# Yuanqi Du

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# **EDUCATIONS**

George Mason University

**Fairfax, VA** *Aug* 2017 - *May* 2021

B.S. in Computer Science GPA: 4.0/4.0 | Major: 16/18 A+

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**Huaqiao University** *B.S. in Computer Science* 

Xiamen, China Aug 2016 - Jun 2017

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GPA: 4.64/5.00

# **RESEARCH INTERESTS**

Representation Learning; Interpretable Machine Learning; Casual Discovery; Deep Graph Learning; Deep Generative Model; AI for Science (Biology/Chemistry/Physics).

## **PUBLICATIONS**

- \* denotes equal contribution, † denotes corresponding author, <u>mentored students</u> are underlined **Conference Papers**
- Xiaojie Guo\*, **Yuanqi Du**\*, Liang Zhao. Deep Generative Model for Spatial Networks, accepted in KDD 2021 conference.
- Xiaojie Guo, **Yuanqi Du**, Liang Zhao. Property Controllable Variational Autoencoder via Invertible Mutual Dependence, accepted in ICLR 2021 conference.
- Pengbo Liu, Hu Han, Yuanqi Du, Heqin Zhu, Yinhao Li, Feng Gu, Honghu Xiao, Jun Li, Chunpeng Zhao, Xinbao Wu, S. Kevin Zhou, Deep Learning to Segment Pelvic Bones: Large-scale CT Datasets and Baseline Models, accepted in IPCAI 2021 conference, published in IJCARS journal [impact factor 2.473].
- Panneer Selvam Santhalingam, Yuanqi Du, Riley Wilkerson, Al Amin Hosain, Ding Zhang, Parth Pathak, Huzefa Rangwala, and Raja Kushalnagar. Expressive ASL Recognition using Millimeterwave Wireless Signals. IEEE International Conference on Sensing, Communication and Networking (SECON) 2020.
- Yuanqi Du, Nguyen Dang, Riley Wilkerson, Parth Pathak, Huzefa Rangwala, Jana Kosecka. American Sign Language Recognition Using an FMCW Wireless Sensor. AAAI Conference on Artificial Intelligence (AAAI) 2020 (Student Abstract).

## **Journal Papers**

• Taseef Rahman, **Yuanqi Du**, Amarda Shehu. Generative Adversarial Learning of Protein Tertiary Structures, accepted in Molecules journal [impact factor: 3.267].

#### **Workshop Papers**

- Yinkai Wang\*, Kaiyi Guan\*, Aowei Ding\*, **Yuanqi Du**†. Ensemble Machine Learning System for Student Academic Performance Prediction. Educational Data Mining (EDM) 2021, Workshop for Undergraduates (W4U).
- Yuanqi Du, Xiaojie Guo, Amarda Shehu, Liang Zhao. Interpretable Property Controlling Molecule Generation. AAAI 2021 Scientific Discovery with AI (SDA) Workshop, Oral Presentation.
- Yuanqi Du, Xiaojie Guo, Amarda Shehu, Liang Zhao. Interpretable Molecule Generation via Disentanglement Learning. ACM Conference of Bioinformatics and Computational Biology (BCB) Workshops: Computational Structural Biology Workshop (CSBW) 2020.

• Yuanqi Du, Xiaojie Guo, Amarda Shehu, Liang Zhao. From Interatomic Distances to Protein Tertiary Structures with a Deep Convolutional Neural Network. ACM Conference of Bioinformatics and Computational Biology (BCB) Workshops: Computational Structural Biology Workshop (CSBW) 2020.

#### Workshops

Payal Chandak, Yuanqi Du<sup>†</sup>, Tianfan Fu, Wenhao Gao, Kexin Huang, Shengchao Liu, Ziming Liu, Gabriel Spadon, Max Tegmark, Hanchen Wang, Adrian Weller, Max Welling, Marinka Zitnik. AI for Science: Mind the Gaps workshop, with NeurIPS 2021 conference.

