Qi Liu

Interests: AI for Science

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EDUCATION

City University of Hong Kong

*Ph.D. candidate at the **Department of Electrical Engineering**, advisor: Dr. Rosa H. M. Chan*   Sept. 2019 - present

*M.Sc. in **Multimedia Information Technology** summa cum laude*   Sept. 2017 - Oct. 2018

Fuzhou University

*B.Eng. in **Software Engineering***   Sept. 2013 - Jun. 2017

SELECTED PUBLICATIONS (* indicates equal contribution)

AI for Science and Healthcare

Q. Liu, R.H.M. Chan, R. Yu.
The Unreasonable Effectiveness of Pretraining in Graph OOD.
Under review *2023.*

Y. Patra, R.H.M. Chan, **Q. Liu**, D. Thomson, D.H.K. Chow, B. Fuller, R.T.H. Cheung.
Tracking Bilateral Lower Limb Kinematics of Distance Runners on Treadmill using a Single Inertial Measurement Unit
EMBC *2023.*

Q. Liu, Y. Du, F. Feng, Q. Ye, J. Fu.
Structural Causal Model for Molecular Dynamics Simulation [OpenReview].
NeurIPS *2022 AI for Science (AI4Science): Progress and Promises workshop* **(Oral presentation)**.

Q. Liu*, S. Mo*, V.C.K. Cheung, B.M.F. Cheung, S. Wang, P.P.K. Chan, A. Malhotra, R.T.H. Cheung, R.H.M. Chan.
Classification of runners' performance levels with concurrent prediction of biomechanical parameters using data from inertial measurement units [DOI].
Journal of Biomechanics *2020.*

Z. Li, Y.W. Lam, **Q. Liu**, A.Y.K. Lau, H.Y. Au-Yeung, R.H.M. Chan.
Machine Learning-Driven Drug Discovery: Prediction of Structure-Cytotoxicity Correlation Leads to Identification of Potential Anti-Leukemia Compounds [DOI].
EMBC *2020.*

General Deep Learning

Z. Wang*, G. Zhang*, K. Yang, N. Shi, W. Zhou, S. Hao, G. Xiong, Y. Li, M.Y. Sim, X. Chen, Q. Zhu, Z. Yang, A. Nik, **Q. Liu**, C. Lin, S. Wang, R. Liu, W. Chen, K. Xu, D. Liu, Y. Guo, J. Fu.
Interactive Natural Language Processing [ArXiv].
preprint *2023.*

F. Feng*, **Q. Liu***, Z. Peng, R. Zhang, R.H.M. Chan.
Community Channel-Net: Efficient channel-wise interactions via community graph topology [DOI].
Pattern Recognition *2023.*

C. Lan*, F. Feng*, **Q. Liu**, Q. She, Q. Yang, X. Hao, I. Mashkin, K-S. Kei, D. Qiang, V. Lomonaco, X. Shi, Z. Wang, Y. Guo, Y. Zhang, F. Qiao, R.H.M. Chan.
Towards lifelong object recognition: A dataset and benchmark [DOI].
Pattern Recognition *2022.*

Q. Liu, J. B. Palmerston, Q. She, R.H.M. Chan.
System and Method for Rendering An Image.
United States patent *US11,393,144. 2022.*

Q. Liu, F. Feng, C. Lan, R.H.M. Chan.
Va2mass: Towards the fluid filling mass estimation via integration of vision and audio learning [DOI].
ICPR *2021 CORSMAL Challenge of Multi-modal Fusion and Learning For Robotics.*

PROFESSIONAL EXPERIENCES

Department of Computer Science and Engineering, UC San Diego   San Diego, CA

Benchmarking pre-trained GNNs in out-of-distribution (OOD) molecular property prediction   Jan. 2023 - Jun. 2023

- Identified the competitiveness of various pre-trained strategies on molecular graph OOD compared with OOD-tailored methods, on well-known molecular datasets (e.g., DrugOOD, MoleculeNet, and TU datasets);
- Explored the impact of critical factors of the pre-trained models in OOD generalization optimization, including initial learning rates, sample size, etc.;
- Proposed the potential of combining pre-trained models with invariant learning or data augmentation techniques to attain improved OOD generalization performance for molecular datasets.

Beijing Academy of Artificial Intelligence   Beijing, P.R.C.

Designing structural causal method for modeling molecular dynamics (MD)   Mar. 2022 – Sept. 2022

- Proposed an efficient approximation algorithm for modeling molecular dynamics via structural causal models;
- Utilized the auto-encoder model to learn dynamic Bayesian network for modeling the atomic dynamics;
- Achieved the accurate MD prediction, validated over single-chain coarse-grained polymers in implicit solvent simulated via LAMMPS, with extremely long sequence.

School of Data Science, The Chinese University of Hong Kong, Shenzhen Shenzhen, P.R.C.
Exploreing the effectiveness of structural and topological priors for deep learning Mar. 2021 – Aug. 2021
- Proposed to incorporate the small-world topology to deep neural networks, inspired by the efficacy of small-worldness in real-world networks and graphs;
- Designed the algorithm for seamlessly adding the structural prior to layer attention models for deep neural networks and updated the structures progressively;
- Achieved well-performing results in terms of network efficiency and accuracy on standard computer vision benchmarks.

SELECTED AWARDS

Travel Funding. *AI for Science: Progress and Promises workshop at NeurIPS 2022* Dec. 2022
2nd runner-up in CORSMAL Challenge of Multi-modal Fusion and Learning for Robotics. *ICPR 2020* Nov. 2020
Outstanding Graduates Award. *Fuzhou University* Jun. 2017

TEACHING

TA for Electronic Devices & Circuits 2020 Fall
TA for Human Computer Interaction 2021, 2022, 2023 Spring
TA for Introduction to Human Bionics 2021 Fall
Tutor for Croucher Summer Courses in Computational Neuroscience 2019 Summer

ACADEMIC SERVICES

Reviewer for ICBINB Workshop at NeurIPS 2023
Reviewer for IEEE Journal of Translational Engineering in Health and Medicine (JTEHM) 2022, 2023
Reviewer for IEEE Journal of Biomedical and Health Informatics (JBHI) 2022

TECHNICAL SKILLS

Drug Discovery Experience with OpenMM simulation, PyMOL visualization & PDB format
Programming Languages Competent in Python (Pytorch & TensorFlow), experience in C, Java & JavaScript/JQuery
Machine Learning Algorithms for drug discovery, graph neural networks & deep generative models
Data Science SQL