Sean Xuefeng Du

College of Computing and Data Science
Nanyang Technological University - NTU Singapore
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Academic Position

Assistant Professor

Sept. 2025-Present

Research Interests Nanyang Technological University - NTU Singapore

Reliable machine learning, foundation model reliability, and related applications, specifically I work on algorithm and theory design for:

- Out-of-distribution (OOD) research: designing adaptive and interpretable learning principles that help ML models detect and generalize on OOD samples, such as semantic/covariate shifts, adversarial and noisy samples.
- Reliability of foundation models: understanding the blindspots of Large Language Models (LLMs) and Multimodal LLMs through uncertainty estimation, such as model hallucination detection and mitigation.
- Security of foundation models: Exploring how foundation models can be strengthened against emerging threats, including prompt injection, jailbreak attacks, and distributional vulnerabilities.
- Other interested topics: LLM alignment, Agentic AI.
- Interdisciplinary research: Biometrics, AI-aided cryo-microscopy/protein structural analysis.

Education

Ph.D. candidate in Computer Sciences

Jan. 2021-May 2025

University of Wisconsin-Madison, Madison, WI

- Ph.D. research in reliable machine learning.
- Advisor: Prof. Sharon Y. Li.
- Dissertation: Foundations of Unknown-aware Machine Learning
- Thesis Committee Members: Profs. Jerry Zhu, Robert D. Nowak, Yong Jae Lee.

B. Eng. in Electrical Engineering

Sept. 2016 - Jun. 2020

Xi'an Jiaotong University, Xi'an, China

- Overall GPA: 91.60/100(3.83/4.0), Rank: 1st/170.
- Honors: National Scholarships (2017, 2018).

Awards

- CS Ivanisevic Award in UW-Madison (\$3,000, awarding to one student in the department with research excellence), 2025.
- Rising Stars in Data Science, September, 2024 (worldwide 30 recipients).
- Jane Street Graduate Research fellowship (\$50,000 grant) (6 selected out of 600), April, 2023.
- NeurIPS Scholar Award, Novemeber, 2022.
- CS departmental research fellowship, UW-Madison, September, 2021.
- National Scholarship (2x), Ministry of Education in China, 2017-2018.

Publications

See full list in my google scholar page, I publish under the name "Xuefeng Du". * indicates Equal Contribution

48. Limited Preference Data? Learning Better Reward Model with Latent Space Synthesis

Leitian Tao, **Xuefeng Du**, Yixuan Li.

NeurIPS 2025.

47. How to Steer LLM Latents for Hallucination Detection?

Seongheon Park, **Xuefeng Du**, Min-Hsuan Yeh, Haobo Wang, Yixuan Li. ICML 2025.

46. Understanding Multimodal LLMs Under Distribution Shifts: An Information-Theoretic Approach

Changdae Oh, Zhen Fang, Shawn Im, **Xuefeng Du**, Yixuan Li. ICML 2025.

45. Challenges and Future Directions of Data-Centric AI Alignment

Min-Hsuan Yeh, Jeffrey Wang, **Xuefeng Du**, Seongheon Park, Leitian Tao, Shawn Im, Yixuan Li.

ICML 2025

44. Robust Palmprint Recognition via Multi-stage Noisy Label Selection and Correction

Huikai Shao, Siyu Shi, **Xuefeng Du**, Dan Zeng, Dexing Zhong. IEEE Transactions on Image Processing.

43. Out-of-Distribution Learning with Human Feedback

Haoyue Bai, **Xuefeng Du**, Katie Rainey, Shibin Parameswaran, Yixuan Li TMLR 2025.

42. Safety-Aware Fine-Tuning of Large Language Models

Hyeong Kyu Choi, Xuefeng Du, Yixuan Li

Advances in Neural Information Processing Systems 2024, Safe Generative AI Workshop.

41. HaloScope: Harnessing Unlabeled LLM Generations for Hallucination Detection

Xuefeng Du, Chaowei Xiao, Yixuan Li

Advances in Neural Information Processing Systems 2024, spotlight.

