Chenqing (William) Hua

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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 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
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.

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-Dec, 2024
Ministre de lconomie et de lInnovation Canada

Neurips2024 Scholar Award Dec, 2024

ICML2023 Travel Award Jul, 2023

Neurips2022 Scholar Award 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, LoG2024 Tutorial 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