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 responsible for developing 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. 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).
  ○ Course Developer - 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., 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] 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. *SIGGRAPH ASIA 2025*.

[7] **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)*.

[8] 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.

[9] **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).

[10] 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.

[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.

[14] 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

- **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.