

Xi He

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Research Profile

My research develops exact and interpretable machine-learning methods for high-stakes decision-making. I combine combinatorial optimization, computational geometry, and constructive algorithm design to obtain formal optimality guarantees for linear models, decision trees, and neural networks. My future programme will develop scalable, dependable machine learning algorithms and causal-identification tools with transparent, explicit guarantees.

Employment and Education

Postdoctoral Researcher, School of Computer Science, Peking University Oct. 2025–Present

Research on formal specification and verification of C programs. Supervisor: Prof. Zhenjiang Hu.

PhD in Computer Science, University of Birmingham Dec. 2021–Apr. 2025

Thesis: *Recursive Optimization: Exact and Efficient Combinatorial Optimization Algorithm Design Principles with Applications to Machine Learning*. Supervisor: Prof. Max A. Little.

- Developed exact algorithmic frameworks for intractable combinatorial optimization problems in machine learning, examples including 0-1 loss classification, neural-network empirical-risk minimization, and decision trees.

BEng in Mechanical Engineering, Zhejiang Normal University Sept. 2017–Jun. 2021

Selected Publications

Deep-ICE: The first globally optimal algorithm for empirical risk minimization of two-layer maxout and ReLU networks

Xi He, Yi Miao, Max A. Little ICLR 2026

Presents the first provably correct algorithm for empirical-risk minimisation of two-layer ReLU and maxout networks under 0–1 loss. The method has polynomial worst-case complexity when the input dimension and number of hidden neurons are fixed, and is implemented in CUDA for small instances.

[Paper](#) | [Code](#)

An efficient, provably optimal, practical algorithm for the 0–1 loss linear classification problem

Xi He, Max A. Little ICLR 2026

Presents a solver-independent exact algorithm based on geometric enumeration for 0–1 loss linear classification, with $O(N^{D+1})$ worst-case time complexity and trivially parallelizable.

[Paper](#) | [Code](#)

Proper decision trees: An axiomatic framework for solving optimal decision tree problems with arbitrary splitting rules

Xi He, Max A. Little Preprint; under review

Introduces a novel framework that first define decision trees through axioms, and then proves that a decision tree satisfies the axiom has a unique K -permutation representation. This characterisation yields a *generic exact dynamic-programming solver for arbitrary splitting rules and objectives*, including depth and leaf-size constraints.

[arXiv:2503.01455](#)

Optimal hypersurface decision trees

Xi He Preprint; under review

Introduces the first exact algorithm for constructing optimal decision trees with hypersurface splits. The framework unifies axis-parallel, hyperplane, and polynomial-hypersurface splits, and design a vectorizable, hardware-friendly algorithm to support efficient GPU parallelization.

[arXiv:2509.12057](#)

Additional Publications and Preprints

Functional design of efficient and parallelizable combinatorial generators using convolution

Xi He, Zhenjiang Hu, Max A. Little

Preprint; under review

[arXiv:2507.03980](https://arxiv.org/abs/2507.03980)

Polymorphic dynamic programming by algebraic shortcut fusion

Max A. Little, **Xi He**, Ugur Kayas

Formal Aspects of Computing, 2024

Vol. 36, no. 2, Article 11. doi:10.1145/3664828

Foundational theory for optimal decision tree problems. I. Algorithmic and geometric foundations

Xi He

Preprint

[arXiv:2509.11226](https://arxiv.org/abs/2509.11226)

Teaching and Supervision Experience

Co-supervisor, MSc Research Project, University of Birmingham

2023–2024

Co-supervised an MSc student on theoretical and experimental aspects of the 0–1 loss linear-classification problem.

Teaching Assistant, School of Computer Science, University of Birmingham

2022–2025

Led tutorials, practical sessions, office hours, and formative assessment across postgraduate and undergraduate modules.

- **Artificial Intelligence and Machine Learning (PGT)** (2024–2025): tutorials and practical sessions for approximately 600 MSc students, focusing on combinatorial algorithms and discrete mathematics in machine learning.
- **Mathematical Foundations of Artificial Intelligence and Machine Learning** (2024–2025): tutorials, office hours, coursework design, and weekly feedback for 300 second-year students; topics included probability, linear algebra, optimization, and foundational machine learning algorithms.
- **Functional Programming and Artificial Intelligence** (2023–2024): Haskell labs and weekly Q&A.
- **Data Structures and Algorithms** (2022–2023; 2023–2024): tutorials for a 500-student first-year module, covering algorithm design and analysis, sorting, searching, and data structures.

Invited Talks

An efficient, provably optimal, practical algorithm for the 0–1 loss linear classification problem

13 June 2023

Invited presentation, *Advances in Data Science and AI Conference 2023*, University of Manchester, UK.

Academic Service

Reviewer (Main Reviewer : Top Reviewer), Conference on Neural Information Processing Systems (NeurIPS).

Reviewer, International Conference on Learning Representations (ICLR).