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EDUCATION

McGill University & Mila-Quebec AI Institute

Sep, 2022 - Dec, 2024

Master of Science (M.Sc)

GPA: 3.75

Computer Science

Thesis: LEARNING FROM GRAPH-STRUCTURED DATA—ADDRESSING DESIGN ISSUES AND EXPLORING PRACTICAL APPLICATIONS IN GRAPH REPRESENTATION LEARNING

Advised by Guy Wolf & Doina Precup

McGill University & Mila-Quebec AI Institute

Sep, 2018 - May, 2022

Bachelor of Science Honours (B.Sc)

GPA: 3.90

Computer Science (First-Class Honours)

Thesis: IS HETEROPHILY A REAL NIGHTMARE FOR GRAPH NEURAL NETWORKS TO DO NODE CLASSIFICATION?

Advised by William Hamilton

RESEARCH

(1) AI for Protein and Enzyme Engineering

(2) AI for Molecule Design

(3) (Equivariant) Graph Neural Network and Graph Transformer

PUBLICATION & PREPRINT (by year)

2024

EnzymeFlow: Generating Reaction-specific Enzyme Catalytic Pockets through Flow Matching and Co-Evolutionary Dynamics

Submitted to ICLR2025

<https://arxiv.org/abs/TBA>

Hua, C., Liu, Y., Zhang, D., Zhang, O., Luan, S., Yang, K.K., Wolf, G., Precup, D., Zheng, S.

ReactZyme: A Benchmark for Enzyme-Reaction Prediction

38th Conference on Neural Information Processing Systems

<https://arxiv.org/abs/2408.13659>

Hua, C.*, Zhong, B.*, Luan, S., Hong, L., Wolf, G., Precup, D., Zheng, S.

Deep Geometry Handling and Fragment-wise Molecular 3D Graph Generation

Submitted to Nature Machine Intelligence

<https://arxiv.org/abs/2404.00014>

Zhang, O., Huang, Y., Cheng, S., Yu, M., Zhang, X., Lin, H., Zeng, Y., Wang, M., Wu, Z., Zhao, H., Hua, C., Kang Y., Cui, S., Pan, P., Hsieh, CY., Hou T.

ECloudGen: Access to Broader Chemical Space for Structure-based Molecule Generation

Submitted to Nature Machine Intelligence

<https://biorxiv.org/content/10.1101/2024.06.03.597263>

Zhang, O., Jin J., Lin H., Zhang J., Hua, C., Huang Y., Zhao H., Hsieh, CY., Hou T.

Effective Protein-Protein Interaction Exploration with PPIretrieval

38th Conference on Neural Information Processing Systems, AIDrugX

<https://arxiv.org/abs/2402.03675>

Hua, C., Coley, C., Wolf, G., Precup, D., Zheng, S.

Are Heterophily-Specific GNNs and Homophily Metrics Really Effective? Evaluation Pitfalls and New Benchmarks

Submitted to LoG2024

<https://arxiv.org/abs/2409.05755>

Luan, S., Lu, Q., Hua, C., Wang, X., Zhu, J., Chang, XW., Wolf, G., Tang, J.

The Heterophilic Graph Learning Handbook: Benchmarks, Models, Theoretical Analysis, Applications and Challenges

<https://arxiv.org/abs/2407.09618>

Luan, S., Hua, C., Lu, Q., Ma, L., Wu, L., Wang, X., Xu, M., Chang, XW., Precup, D., Ying R., Li, SZ., Tang, J., Wolf, G., Jegelka, S.

2023

MUDiff: Unified Diffusion for Complete Molecule Generation

2nd Learning on Graphs Conference

<https://arxiv.org/abs/2304.14621>

Hua, C., Luan, S., Xu, M., Ying, R., Fu, J., Ermon, S., Precup, D.

When Do Graph Neural Networks Help with Node Classification?

Investigating the Homophily Principle on Node Distinguishability

37th Conference on Neural Information Processing Systems

<https://arxiv.org/abs/2304.14274>

Luan, S., Hua, C., Xu, M., Lu, Q., Zhu, J., Chang, XW., Fu, J., Leskovec, J., Precup, D.

