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EDUCATION

Stanford University

Jan, 2025 - Sep, 2025

Visiting Student

Topic: PROTEIN AND RNA ENGINEERING

Advised by Le Cong

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 Doina Precup & Guy Wolf

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 Design

(2) AI for Drug Discovery

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

PUBLICATION & PREPRINT (by topic)

Protein and Enzyme Engineering

EnzymeCAGE: A Geometric Deep Learning Model for Catalytic-Specified Enzyme Retrieval and Function Prediction with Evolutionary Insights

Submitted to Nature Methods

<https://www.biorxiv.org/content/10.1101/2024.12.15.628585v1>

Liu, Y., Hua, C., Zeng, T., Rao, J., Wu, R., Coley, C., Zheng, S.

Reaction-conditioned De Novo Enzyme Design with GENzyme

<https://arxiv.org/abs/2411.16694>

Hua, C.*, Lu, J.*, Liu, Y., Zhang, O., Tang, J., Ying, R., Jin, W., Wolf, G., Precup, D., Zheng, S.

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

Submitted to ICLR2025; 38th Neural Information Processing Systems, AIDrugX

<https://arxiv.org/abs/2410.00327>

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.

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.

Molecule Design

FragGen: Towards 3D Geometry Reliable Fragment-based Molecular Generation
Chemical Science, Royal Society of Chemistry

<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.

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.

Graph Neural Network Architecture

Learning From Graph-Structured Data: Addressing Design Issues and Exploring Practical Applications in Graph Representation Learning

Master Thesis

<https://arxiv.org/abs/2411.07269>

Hua, C.

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.

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.

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.

Graph Neural Network Principle

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

<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.

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.

Graph Neural Networks Intersect Probabilistic Graphical Models: A survey

50th IEEE International Conference on Acoustics, Speech and Signal Processing, 2022

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

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

RESEARCH ROLE	Stanford University <i>Supervisor: Le Cong</i> <i>Protein and RNA Engineering</i>	Jan, 2025-Present
	Harvard & MIT <i>Supervisor: Omar Abudayyeh & Jonathan Gootenberg</i> <i>Protein Evolution, Protein Mutation</i>	Dec, 2024-Present
	Aureka Biotechnologies <i>Supervisor: Shuangjia Zheng</i> <i>Protein and Enzyme Engineering, Generative Model</i>	Sep, 2023-Present
	Mila-Quebec AI Institute <i>Supervisor: Yoshua Bengio</i> <i>Generative Flow Network, Molecule Design</i>	May, 2022-Dec, 2022
	Mila-Quebec AI Institute <i>Supervisor: Jian Tang & Guillaume Rabusseau</i> <i>Graph Neural Network, Tensor Method</i>	Jun, 2021-Jan, 2022
	Mila-Quebec AI Institute <i>Supervisor: William Hamilton</i> <i>Graph Neural Network, Heterophily</i>	Dec, 2020-Apr, 2021
HONOR & AWARD	Scholarship of FACS-Acuity Project Ministre de l'conomie et de l'Innovation Canada	May, 2022-Dec, 2024
	Neurips2024 Scholar Award	Dec, 2024
	ICML2023 Travel Award	Jul, 2023
	Neurips2022 Scholar Award	Dec, 2022
	Scholarship of CIFAR AI chair program Canadian Institute for Advanced Research	May, 2021-Aug, 2021
	Scholarship of Discovery program Natural Sciences and Engineering Research Council of Canada	May, 2021-Aug, 2021
	Funding of Calcul Quebec Calcul Quebec	May, 2021-Aug, 2021
	Funding of Digital Research Alliance of Canada Digital Research Alliance of Canada	May, 2021-Aug, 2021
	Funding of NVIDIA NVIDIA	May, 2021-Aug, 2021
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, LoG2024 Tutorial	Organizer
TEACHING	MGSC695 Teaching Assistant MGSC695 Intro to AI & Deep Learning II TA at McGill, Montreal	Summer 2022
	MGSC673 Teaching Assistant MGSC673 Intro to AI & Deep Learning I TA at McGill, Montreal	Winter 2022
	MATH340 Grader MATH340 Discrete Mathematics grader at McGill, Montreal	Winter 2020