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. In addition, I am leading the development AI and Machine Learning modules for Heriot-Watt's MSc Online Coursera course.

Expertise and 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. 2019*
  (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 (Nominated Postdoc with Global Talent Visa, 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).
  - Course Developer and Lecturer - F91DM Data Mining and Machine Learning & F91AI Artificial Intelligence, First UK Coursera MSc Online Course, Heriot-Watt University.

Selected Publications

∗ means corresponding author, † means equal contribution

[1] Yang, Z., Yang, Z., Zhan, S., Yue, T., Pang, W. and **Yuan, Y**.*, 2026. SVAgent: Storyline-guided Long Video Understanding via Cross-modal Multi-agent Collaboration. *Accepted by Conference on Computer Vision and Pattern Recognition 2026.* **CCF A, CORE A***

[2] Yang, Z., Wang, X., Xu, D., Zhang, Y., Chen, K., Pang, W. and **Yuan, Y**.*, 2026. Do Vision and Text Cues Exhibit Evidential Coupling? Compositional Multimodal Reasoning in Unified Foundation Models. *Submitted to International Conference on Machine Learning 2026*.

[3] Yang, Z., Xu, D., Pang, W. and **Yuan, Y**.*, 2025. Script: Graph-Structured and Query-Conditioned Semantic Token Pruning for Multimodal Large Language Models. *Transactions on Machine Learning Research*.

[4] Yang, Z., Song, J., Song, S., Pang, W. and **Yuan, Y**.*, 2025. MERMAID: Multi-perspective Self-reflective Agents with Generative Augmentation for Emotion Recognition. *In Proceedings of the 2025 Conference on Empirical Methods in Natural Language Processing* (pp. 24650-24666). **CORE A***

[5] Liu, Z., Li, Y., Xu, Y., Wang, Y., **Yuan, Y**. and Yang, Z., 2025. Evaluating Text Generation Quality Using Spectral Distances of Surprisal. *In Findings of the Association for Computational Linguistics: EMNLP 2025* (pp. 2444-2463). **CORE A***

[6] Yang, Z.†, **Yuan, Y**.†, Jiang, X., An, B. and Pang, W., 2025. InEx: Hallucination Mitigation via Introspection and Cross-Modal Multi-Agent Collaboration. *Accepted by AAAI 2026*. **CCF A, CORE A***

[7] Yang, Z., Pang, W. and **Yuan, Y**.*, 2025. X^R: Cross-Modal Agents for Composed Image Retrieval. *Accepted by The Web Conference 2026*. **CCF A, CORE A***

[8] Yang, Z., Song, J., Luo, Z., Yang, Z., Xu, Y., Lan, J., Zhang, Y., Pang, W., Song, S. and **Yuan, Y**.*, 2025. ReChar: Revitalising Characters with Structure Preserved and User-Specified Aesthetic Enhancements. *In Proceedings of the SIGGRAPH Asia 2025 Technical Communications* (pp. 1-5). **CORE A***

[9] **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. *In 2025 International Joint Conference on Neural Networks (IJCNN)* (pp. 1-10). IEEE. (Oral). **CCF C, CORE B**

[10] 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. **Q2**

[11] **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). **CCF C, CORE A**

[12] 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. **CCF A, CORE A***

[13] **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). **CORE A**

[14] **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). **CCF C, CORE A**

[15] **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. **CORE B**

[16] 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.

PROJECTS

- **Agentic AI for Causality Rules in Green Hydrogen Certificate Markets, £7K** *Jan. 2026 - Apr. 2026*
  Co-investigator
- **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

◦ **Gold Medal**
2025 iGEM Competition, Team: OUC-China. *2025*

◦ **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 and Lecturer** *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*
2 Undergraduate, 1 Postgraduate, and 1 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; CVPR; LOG; ICME; IJCNN; ICCV; ACAIT.

Journal: Information Science; npj Artificial Intelligence; IEEE Transactions on Emerging Topics in Computational Intelligence; Transactions on Parallel and Distributed Systems; 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.
∗ £4 million UKRI Metascience AI Early Career Fellowships.

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.