#### **Preprints**

- **Yuanqi Du**, Xiaojie Guo, Hengning Cao, Yanfang Ye, Liang Zhao. Spatiotemporal Graph Generative Representation Learning, under review in NeurIPS 2021 conference.
- Xiaojie Guo\*, **Yuanqi Du**\*, Liang Zhao. Interpretable Deep Graph Generation via Information Bottelneck, under review in TKDE journal.
- Xiaojie Guo\*, **Yuanqi Du\***, Liang Zhao. Scalable Deep Generative Models for Spatial Networks, under review in TNNLS journal.
- Yuanqi Du, Xiaojie Guo, Amarda Shehu, Liang Zhao. Interpretable Molecular Graph Generation via Monotonic Constraints, under review in ICDM 2021 conference.
- Yuanqi Du, Quan Quan, Hu Han, S. Kevin Zhou. Where is the disease? Semi-supervised pseudo-normality synthesis from an abnormal image, under review in BMVC 2021 conference.
- Yuanqi Du, Xiaojie Guo, Amarda Shehu, Liang Zhao. Disentangled Representation Learning for Interpretable Molecule Generation, under review in IJMS journal.
- Yuanqi Du, Xiaojie Guo, Hengning Cao, Liang Zhao, et al. GraphGen: A Large-sclae Graph Generative Dataset Collection. In preparation.
- Runsheng Xu\*, Zhengzhong Tu\*, Yuanqi Du\*, Xiao Yu, Jinlong Li, Zibo Meng, Hongkai Yu. ROM-Net: Renovate the Old Memories, under review.
- Xiaojie Guo, **Yuanqi Du**, Sivani Tadepalli, Liang Zhao, Amarda Shehu. Generating Tertiary Protein Structures via Interpretable Graph Variational Autoencoders, under review.
- Quan Quan, Qiyuan Wang, Liu Li, Yuanqi Du, S. Kevin Zhou, CT Film Recovery via Disentangling Geometric Deformation and Photometric Degradation: Simulated Datasets and Deep Models, arXiv preprint arXiv:2012.09491, under review.

#### PROFESSIONAL & RESEARCH EXPERIENCES

The Chinese University of Hong Kong

Hong Kong, China

Research Intern (MM Lab)

Iune 2021 - Present

Topic: Deep Generative Models in Scientific Discovery, Advisor: Bolei Zhou

University of Amsterdam

Amsterdam, Netherlands

Visiting Student (AMLAB & AI4Science)

June 2021 - Present

Topic: Modeling Chemical Systems with Equivariant Neural Nets, Advisor: Max Welling

George Mason University

Atlanta, US

Research Assistant

Feb 2020 - Present

Topic: Deep Graph Learning and Applications, Advisor: Liang Zhao

Microsoft Research Asia

Beijing, China

Research Intern (Machine Learning & Computational Biology Group)

Nov 2020 - May 2021

Topic: Protein Structure Prediction, Advisor: Jianwei Zhu

George Mason University

Fairfax, US

Research Assistant Jan 2020 - May 2021 Topic: Learning Protein Structures and Dynamics, Advisor: Amarda Shehu, Liang Zhao

Chinese Academy of Sciences

Beijing, China

Research Intern (MIRACLE Group) Aug 2020 - Nov 2020

Topic: Medical Image Analysis, Advisors: S. Kevin Zhou, Hu Han

George Mason University

Fairfax, US Research Assistant *Apr* 2019 - May 2020

Topic: Application of Millimeter-wave Radar Signals, Advisor: Parth Pathak

## TEACHING & MENTORING EXPERIENCES

George Mason University Fairfax, US

Research Mentor Aug 2020 - Feb 2021

Topic: Education Data Mining with Focus on Student Performance Prediction

George Mason University Fairfax, US

Aug 2018 - Dec 2019 **Undergraduate Teaching Assistant** 

Courses: Object-oriented Programming, Data Structures, Data Mining

George Mason University Fairfax, US

Peer Mentor Feb 2019 - Dec 2019

Courses: Engineering Courses & Careers Services

# PROFESSIONAL SERVICES

• Reviewer for NeurIPS-W (2021-), KDD (2021-), TKDD (2021-), BMVC (2021-), CIKM (2021-), ICDM (2021-), DLG-KDD (2021-), IRS-KDD (2021-), BioKDD (2021-)

- Co-organize workshops DLG-KDD 2021 (Web Chair), DeepSpatial-KDD 2020/2021 (Web/Publicity Chair)
- Co-organize conferences KDD 2021 (Web Team), AAAI 2021 (Student Technical Team)
- Contribute to the open-source community (e.g. DeepChem, Graph4NLP, GNNBook)

#### AWARDS & ACHIEVEMENTS

MSRA Star of Tomorrow Award	2021
Distinguished Academic Achievement Award	2021
Outstanding Graduate Student	2021
NeurIPS, AIJ AIIDE Travel Award	2020
NSF REU Fellowship	2019-2020
Distinguished Undergraduate Research Award	2019-2020
Distinguished Undergraduate Teaching Assistant Award	2019-2020
GMU OSCAR Fellowship	Summer 2019
Outstanding Undergraduate Teaching Award	2018-2019
• League of Legends Challenger (world top 0.01%)	2016
• StarCraft II GrandMaster (world top 0.2%)	2015

# **VOLUNTEERS & LEADERSHIPS**

- GMU NSF REU Student Mentor 2021
- ICLR, ICML Student Volunteer 2021
- GMU SCAN (Career) Mentor, 2021
- Microsoft Learn Student Ambassador (2021-)
- Student Member of ACM, IEEE, IEEE Computer Society, AAAI, SIAM, ASA Community (2020-)
- Activities: NetBrain Club Research Director

# **MISCELLANEOUS**

•	Coursera Certificates: Machine Learning; Deep Learning; Deep Neural Network with PyT	lorch;
	Probabilistic Graphical Models;	