# Yuanqi Du

#### **EDUCATIONS**

George Mason University

Fairfax, VA B.S. in Computer Science Aug 2017 - May 2021

GPA: 4.0/4.0 | Major: 16/18 A+

**Huaqiao University** Xiamen, China Aug 2016 - Jun 2021 B.S. in Computer Science

GPA: 4.6/5.0

### REPRESENTATIVE PUBLICATIONS

\* denotes equal contribution, † denotes correspondence, full list can be found in personal website including in-submissions.

# **Conference Papers**

- Yuanqi Du\*, Shiyu Wang\*, Xiaojie Guo, et al. GraphGT: Machine Learning Datasets for Graph Generation and Transformation, accepted in NeurIPS 2021 Benchmark and Dataset Track.
- Xiaojie Guo\*, Yuanqi Du\*, Liang Zhao. Deep Generative Model for Spatial Networks, published in KDD 2021.
- Xiaojie Guo, **Yuanqi Du**, Liang Zhao. Property Controllable Variational Autoencoder via Invertible Mutual Dependence, published in ICLR 2021.
- Yuanqi Du, Yinkai Wang, Fardina Alam, Yuanjie Lu, Xiaojie Guo, Liang Zhao, and Amarda Shehu. Deep Latent-Variable Models for Controllable Molecule Generation, accepted in BIBM 2021.

#### **Journals**

• Xiaojie Guo\*, Yuanqi Du\*, Sivani Tadepalli, Liang Zhao, Amarda Shehu. Generating Tertiary Protein Structures via an Interpretative Variational Autoencoder, accepted in Bioinformatics Advances.

#### **Workshop Papers**

- Yuanqi Du, Xian Liu, Shengchao Liu, Jieyu Zhang, Bolei Zhou. Interpreting Molecule Generative Models for Interactive Molecule Discovery, accepted in ELLIS ML4Molecules workshop 2021 (Oral).
- Yuanqi Du, Xiaojie Guo, Hengning Cao, Yanfang Ye, Liang Zhao. Learning Disentangled Representation for Spatiotemporal Graph Generation, accepted in NeurIPS 2021 DGMs Apps workshop.
- Ziming Liu, Yunyue Chen, Yuanqi Du, Max Tegmark. Physics-Augmented Learning: A New Paradigm Beyond Physics-Informed Learning, accepted in NeurIPS 2021 AI for Science workshop.

#### Workshop Organization

- 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 (alphabetic order). AI for Science: Mind the Gaps workshop, with NeurIPS 2021.
- Yuanqi Du<sup>†</sup>, Adji Bousso Dieng, Yoon Kim, Rianne Van Den Berg, Yoshua Bengio. Deep Generative Models for Highly Structured Data, (tentative) with ICLR 2022.

## PROFESSIONAL & RESEARCH EXPERIENCES

**DP Technology** Beijing, China Researcher Oct 2021 - Present

Topic: AI for Drug Discovery, Supervisor: Linfeng Zhang

**Princeton University** Princeton, US Visiting Student Oct 2021 - Present Topic: Highly Structured Scientific Data Modeling, Advisor: Adji Bousso Dieng

University of Amsterdam

Amsterdam, Netherlands

Visiting Student (AMLAB & AI4Science)

June 2021 - Present

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

The Chinese University of Hong Kong

Hong Kong

Visiting Student (MM Lab)

*June* 2021 - Dec 2021

Topic: Deep Generative Models for Molecule Generation and Manipulation, Advisor: Bolei Zhou

George Mason University

Fairfax, US

Research Assistant

Jan 2020 - Oct 2021

Topic: Deep Graph Learning and Molecule/Protein Structure & Dynamic Learning

Advisor: Liang Zhao, Amarda Shehu

Beijing, China

Microsoft Research Asia

2020 14 2021

Research Intern (Machine Learning & Computational Biology Group)

Nov 2020 - May 2021

Topic: Protein Structure Prediction, Advisor: **Jianwei Zhu** 

**Chinese Academy of Sciences** 

Beijing, China

Visiting Student (MIRACLE Group)

Aug 2020 - Nov 2020

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

#### 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

# TEACHING & MENTORING EXPERIENCES

George Mason University Fairfax, US
Undergraduate Teaching Assistant Aug 2018 - Dec 2019

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

George Mason University

Peer Mentor

Feb 2019 - May 2019

Courses: Research Advisor & Engineering Courses & Careers Services

# PROFESSIONAL SERVICES

- Reviewer for TPAMI, ICLR, AISTATS, TNNLS, NeurIPS-W, KDD, TKDD, BMVC, CIKM, ICDM, J. Adv. Transp., NeurIPS-AI4Sci, DLG-KDD, IRS-KDD, BioKDD
- Co-organize conferences KDD 2021/AAAI 2021 (Web Team), Co-organize workshops DLG-KDD/AAAI 2021/2022, DeepSpatial-KDD 2020/2021, open-source community (e.g. GraphGT, GNNBook, Graph4NLP, DeepChem)