40. Exploring Transition States of Protein Conformational Changes via Out-of-Distribution Detection in the Hyperspherical Latent Space

Bojun Liu, Jordan G Boysen, Ilona Christy Unarta, **Xuefeng Du**, Yixuan Li, Xuhui Huang

Nature Communications, 2024

39. When and How does In-distribution Label Help Out-of-distribution Detection? **Xuefeng Du**, Yiyou Sun, Yixuan Li

International Conference on Machine Learning (ICML) 2024.

38. How does Unlabeled Data Provably Help Out-of-distribution Detection? **Xuefeng Du***, Zhen Fang*, Ilias Diakonikolas, Yixuan Li International Conference on Learning Representations (ICLR) 2024.

37. Feed Two Birds with One Scone: Exploiting Wild Data for Both Out-of-Distribution Generalization and Detection

Haoyue Bai, Gregory Canal, **Xuefeng Du**, Jeongyeol Kwon, Robert D Nowak, Yixuan Li

International Conference on Machine Learning (ICML) 2023.

- 36. Dream the Impossible: Outlier Imagination with Diffusion Models Xuefeng Du, Yiyou Sun, Jerry Zhu, Yixuan Li Advances in Neural Information Processing Systems (NeurIPS) 2023.
- 35. OpenOOD v1.5: Enhanced Benchmark for Out-of-Distribution Detection Jingyang Zhang, Jingkang Yang, Pengyun Wang, Haoqi Wang, Yueqian Lin, Haoran Zhang, Yiyou Sun, **Xuefeng Du**, Kaiyang Zhou, Wayne Zhang, Yixuan Li, Ziwei Liu, Yiran Chen, Hai Li Journal of Data-centric Machine Learning Research.
- 34. Non-parametric Outlier Synthesis Leitian Tao, **Xuefeng Du**, Jerry Zhu, Yixuan Li International Conference on Learning Representations (ICLR) 2023.
- 33. Noise-robust Graph Learning by Estimating and Leveraging Pairwise Interactions

Xuefeng Du, Tian Bian, Yu Rong, Bo Han, Tongliang Liu, Tingyang Xu, Wenbing Huang, Yixuan Li, Junzhou Huang Transactions on Machine Learning Research (TMLR) 2023

- 32. SIREN: Shaping Representations for Detecting Out-of-distribution Objects **Xuefeng Du**, Gabriel Gozum, Yifei Ming, Yixuan Li Advances in Neural Information Processing Systems (NeurIPS) 2022.
- 31. OpenOOD: Benchmarking Generalized Out-of-Distribution Detection Jingkang Yang, Pengyun Wang, Dejian Zou, Zitang Zhou, Kunyuan Ding, Wenxuan Peng, Haoqi Wang, Guangyao Chen, Bo Li, Yiyou Sun, **Xuefeng Du**, Kaiyang Zhou, Wayne Zhang, Dan Hendrycks, Yixuan Li, Ziwei Liu Advances in Neural Information Processing Systems (NeurIPS) Datasets and Benchmarks Track, 2022.
- 30. Unknown-Aware Object Detection: Learning What You Don't Know from Videos in the Wild

Xuefeng Du, Xin Wang, Gabriel Gozum, Yixuan Li IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR) 2022, **oral**.

29. Performance-Aware Mutual Knowledge Distillation for Improving Neural Architecture Search

Pengtao Xie, **Xuefeng Du** IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR) 2022.

