Xiaoyin Chen

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Education

Mila, Université de Montreal — Sept. 2023 – Present
Doctor of Philosophy, Computer Science, Advisor: Prof. Yoshua Bengio — *GPA: 4.00/4.00*

Duke University — Aug. 2021 – May 2023
Master of Science, Computer Science, Advisor: Prof. Sam Wiseman — *GPA: 4.00/4.00*

University of California, Irvine — Sept. 2016 – Mar. 2020
Bachelor of Science, Computer Science, Minor in Statistics — *GPA: 3.94/4.00, Major GPA:3.99/4.00*

Publications & Preprints

Peer-reviewed conference, journal, and workshop

Structure Language Models for Protein Conformation Generation
Jiarui Lu*, **Xiaoyin Chen***, Stephen Zhewen Lu, Chence Shi, Hongyu Guo, Yoshua Bengio, Jian Tang.
International Conference on Learning Representations 2025, https://arxiv.org/abs/2410.18403, 2024.

HarmAug: Effective Data Augmentation for Knowledge Distillation of Safety Guard Models
Seanie Lee, Haebin Seong, Dong Bok Lee, Minki Kang, **Xiaoyin Chen**, Dominik Wagner, Yoshua Bengio, Juho Lee, Sung Ju Hwang.
International Conference on Learning Representations 2025, https://arxiv.org/abs/2410.01524, 2024.

Proof Flow: Preliminary Study on Generative Flow Network Language Model Tuning for Formal Reasoning
Matthew Ho, Vincent Zhu, **Xiaoyin Chen**, Moksh Jain, Nikolay Malkin, Edwin Zhang.
System-2 Reasoning at Scale Workshop at NeurIPS 2024, https://arxiv.org/abs/2410.13224, 2024.

Inference and Verbalization Functions During In-Context Learning
Junyi Tao*, **Xiaoyin Chen***, Nelson F. Liu.
Findings of Empirical Methods in Natural Language Processing (EMNLP) 2024, https://arxiv.org/abs/2410.09349, 2024.

Efficient Causal Graph Discovery Using Large Language Models
Thomas Jiralerspong*, **Xiaoyin Chen***, Yash More, Vedant Shah, Yoshua Bengio.
AGI Workshop at ICLR 2024, https://arxiv.org/abs/2402.01207, 2024.

Learning Consistent Deep Generative Models from Sparse Data via Prediction Constraints
Gabriel Hope, Madina Abdrakhmanova, **Xiaoyin Chen**, Michael C. Hughes, Erik B. Sudderth.
4th Symposium on Advances in Approximate Bayesian Inference, 2022. arxiv.org/abs/2012.06718.

On the Current Failure – But Bright Future – of Topology-driven Biological Network Alignment
Siyue Wang, **Xiaoyin Chen**, Brent J. Frederisy, Benedict A. Mbakogu, Amy D. Kanne, Pasha Khosravi, Wayne B. Hayes.
Advances in Protein Chemistry and Structural Biology: Protein interaction networks, Volume 131.
https://arxiv.org/abs/2204.11999.

Cross-species Prediction of Protein Function by Global Network Alignment
Siyue Wang, **Xiaoyin Chen**, Brent J. Frederisy, Benedict A. Mbakogu, Amy D. Kanne, Pasha Khosravi, Giles R.S. Atkinson, Wayne B. Hayes.
28th Conference on Intelligent Systems for Molecular Biology (protein prediction track), 2020.
https://www.iscb.org/cms_addon/conferences/ismb2020/tracks/functioncosi.

Preprints & Under Review

Aligning Protein Conformation Ensemble Generation with Physical Feedback
Jiarui Lu*, **Xiaoyin Chen***, Stephen Zhewen Lu, Aurelie Lozano, Aurelie Lozano, Vijil Chenthamarakshan, Payel Das, Jian Tang.
Submitted to ICML 2025, 2025.

BM25 Query Augmentation Learned End-to-End
Xiaoyin Chen, Sam Wiseman.
arXiv preprint arXiv: 2305.14087, https://arxiv.org/abs/2305.14087, 2023.

An Early Warning System for Democratic Resilience: Predicting Shocks to Civic Space
Xiaoyin Chen, Jeremy Springman, Erik Wibbels.
Technical report, 2022.

Selected Projects

Interactive Inductive Reasoning May 2024

- Introduced an interactive benchmark that allows agents to propose queries and iteratively refine hypotheses based on feedback from an oracle;
- Built from abstract inductive reasoning tasks, e.g., program synthesis, but the initial observations do not fully specify the underlying rules;
- Leveraged programs as the oracle to provide feedback on agent queries;
- Enhanced the evaluation of LLM reasoning by introducing information-seeking capabilities, in contrast to traditional static evaluations.
- Demonstrated that LLMs achieve higher accuracy in rule induction through active querying compared to a non-interactive environment.

Commonsense Reasoning via Knowledge Infused Text Generation Dec. 2022

- Improved and implemented a general framework for applying arbitrary non-differentiable constraints to text generation inspired by cognitive Dual-System approach;
- Formulated text generation as a tree search problem and applied a modified Monte Carlo Tree Search algorithm;
- Utilized GPT-3 for fact checking to ensure the generated sentences are consistent with commonsense;
- Improved the average constraint satisfaction rate from 90.1% to 98.4% compared to the baseline.

Evaluating and Improving Logical Reasoning Capability with Syllogisms Dec. 2022

- Proposed and implemented a pipeline for automatically generating logical questions without any human labeling;
- Developed an algorithm that samples logical questions in symbolic form by composing all 24 valid syllogisms;
- Written 100+ templates for verbalizing symbolic expressions to ensure the variety of utterances;
- Demonstrated that GPT-3 is unable to consistently infer syllogisms and generalize to a greater depth, even when all rules are given in the prompt;
- Improved logical QA accuracy on a human-written dataset by 3% by pre-training with synthetic data.

Work Experience

Visiting Researcher Nov. 2024 – Present

ServiceNow Research, Montreal, Canada

- Worked on training reasoning models and LLM agents.

Deep Learning Engineer Intern Jul. 2018 – Sept. 2018

Tencent, Guangzhou, China

- Deep learning for semantic matching and information retrieval;
- Implemented and tested 8+ models from related papers;
- Proposed a novel padding method by dynamical expanding;
- Developed a joint model CNN and LSTM that achieved the best performance on the internal dataset.

Teaching Experience

Teaching Assistant

Duke University

- **CS590.05 Spring 2023**: Computational Biology.

Undergrad Tutor & Grader

University of California, Irvine

- **ICS-33 Spring 2017**: Intermediate Programming in Python;
- **ICS-46 Fall 2018**: Data Structure Implementation and Analysis in C++.

Service

Reviewer: ACL, EMNLP, Neurips