal Large Language Models. *Submitted to TMLR*.

[2]] Yang, Z., Song, J., Song, S., Pang, W. and **Yuan, Y***., 2025. MERMAID: Multi-perspective Self-reflective Agents with Generative Augmentation for Emotion Recognition. *Conference on Empirical Methods in Natural Language Processing (EMNLP 2025)*.

[3]] Liu, Z., Li, Y., Xu, Y., Wang, Y., **Yuan, Y**. and Yang, Z., 2025. Evaluating Text Generation Quality Using Spectral Distances of Surprisal. *Conference on Empirical Methods in Natural Language Processing (EMNLP 2025)*.

[4]] Yang, Z†., **Yuan, Y**†., Jiang, X., An, B. and Pang, W., 2025. InEx: Hallucination Mitigation via Introspection and Cross-Modal Multi-Agent Collaboration. *Submitted to AAAI 2026*.

[5]] Yang, Z., Pang, W. and **Yuan, Y***., 2025. X^{R}: Cross-Modal Agents for Composed Image Retrieval. *Submitted to WWW 2026*.

[6]] **Yuan, Y**†., Chen, K†., Riziv, M., Baillie, L. and Pang, W., 2025, Quantifying the Cross-sectoral Intersecting Discrepancies within Multiple Groups Using Latent Class Analysis Towards Fairness. *International Joint Conference on Neural Networks (IJCNN 2025) (Oral)*.

[7]] 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.

[8]] **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).

[9]] Yang, Z†., **Yuan, Y**†., Xu, Y†., Zhan, S., Bai, H. and Chen, K., 2023. FACE: Evaluating Natural Language Generation with Fourier Analysis of Cross-Entropy. *Advances in Neural Information Processing Systems (NeurIPS 2023), 36*, pp. 17038-17056.

[10]] 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.

[11]] **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).

[12]] **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).

[13]] **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.

PROJECTS

- **Engineering and Physical Sciences Research Council - Digital Circular Chemical Economy, £1.1M** *Feb. 2023 - Apr. 2025*
  Researcher
  ◦ Examined public attention on the circular economy and group attitudes toward environment-friendly detergent products through multi-objective topic modelling and latent class analysis.
- **Natural Environment Research Council - Explainable Artificial Intelligence Approaches to Understand and Communicate Spatial and Temporal Patterns of Toxic Chemicals, £7K** *Feb. 2022 - March. 2022*
  Research Programmer
  ◦ Identified key factors influencing soil toxicity using an Explainable AI (XAI) approach.
- **Engineering and Physical Sciences Research Council - Manufacturing Immortality, £2.69M** *Jun. 2021 - Jul. 2021*
  Research Assistant
  ◦ Contributed to the development of self-healing materials by applying machine learning to predict molecular properties.
- **Engineering and Physical Sciences Research Council - Low Carbon Jet Fuel, £1.8M** *Nov. 2020 - Dec. 2020*
  Research Assistant
  ◦ Applied topic modelling to analyse texts and identify stakeholder attitudes and actions.

GRANT

◦ **Graph Neural Networks for Recommendation System with Fairness and Safety**, *Apr. 2023 - Jun. 2023*
Principle Investigator, total value: £8,690.72, EPSRC IAA.

AWARDS

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

◦ **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*

Teachning and Supervision

- **Course Developer** *Oct. 2024 - present*
  Data Mining and Machine Learning & Artificial Intelligence (Coursera MSc Online Course), Heriot-Watt University
- **Lecturer** *Feb. 2025 - Feb. 2025*
  F90AM Advanced Machine Learning, Heriot-Watt University
- **Supervisor/Co-supervisor** *2023 - present*
  Undergraduate, Postgraduate, and PhD students, Heriot-Watt University
- **Guest Lecturer** *Oct 2024 and Oct 2023*
  Exploring Graph Neural Networks: Techniques and Application
- **Teaching Assistant** *2020 - 2022*
  F20ML Statistical Machine Learning, F20BC/F21BC Bioinspired Computation, Heriot-Watt University
- **Teaching Assistant** *2018 - 2020*
  CS551G Data Mining and Visualisation, Aberdeen University.

Skills And Services

- **Programming Languages:** Python, C, Java, HTML+C, Latex
- **Languages:** Mandarin (Native), English (Proficiency)
- **Operation System:** Windows (advanced), Linux (advanced)
- **Reviewer Services:**

  Conference: ICLR; AAAI; LOG; ICME; IJCNN; ICCV; ACAIT.

  Journal: Information Science; npj Artificial Intelligence; IEEE Transactions on Emerging Topics in Computational Intelligence; Complex & Intelligent Systems; Journal of Heuristics; Applied Artificial Intelligence; Information Processing and Management.
- **Data Science Coach:** Data Lab Innovation Week 2020.
- **Vice President:** Chinese Students and Scholars Association, Heriot-Watt University, Sep 2023 - present.
- **Funding Reviewer:** REPHRAIN, £8.6 million three-year UKRI Research Centre of Excellence; UKRI Metascience Research Grants.

Academic Referee

1. Prof. Wei Pang, MACS, Heriot-Watt University, w.pang@hw.ac.uk.
2. Prof. John Woodward, Head of MACS (Dubai), Heriot-Watt University, j.woodward@hw.ac.uk.