- 28. VOS: Learning What You Don't Know by Virtual Outliers Synthesis **Xuefeng Du**, Eric Wang, Mu Cai, Yixuan Li International Conference on Learning Representations (ICLR) 2022.
- 27. Learning Diverse-Structured Networks for Adversarial Robustness Xuefeng Du, Jingfeng Zhang, Bo Han, Tongliang Liu, Yu Rong, Gang Niu, Junzhou Huang, Masashi Sugiyama International Conference on Machine Learning (ICML) 2021.
- 26. How to save your annotation cost for Panoptic Segmentation? **Xuefeng Du**, Chenhan Jiang, Hang Xu, Gengwei Zhang, Zhenguo Li The AAAI Conference on Artificial Intelligence (AAAI) 2021.
- 25. Active learning to classify macromolecular structures in situ for less supervision in cryoelectron tomography

Xuefeng Du, Haohan Wang, Zhenxi Zhu, Xiangrui Zeng, Yi-Wei Chang, Jing Zhang, Eric Xing, Min Xu Bioinformatics, 2021 24. Node Classification on Graphs with Few-Shot Novel Labels via Meta Transformed Network Embedding

Lin Lan, Pinghui Wang, **Xuefeng Du**, Kaikai Song, Jing Tao, Xiaohong Guan Advances in Neural Information Processing Systems (NeurIPS) 2020.

23. A deep biometric hash learning framework for three advanced hand-based biometrics.

Huikai Shao, Dexing Zhong, **Xuefeng Du** IET Biometrics.

22. Few-shot learning for palmprint recognition via meta-siamese network Huikai Shao, Dexing Zhong, **Xuefeng Du**, Shaoyi Du, Raymond NJ Veldhuis IEEE transactions on instrumentation and measurement.

21. Deep distillation hashing for unconstrained palmprint recognition Huikai Shao, Dexing Zhong, **Xuefeng Du**

IEEE transactions on instrumentation and measurement.

20. Cross-domain palmprint recognition via regularized adversarial domain adaptive hashing

Xuefeng Du, Dexing Zhong, Huikai Shao

IEEE Transactions on Circuits and Systems for Video Technology.

19. Effective deep ensemble hashing for open-set palmprint recognition Huikai Shao, Dexing Zhong, **Xuefeng Du** Journal of Electronic Imaging.

18. Cross-domain palmprint recognition based on transfer convolutional autoencoder

Huikai Shao, Dexing Zhong, Xuefeng Du

IEEE International Conference on Image Processing (ICIP) 2019.

17. Continual palmprint recognition without forgetting

Xuefeng Du, Dexing Zhong, Huikai Shao

IEEE International Conference on Image Processing (ICIP) 2019.

16. Building an active palmprint recognition system

Xuefeng Du, Dexing Zhong, Huikai Shao

IEEE International Conference on Image Processing (ICIP) 2019.

15. Low-shot palmprint recognition based on meta-siamese network **Xuefeng Du**, Dexing Zhong, Pengna Li

IEEE International Conference on Multimedia and Expo (ICME) 2019.

14. A hand-based multi-biometrics via deep hashing network and biometric graph matching

Dexing Zhong, Huikai Shao, Xuefeng Du

IEEE Transactions on Information Forensics and Security.

13. Decade progress of palmprint recognition: A brief survey

Dexing Zhong, **Xuefeng Du**, Kuncai Zhong Neurocomputing.

12. Classification in Cryo-Electron Tomograms

Ilja Gubins, Gijs van der Schot, Remco C Veltkamp, Friedrich Förster, **Xuefeng Du**, Xiangrui Zeng, Zhenxi Zhu, Lufan Chang, Min Xu, Emmanuel Moebel, Antonio Martinez-Sanchez, Charles Kervrann, Tuan M Lai, Xusi Han, Genki Terashi, Daisuke Kihara, Benjamin A Himes, Xiaohua Wan, Jingrong Zhang, Shan Gao, Yu Hao, Zhilong Lv, Xiaohua Wan, Zhidong Yang, Zijun Ding, Xuefeng Cui, Fa Zhang

Eurographics 2019.

 Open-set Recognition of Unseen Macromolecules in Cellular Electron Cryo-Tomograms by Soft Large Margin Centralized Cosine Loss Xuefeng Du, Xiangrui Zeng, Bo Zhou, Alex Singh and Min Xu

British Machine Vision Conference (BMVC) 2019, **Spotlight**.

