# Ya Shi **Zhang**

Machine Learning Researcher

*Location: Chicago, USA  Citizenship: Canada*

(+1) 347-554-4707 | ysz23@cantab.ac.uk | yashizhang.github.io | Google Scholar

## Summary

I am a machine learning researcher passionate about the interplay between theory, empirics, and application. Currently, my interests are in Generative AI, high-dimensional statistics and reinforcement learning, and their downstream applications in agentic AI, drug discovery, and finance.

## Education

### MILA - Quebec AI Institute

*Montreal, Canada*

Ph.D. in Computer Science — *Incoming 08/2025*

- Advisor: Jian Tang and Kirill Neklyudov; Fully funded by NSERC
- Deep learning, generative modeling, reinforcement learning, applications in biology and finance

### Faculty of Mathematics, University of Cambridge

*Cambridge, UK*

M.A.St. in Mathematics (Part III of the Mathematical Tripos), with Honours — *10/2023 - 06/2024*

- Ph.D. level coursework
- Selected awards: College Travel Award (£1000) in 2024
- Declined awards: Computer Science Pre-Doctoral Fellowship (University of Chicago, $40,000) in 2024; Fellowship for Research in Manifold Machine Learning (Nanyang Technological University, S$30,000) in 2024
- Thesis: Sampling from High-dimensional Distributions (Link). Advised by Randolf Altmeyer.

### Courant Institute, New York University

*New York, USA*

B.A. in Mathematics with High Honors, B.A. in Computer Science with High Honors — *09/2019 - 05/2023*

- Selected awards: Alumni Award (Excellence in Research) in 2024; University Honors Scholar in 2023; Dean's List from 2019-2023; Courant Institute SURE Fellowship ($3,500) in 2022; Dean's Undergraduate Reseacrh Fund Recipient (Awarded 3x, $3,000, Top 50 among 400+ candidates) in 2022
- Other awards: 2019 International Baccalaureate Further Mathematics Examination Prize (Top 30 / 180,000+); University of California, Berkeley Pre-Collegiate Scholar in 2018, 2nd out of 30+ in National Team Mathematics Contest in 2018
- Thesis: Computing Interval Range Approximations for Smooth Real Functions with Applications in Real-root Isolation (Link). Advised by Chee Yap.

## Publications

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|---|---|---|
| 2024 | **Mind the GAP: Improving Robustness to Subpopulation Shifts with Group-Aware Priors** , Tim G. J. Rudner, Ya Shi Zhang, Andrew G. Wilson, Julia Kempe. | *AISTATS Oral **(2%)*** |
| 2023 | **On the Robustness of Neural Collapse and the Neural Collapse of Robustness** , Jingtong Su, Ya Shi Zhang, Nikolaos Tsilivis, Julia Kempe. | *NeurIPS Workshop, TMLR* |
| 2023 | **Range Functions of Any Convergence Order and their Amortized Complexity Analysis** , Kai Hormann*, Chee Yap*, Ya Shi Zhang* (Equal Contribution). | *CASC, LNCS* |

## Experiences

### Kempner Institute at Harvard University and Google DeepMind

*Cambridge, USA*

Research Assistant — *12/2024 - Present*

- Advisor: Yilun Du
- Working on the composition and steerability of deep diffusion and flow-matching models

### Toyota Technical Institute at Chicago and University of Chicago

*Chicago, USA*

Research Scientist Intern — *06/2024 – Present*

- Advisor: Jinbo Xu, Yilun Du; Fully funded by MoleculeMind
- Reviewed articles on structure/sequence prediction, enzyme design, enzymatic function prediction, protein-protein/DNA/RNA/small molecule conditional design, and rototranslation-invariant generative models
- Implemented training and fine-tuning algorithms for the RFDiffusion-AllAtom model
- Leading a project on designing a flexible compositional diffusion model for protein sequence design by utilizing the representations of large protein language models with computationally efficient guidance classifiers

