Zhiqing Xu

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EDUCATION

Ph.D., Chemical Engineering, University of Toronto (2020 - Present)
  PhD Thesis: *A Deep Learning and GenAI-Guided Directed Evolution Framework for Protein Design*
  Supervisor: *Radhakrishnan Mahadevan, krishna.mahadevan@utoronto.ca*

M.A.Sc, Chemical Engineering, University of Toronto , **cGPA 3.9** (2017 - 2019)
  Thesis: *Deep Learning-Based Biochemical Reaction Pathway Prediction*

B.A.Sc, Chemical Engineering, University of Toronto (2013 - 2017)
  Graduate with Honour

Relevant Courses: Natural Language Processing, Deep Learning in Finance, Cloud-Based Data Analytics, Statistical Methods for Machine Learning, Probability, Applied Stochastic Processes, Time Series Analysis, Mathematical Statistics, Statistical Computation, Database.

Academic Awards:
- Doctoral Completion Award, University of Toronto. (2024, 2025).
- School of Graduate Study (SGS) Award, University of Toronto. (2020, 2023).
- UTEA, University of Toronto Excellence Award. (2017).

SKILLS SUMMARY

Frameworks	PyTorch, TensorFlow, MXNet, NLTK, SpaCy, NodeJS, Apache Spark
Programming	Python, C/C++, JavaScript, HTML5, CSS, SQL, Matlab, R, Bash
DevOps	Bash, Git, Docker, PostgreSQL, MySQL, Databricks
Platforms	Azure, AWS, GCP, Alibaba Cloud
CAD Tools	SolidWorks, Autodesk CFD, Inventor, Blender, AutoCAD

SELECTED PUBLICATIONS

- Xu, Z., Barghout, R. A., Wu, J., Garg, D., Song, Y. S., Mahadevan, R. (2025). **CPI-Pred: A deep learning framework for predicting compound-protein interactions** *Preprint* ⬈

- Barghout, R. A, Xu, Z., Mahadevan, R. (2023). **Advances in generative modeling methods and datasets to design novel enzymes for renewable chemicals and fuels** *Biotechnology*, 84, 103007 ⬈

- Xu, Z., Mahadevan, R. (2022). **Efficient Enumeration of Branched Novel Biochemical Pathways Using a Probabilistic Technique** *Ind. Eng. Chem. Res.*, **61**, 25, 8645–8657 ⬈

- Xu, Z., Wu, J., Song, Y.S., Mahadevan, R. (2022). **Enzyme Activity Prediction of Sequence Variants on Novel Substrates using Improved Substrate Encodings and Convolutional Pooling** *Proceedings of the 16th Machine Learning in Computational Biology meeting*, PMLR, **165**, 78–87 ⬈

- Biz, A., Proulx, S., Xu, Z., Siddartha, K., Indrayanti, A.M., Mahadevan, R. (2019). **Systems biology based metabolic engineering for non-natural chemicals** *Biotechnology advances*, **37**, (6):107379 ⬈

RESEARCH & TECHNICAL EXPERIENCE

Ph.D. Candidate, LMSE Lab, lmse.utoronto.ca (2020 – Present)
University of Toronto

- Built reaction-guided **generative AI (genAI)** models for protein design with discrete denoising diffusion models.
- Developed heterogeneous graph neural networks for compound-protein interaction and reaction property prediction.
- Built deep learning models for protein function prediction using **natural language processing (NLP)** techniques.
- Implemented large-scale sequence representation learning for protein functional annotation.

Research Assistant & M.A.Sc. Student (2017 – 2019)
University of Toronto

- Developed a biochemical pathway design computation tool using autoencoders and graph neural networks.
- Designed deep learning models for molecular property prediction, improving accuracy over SOTA models.

Research Assistant (2016 – 2017)
Southern Ontario Centre for Atmospheric Aerosol Research (SOCAAR)

- Designed and built a device to isolate PM2.5 from street dust, enabling precise elemental composition analysis.
- Conducted air pollution assessments on train emissions, analyzing particulate matter composition and distribution.
- Developed data visualization pipelines for managing and interpreting large-scale environmental datasets.

Engineer Intern (2016 – 2017)
Bombardier Aerospace

- Worked collectively to develop a portable system to evaluate the remaining life of aircraft air filters.
- Performed computational fluid dynamics (CFD) simulations using Autodesk CFD to optimize system design.
- Modeled the measuring system in SolidWorks/Inventor and built a functional prototype.