10. Semi-supervised Macromolecule Structural Classification in Cellular Electron Cryo-Tomograms using 3D Autoencoding Classifier

Siyuan Liu, **Xuefeng Du**, Rong Xi, Fuya Xu, Xiangrui Zeng, Bo Zhou and Min Xu

British Machine Vision Conference (BMVC) 2019.

 Efficient Deep Palmprint Recognition via Distilled Hashing Coding Huikai Shao, Dexing Zhong and Xuefeng Du IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR) Workshops 2019.

8. Palm vein recognition with deep hashing network Dexing Zhong, Shuming Liu, Wenting Wang, **Xuefeng Du** Pattern Recognition and Computer Vision 2019.

7. Palmprint recognition using siamese network Dexing Zhong, Yuan Yang, **Xuefeng Du**

13th Conference of Biometric Recognition, CCBR 2018.

Preprints

- VLMGuard: Defending VLMs against Malicious Prompts via Unlabeled Data Xuefeng Du, Reshmi Ghosh, Robert Sim, Ahmed Salem, Vitor Carvalho, Emily Lawton, Yixuan Li, Jack W. Stokes. arXiv preprint arXiv:2410.00296.
- The Ghanaian NLP Landscape: A First Look Sheriff Issaka, Zhaoyi Zhang, Mihir Heda, Keyi Wang, Yinka Ajibola, Ryan De-Mar, Xuefeng Du arXiv preprint arXiv:2405.06818.
- 4. Learning by Passing Tests, with Application to Neural Architecture Search **Xuefeng Du**, Pengtao Xie arXiv preprint arXiv:2011.15102.
- Skillearn: Machine Learning Inspired by Humans' Learning Skills Pengtao Xie, Xuefeng Du, Hao Ban arXiv preprint arXiv:2012.04863.
- Small-Group Learning, with Application to Neural Architecture Search Xuefeng Du, Pengtao Xie arXiv preprint arXiv:2012.12502.
- 1. Towards efficient unconstrained palmprint recognition via deep distillation hashing

Huikai Shao, Dexing Zhong, **Xuefeng Du** arXiv preprint arXiv:2004.03303.

Patents

- VisionGuard: Detecting Multimodal AI Systems from Indirect Prompt Injections (pending)
 Xuefeng Du, Reshmi Ghosh, Vitor Carvalho, Robert Sim, Emily Lawton, Jay Stokes, Lukas Wutschitz, Reshmi Ghosh, Ahmed Salem
- A kind of cross-platform palm grain identification method Dexing Zhong, Huikai Shao, Xuefeng Du, Runzhao Yao

 A kind of vehicle early warning vehicle intelligent system based on multisensor Dexing Zhong, Huikai Shao, Xuefeng Du

Grants TBD

Service *Area Chair for* ICLR 2026

Reviewer for

- NeurIPS, ICML, ICLR
- CVPR, ECCV, ICCV
- WACV, AAAI, IJCAI, MICCAI
- TMLR, Nature Communications, IJCV, IEEE TCSVT, TMM, TIP, TIFS

Department Service

• UM-Madison, Admission Committee, Master for Data Science Program, 2024.

Students and Mentees

Students

Mentees

- 9. Seongheon Park, PhD student at UW-Madison, now PhD student at UW-Madison.
- 8. Sheriff Issaka, undergraduate student at UW-Madison, 2024, now PhD student at UCLA.
- Leitian Tao, undergraduate student at WHU, 2022, now PhD student at UW-Madison.
- 6. Tian Bian, PhD student at CUHK, 2021, now PhD student at CUHK.
- 5. Gabriel Gozum, undergraduate student at UW-Madison, 2021, now perception engineer at Applied Intuition.
- Eric Wang, undergraduate student at UW-Madison, 2021, now research assistant at UCSD.
- 3. Zhenxi Zhu, undergraduate student at BUPT, 2019, now PhD student at Nanjing University.
- 2. Alex Singh, undergraduate student at CMU, 2019, now AI Engineer at Tesla.
- 1. Pengna Li, undergraduate student at XJTU, 2019, now PhD student at XJTU.