### Exact Geometric Computation Group (EGC Group)

*New York, USA*

Research Assistant — *02/2022 – 01/2023*

- Advisor: Chee Yap, Kai Hormann; Fully funded by New York University
- Published "Range Functions of Any Convergence Order and their Amortized Complexity Analysis" with Prof. Chee Yap from the Courant Institute of Mathematical Sciences at NYU and Prof. Kai Hormann from Università della Svizzera Italiana Lugano
- Expanded the Cornelius-Lohner (CL) framework to develop a new method for enclosing the image of a function under an interval with tightness and convergence guarantees
- Searched through numerical analysis literature to prove convergence of our state-of-the-art method
- Contributed to the CORE library for C++ with the new algorithm and optimized the rest of the codebase
- Helped develop the proof for the amortized complexity analysis of the algorithm by examining and generalizing the subdivision algorithm to higher dimensions

### Kempe Lab

*New York, USA*

Research Assistant — *09/2022 – 12/2023*

- Advisor: Julia Kempe, Tim G. J. Rudner, Andrew G. Wilson; Partially funded by New York University
- **Project:** Mind the GAP: Improving Robustness to Subpopulation Shifts with Group-Aware Priors
  - Worked with Prof. Tim G. J. Rudner, Prof. Julia Kempe, and Prof. Andrew G. Wilson on a empirical Bayesian deep learning framework for mitigating dataset subpopulation shifts
  - Reviewed literature on fairness-aware and group-robust machine learning methods and bench-marking metrics and baselines
  - Devised and implemented experiments, ablations, and performance tuning in JAX and PyTorch
  - Accepted as oral presentation (2% acceptance rate) at AISTATS 2024
- **Project:** On the Robustness of Neural Collapse and the Neural Collapse of Robustness
  - Worked with Prof. Julia Kempe and two PhD students on the interplay of adversarial robustness and neural collapse; examined conditions when neural collapse occurs in adversarially robust neural networks
  - Studied the stability and statistical properties of simplices formed in the pen-ultimate neural network layer by training and testing data
  - Devised and implemented experiments in PyTorch for training neural networks with various robust optimization methods to measure neural collapse metrics under unperturbed and perturbed training data
  - Discovered the 'cluster-leaping' phenomenon, and clearly outlined conditions to induce neural collapse
  - Supported by Dean's Undergraduate Research Fund
  - Cited for U.S. Dept. of Defense Air Force research (Topic Number AF24B-T002)

### Government of Canada, Natural Resources Canada

*Ottawa, Canada*

Machine Learning Engineer — *05/2021 - 08/2021*

- Utilized satellite image data to perform heating load estimation in remote Canadian communities
- Fitted random forest, convolutional neural networks, among other models with GIS data to maximize AUROC metric
- Presented solution and suggestions to the minister of the department

## Teaching & Service

2023 **Ethics Reviewer**, Neural Information Processing Systems (NeurIPS) — *New Orleans, USA*

2023 **Courant Tutor**, Courant Institute of Mathematical Sciences — *New York, USA*

## Extracurricular Activity

### Phi Chi Theta Business Fraternity

*New York, USA*

Former Treasurer/Alumni Member — *09/2019 - Present*

- Learned Discounted Cash Flow (DCF), Leveraged Buyout (LBO), SWOT Analysis, Porter's Five Forces, and other key concepts in finance, consulting, and marketing
- Wrote a 50-page start-up business plan, outlining ideas, conducting market analysis, developing partnerships, and building a DCF model to valuate the company with three team members
- Conducted a SWOT analysis of Ferrari and offered advice in attracting potential customers and suggesting ways to boost client retention
- Guided first and second year students, offering career advice, course selection, interview preparation, and internship information

### Quantitative Finance Society

*New York, USA*

Quantitative Analyst – Quant Trading Team — *01/2020 - 06/2023*

- Utilized statistical modeling to take advantage of capital market inefficiencies
- Examined impact of variations of moving averages in mean-reversion trading strategies, using Sharpe ratios as a performance indicator
- Fine-tuned natural language model BERT to perform automated sentiment analysis of online forums to predict price action

### Mathematical Finance Group

*New York, USA*

Co-lead/Mentor – Academic Team — *03/2021 - 06/2023*

- Wrote 7 quantitative interview questions to screen and recruit 10+ members
- Implemented lesson plans for courses such as probability theory, stochastic processes, and option theory, teaching 6+ sophomores
- Instructed second-year students on efficient paper-reading in quantitative finance

## Skills & Interests

**Programming:** Python (PyTorch, JAX), R, C/C++, MATLAB, HPC (Slurm, Singularity, Bash Scripting), Git, LaTeX