



Xiaotian Liu

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Summary

Ph.D. candidate specializing in **AI for Science** with experience in neural operators, iterative refinement, and flow-based models. Extensive experience training large-scale models on multi-GPU clusters with massive scientific datasets (ERA5 weather, turbulent flows, active matter). Published and accepted work spans neural operators for scientific computing (**ICML 2026 Spotlight, top 2.2%**), ensemble learning optimization theory (**NeurIPS 2024**), and multi-modal contrastive learning (**IEEE TPAMI 2022**).

Education

Dartmouth College, Ph.D. in Computer Science	Sept. 2023 – Present
• Advisor: Dr. Yaoqing Yang Focus: AI4Science, Neural Operators, Scientific ML	
Wake Forest University, M.S. in Computer Science	Sept. 2020 – May 2023
• GPA: 4.0/4.0, Advisor: Dr. Gray Ballard	
Wake Forest University, B.S. in Mathematics and Computer Science	Sept. 2016 – May 2020
• GPA: 3.68/4.0, <i>Magna Cum Laude</i>	













Technical Skills

Languages: Python, MATLAB, C++, Java, LaTeX

Frameworks & Tools: PyTorch, TensorFlow, Open MPI, Slurm, Hugging Face

Data Processing: NumPy, Pandas, Scikit-learn, SciPy, Matplotlib

Selected Publications

1. X. Liu, S. Shang, X. Wang, P. Ren, Y. Yang, "Iterative Refinement Neural Operators are Learned Fixed-Point Solvers: A Principled Approach to Spectral Bias Mitigation," *International Conference on Machine Learning (ICML), 2026*.
Spotlight presentation, top 2.2%.
 AI4Science  Neural Operators
2. J. Xiong, X. Liu, R. Wang, Z. Liu, Y. Zhou, Y. Yan, Y. Yang, "RL4RLA: Teaching ML to Discover Randomized Linear Algebra Algorithms through Curriculum Design and Graph-based Search," *International Conference on Machine Learning (ICML), 2026*.
 RL for Algorithms  Randomized Linear Algebra
3. H. Lu, X. Liu, Y. Zhou, Q. Li, K. Keutzer, M.W. Mahoney, Y. Yan, H. Yang, Y. Yang, "Sharpness-diversity tradeoff: improving flat ensembles with SharpBalance," *Advances in NeurIPS 2024*. [paper] | [code]
 Data Selection  Ensemble Learning  Optimization Theory
4. Y. Lin, X. Liu, Y. Gou, J. Bai, J. Lv, and X. Peng, "Dual Contrastive Prediction for Incomplete Multi-View Representation Learning," in *IEEE Transactions on Pattern Analysis and Machine Intelligence, 2022*. [paper] | [code]
 Multi-modal Learning  Contrastive Learning
5. R. Minster, I. Viviano, X. Liu, and G. Ballard, "CP Decomposition for Tensors via Alternating Least Squares with QR Decomposition," in *Numerical Linear Algebra with Applications, 2021*. [paper] | [code]
 HPC  Tensor Decomposition  Numerical Linear Algebra

Research Experience

Graduate Research Assistant, Dartmouth College – Hanover, NH Sept. 2023 – Present
Advisor: Dr. Yaoqing Yang

Iterative Refinement Neural Operators **ICML 2026 Spotlight, top 2.2%**  AI4Science  Neural Operators

- Developed **Iterative Refinement Neural Operators (IRNO)**, an **ICML 2026 Spotlight** method that augments pre-trained neural operators with a shared-weight refinement module to iteratively correct residual errors without re-training the base model
- Established rigorous **convergence guarantees** with geometric convergence rate and iteration complexity $O(\log(\|e_0\|/\epsilon))$ under fixed-point iteration and contraction theory.

- Conducted large-scale distributed training across **12 A100 GPUs** on massive scientific datasets: *turbulent radiative layer 2D*, *active matter system* (51.3 GB), and *ERA5 global weather reanalysis* (4.7 TB)
- Achieved **50-80% relative error reduction** across benchmarks in fluid dynamics, biological active matter, and climate modeling, with strong extrapolation beyond the training horizon and computational efficiency comparable to base models

Autonomous Algorithm Discovery via Reinforcement Learning

ICML 2026  [RL for Algorithms](#)  [Numerical Methods](#)

- Developed **RL4RLA**, an **ICML 2026** framework for discovering interpretable, symbolic randomized linear algebra algorithms from low-level primitives through curriculum-guided search
- **Leveraged Monte Carlo Graph Search (MCGS)** with **DAG-aware exploration (UCD)** to navigate the algorithmic space, effectively handling state transpositions (node merging) and achieving **2-3× reduction** in search cost compared to standard MCTS
- Engineered an **adaptive curriculum generator** to synthesize progressively harder problems, decomposing deep algorithmic search into shallow refinements by progressively introducing numerical failure modes
- Successfully **rediscovered 11 distinct classical algorithms** including sketch-and-precondition solvers (Blendenpik, LSRN), Randomized Kaczmarz, and Newton Sketch, with **10× improvement** in multi-objective performance balancing accuracy, speed, and stability

Sharpness-Diversity Trade-off in Ensemble Learning  [Robust ML](#)  [Optimization Theory](#)  [Ensemble Methods](#)

- Developed theoretical framework using random matrix theory characterizing fundamental trade-off between model sharpness and ensemble diversity, with implications for robust scientific ML systems
- Created SharpBalance algorithm achieving **2.5% accuracy improvement** on out-of-distribution tasks with <1% computational overhead, relevant for robust deployment of ML models in scientific applications

Research Assistant, Wake Forest University – Winston-Salem, NC

May 2021 – Dec. 2022

Advisor: Dr. Gray Ballard

Tensor Decomposition for Scientific Data  [HPC](#)  [Tensor Methods](#)  [Numerical Linear Algebra](#)

- Optimized CP-ALS tensor decomposition algorithms by integrating QR decomposition, enhancing **numerical stability and convergence** for large-scale scientific datasets
- Implemented and benchmarked parallel tensor decomposition methods on HPC clusters, demonstrating improved performance for multi-dimensional scientific data analysis
- **Publication:** Accepted in **Numerical Linear Algebra with Applications**

Professional Experience

Data Scientist Intern, Brunswick Group – Shanghai, China

Sept. 2021 – Dec. 2021

- Applied NLP methods (topic modeling, embeddings, NER) to analyze large-scale unstructured data
- Built automated data pipelines processing multi-source survey and social media data into actionable insights
- Translated complex analyses into strategic recommendations for pharmaceutical clients

Honors & Awards

- **ICML Spotlight Presentation** (Top 2.2%), 2026
- **Best Reviewer Award** (Rated top 4%), AISTATS 2025
- **NeurIPS Scholar Award**, 2024
- Graduate Excellence Award, Wake Forest University, 2021
- Walter Low Tatum Scholarship in Mathematics (Awarded to **2/110** mathematics majors), 2019
- Wake Forest Research Fellowship, 2019

Service & Teaching

Reviewer: ICLR (25, 26), ICML (26), AISTATS (25, 26), ACL (24), IEEE TNNLS, IEEE TPAMI

Teaching Assistant (Dartmouth): Intro to Algorithms (Head TA), Discrete Mathematics

Teaching Assistant (WFU): Data Visualization, Fundamentals of CS, Intro to CS