Talks

- Talk at University of Queensland, 6/2025
- Talk at MBZUAI, 5/2025
- Talk at Microsoft Research, 4/2025
- Talk at Pennsylvania State University, 3/2025
- Talk at University of Texas at Arlington, 3/2025
- Talk at Oregon State University, 2/2025
- Talk at UC Riverside, Statistics and CS departments, 2/2025 and 3/2025
- Talk at Rochester Institute of Technology, 2/2025
- Talk at Johns Hopkins University, 2/2025
- Talk at OpenAI, 1/2025
- Talk at NTU CCDS, 1/2025

- Talk at HKUST CSE, 12/2024
- Talk at MLOPT Seminar, UW-Madison, 12/2024
- Talk at UCSD, 11/2024
- Talk at Microsoft, 08/2024
- Talk at Jane Street, 04/2023
- Talk at AI talks, 02/2023
- Talk at MLOPT Seminar, UW-Madison, 05/2022
- Talk at Google Research, 01/2022
- Talk at Adobe Research, 12/2021
- Talk at Microsoft Research, 12/2021

Teaching

Teaching Assistant for

- CS762 (graduate course), UW-Madison: Advanced Deep Learning, Fall 2022.
 Designing lectures on topics in trustworthy machine learning, grading students' written papers, holding office hours, leading discussions and answering questions.
- CS540 (undergraduate course), UW-Madison: Intro to AI, Spring 2021.
 Designing lectures on topics in unsupervised learning, deep learning, and reinforcement learning. Preparing all the homework related to the topic of deep learning, and design final exams, guiding students on final projects, holding office hours, and delivering discussion sections.

Research Experience

Research Intern

June 2024 – Sept. 2024

Microsoft Research, Redmond, WA, USA

- Hosts: Dr. Robert Sim, Jay Stokes and Reshmi Ghosh.
- Research on Malicious prompt detection for vision language models

Student Researcher

June 2022 – Sept. 2022

Google Research, Sunnyvale, CA, USA

- Hosts: Dr. Zizhao Zhang, Ting Chen and Han Zhang.
- Research on Open-vocabulary object detection with language models

Research Intern

Mar. 2021 - June 2021

Tencent AI Lab, Shenzhen, China

- Supervised by Dr. Yu Rong and Junzhou Huang.
- Research on Robust graph neural networks against noisy labels .

Research Assistant

Oct. 2020 - Jan. 2021

Department of Computer Science, Hong Kong Baptist University, Hong Kong

- Supervised by Dr. Bo Han.
- Research on Effective network architecture for adversarial robustness.

Research Engineer Intern

Aug. 2020 -Sept. 2020

AI Lab, Bytedance Inc., Beijing, China

- Supervised by Dr. Changhu Wang.
- Research on Fine-grained image classification.

Research Intern Dec. 2019 -July 2020

AI Theory Group, Noah's Ark Lab, Shenzhen, China

- Supervised by Dr. Hang Xu and Chenhan Jiang.
- Research on *Hybrid supervised panoptic segmentation*.

Student Intern July 2018 – Feb. 2020

Department of Computational Biology, CMU, Pittsburgh, PA, USA

- Supervised by Dr. Min Xu and Dr. Haohan Wang.
- Research on *Deep learning for cellular electron cryo-tomography analysis*.

Research Assistant Nov. 2018 – Jun. 2020

Intelligent Networks and Network Security Lab, XJTU, Xi'an, China

- Supervised by Dr. Pinghui Wang.
- Research on Few-shot node classification with meta learning.

Research Assistant Jun. 2017 - Apr. 2019

Institute of Automatic Control, XJTU, Xi'an, China

- Supervised by Dr. Dexing Zhong.
- Research on Machine learning for hand-based biometrics.

Additional Information

Language skills

• Native speakers of Mandarin with professional English speaking capability.

Programming skills

• Proficient with Python, TensorFlow, PyTorch. Familiar with C, Matlab, C++.