When Do We Need GNN for Node Classification?

12th International Conference on Complex Networks and their Applications

<https://arxiv.org/abs/2210.16979>

Luan, S., Hua, C., Lu, Q., Zhu, Jia., Chang, X. W., Precup, D.

2022

Complete the Missing Half: Augmenting Aggregation Filtering with

Diversification for Graph Convolutional Networks

36th Conference on Neural Information Processing Systems, GLFrontiers (Oral)

<https://arxiv.org/abs/2008.08844>

Luan, S.*, Zhao, M.*, Hua, C.*, Chang, X. W., Precup, D.

Revisiting Heterophily For Graph Neural Networks

36th Conference on Neural Information Processing Systems (Spotlight)

<https://arxiv.org/abs/2210.07606>

Luan, S., Hua, C., Lu, Q., Zhu, Jia., Zhao, M., Zhang, S., Chang, XW., Precup, D.

High-Order Pooling for Graph Neural Networks with Tensor Decomposition

36th Conference on Neural Information Processing Systems

<https://arxiv.org/abs/2205.11691>

Hua, C., Rabusseau, G., Tang, J.

2021

Graph Neural Networks Intersect Probabilistic Graphical Models: A survey

<https://arxiv.org/abs/2206.06089>

Hua, C., Luan, S., Zhang, Q., Fu, J.

Is Heterophily A Real Nightmare For Graph Neural Networks To Do Node Classification?

<https://arxiv.org/abs/2109.05641>

Luan, S.*, Hua, C.*, Chang, XW., Precup, D.

INTERNSHIP

Aureka Biotechnologies

Sep, 2023 - Present

Supervisor: Shuangjia Zheng

Protein and Enzyme Engineering, Generative Model

Mila-Quebec AI Institute

May, 2022 - Dec, 2022

Supervisor: Yoshua Bengio

Generative Flow Network, Molecule Design

Mila-Quebec AI Institute

Jun, 2021 - Jan, 2022

Supervisor: Jian Tang & Guillaume Rabusseau

Graph Neural Network, Tensor Method

Mila-Quebec AI Institute

Dec, 2020 - Apr, 2021

Supervisor: William Hamilton

Graph Neural Network, Heterophily

**HONOR &
AWARD**

Scholarship of FACS-Acuity Project

May, 2022-Present

Ministre de l'conomie et de l'Innovation Canada

ICML2023 Travel Award

July, 2023

Neurips 2022 Scholar Award

Nov, 2022-Dec, 2022

	Scholarship of CIFAR AI chair program	May, 2021-Aug, 2021
	Canadian Institute for Advanced Research	
	Scholarship of Discovery program	May, 2021-Aug, 2021
	Natural Sciences and Engineering Research Council of Canada	
	Funding of Calcul Quebec	May, 2021-Aug, 2021
	Calcul Quebec	
	Funding of Digital Research Alliance of Canada	May, 2021-Aug, 2021
	Digital Research Alliance of Canada	
	Funding of NVIDIA	May, 2021-Aug, 2021
	NVIDIA	
SERVICE	ICML2022, LoG2022, NeurIPS2022 AI4Mat, NeurIPS2022 GLFrontier, ICML2023, NeurIPS2023, KDD2023 PhD Consortium, LoG2023, ICLR2024, ICLR2024 GEM, ICLR2024 AGI, ICML2024, LoG2024, NeurIPS2024, AAAI2025, ICLR2025	Reviewer
	NeurIPS2023 GLFrontier	Area Chair
	LoG2023 Montreal Meetup	Organizer
TEACHING	MGSC695 Teaching Assistant	Summer 2022
	MGSC695 Intro to AI & Deep Learning II TA at McGill, Montreal	
	MGSC673 Teaching Assistant	Winter 2022
	MGSC673 Intro to AI & Deep Learning I TA at McGill, Montreal	
	MATH340 Grader	Winter 2020
	MATH340 Discrete Mathematics grader at McGill, Montreal	