Chenghui Zhou

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Profile

I am a graduating machine learning PhD student from Carnegie Mellon University. My thesis is on generative models and their applications to discrete structured data, such as molecules, programs, and text. During my time at CMU and industry internships, I have gained hands-on experiences with diffusion models, VAEs, GANs, transformers and RNNs in real world settings.

Education

Ph.D. in Machine Learning – Carnegie Mellon University   April 2024 (Expected)
Thesis Topic: Generative Models and Their Applications to Discrete Structured Data
Advisor: Barnabás Póczos

M.S. in Machine Learning – Carnegie Mellon University   December 2018
Related Coursework: Deep Reinforcement Learning, Probabilistic Graphical Model, Intermediate Statistics, Statistical Machine Learning, Convex Optimization

B.S. in Honours Computer Science – McGill University   May 2016
Minor in Statistics
Advisor: Joelle Pineau

Industry & Research Experience

Applied Scientist Intern   May 2020 – August 2020
CodeGuru team, Amazon Web Service, Inc.

- Leveraging CodeBERT for effective code retrieval from repositories using contrastive learning

Research Intern   May 2018 – August 2018
Predictive Algorithm team, Zoll LifeVest

- Applying sequence modeling techniques for robust classification of cardiac rhythms in ECG segments

Undergraduate Research Assistant   May 2014 – August 2015
Reasoning and Learning Lab, McGill University

- Improving predictions for tracking in robotics by learning a predictive linear Gaussian model

Publications & Working Papers

- **Chenghui Zhou**, Kaushal Gumpula, Barnabás Póczos
  Generating Molecules in 3D at Equilibrium with Equivariant Diffusion Model
  In Progress

- **Chenghui Zhou**, Barnabás Póczos
  Objective-Agnostic Enhancement of Molecule Properties via Multi-Stage VAE
  Submitted to *International Conference on Machine Learning (ICML)*, 2024

- **Chenghui Zhou**, Barnabás Póczos
  Improving Molecule Properties Through 2-Stage VAE
  Machine Learning for Structural Biology Workshop, NeurIPS, 2022.

- **Chenghui Zhou***, Frederic Koehler*, Viraj Mehta*, Andrej Risteski
  Variational Autoencoders in the Presence of Low-Dimensional Data: Landscape and Implicit Bias
  International Conference on Learning Representations (ICLR), 2022.

- **Chenghui Zhou**, Chun-Liang Li, Barnabás Póczos
  Unsupervised Program Synthesis for Images by Sampling without Replacement
  Conference on Uncertainty in Artificial Intelligence (UAI), 2021.

- **Chenghui Zhou**, Chun-Liang Li, Barnabás Póczos
  Unsupervised Program Synthesis for Images Using Tree-Structured LSTM
  Deep Reinforcement Learning Workshop & Learning with Rich Experience Workshop (one of two selected oral presentations) *NeurIPS*, 2019.

- Robin Schmucker, **Chenghui Zhou**, Manuela Veloso
  Multimodal Movement Activity Recognition Using a Robot's Proprioceptive Sensors
  RoboCup Symposium, 2018.

- **Chenghui Zhou**, Manuela Veloso
  Interception in Continuous Space Using Deep Reinforcement Learning
  Submitted to *International Conference on Robotics and Automation (ICRA)*, 2018.

- Michiel de Jong, Kevin Zhang, Travers Rhodes, Aaron Roth, Robin Schmucker, **Chenghui Zhou**, Sofia Ferreira, João Cartucho, Manuela Veloso
  Towards a Robust Interactive and Learning Social Robot
  International Conference on Autonomous Agents and Multiagent Systems (AAMAS), 2018.

- **Chenghui Zhou**, Borja Balle, Joelle Pineau
  Learning Time Series Models for Pedestrian Motion Prediction
  International Conference on Robotics and Automation (ICRA), 2016.

TEACHING

2021	Teaching assistant for **Convex Optimization** (Carnegie Mellon University)
2018	Teaching assistant for **Statistical Machine Learning** (Carnegie Mellon University)
2016	Teaching assistant for **Introduction to Software Systems** (McGill University)
2015	Teaching assistant for **Foundations of Programming** (McGill University)

COMMUNITY SERVICE

2022 – Now	Served as a mentor in the **PhD Peers Program** of Machine Learning Department
2019	Served on the **Retreat Committee** of Machine Learning Department
2018 – 2020	Served as **SCS4ALL Representative** for Machine Learning Department

COMPUTER SKILLS

Languages	Python, Java, C, Matlab, LaTeX
Operating systems	Linux, Windows, OS X
ML packages	PyTorch, Keras, JAX, Tensorflow, Sklearn
Chemistry packages	RDKit, OpenBabel, OpenMM

LANGUAGES

English	Fluent
Chinese	Fluent
French	Elementary

SCHOLARSHIPS & AWARDS

2013 – 2016	**Dean's Honours List** – McGill University Faculty of Science
2015	**Science Undergraduate Research Award** – McGill University
2015	**Emily Ross Crawford Scholarship** – McGill University
2014	**Scholarship for BSc Computer Science Honours Student** – Le Réseau ACTION TI
2013	**Faculty of Science Scholarship** – McGill University