



Education

University of Illinois Urbana Champaign

2017 - 2022

Doctor of Philosophy in **Computer Science**

Dissertation: **Machine learning for drug discovery and beyond** (advisor: Jian Peng)

GPA: 4.00 / 4.00

Awards: **University Fellowship, Richard T. Cheng Endowed Fellowship**

Brandeis University

2013 - 2017

Bachelor of Science in **Computer Science** and **Neuroscience**

Senior Thesis: **Graph matching, pattern learning, and protein modeling** (advisor: Pengyu Hong)

GPA: **3.96** / 4.00 (Overall) **4.00** / 4.00 (CS)

Awards: **Summa Cum Laude, Phi Beta Kappa (junior), Schiff Fellowship, Collaborative Research Grant**

Experience

Student Researcher | Google

MAY 2018 - PRESENT

- ▶ I spend part of my Ph.D. working with the talented folks from Google Brain and Accelerated Science.
- ▶ Since 2020, I have been working on drug-target interactions and transfer learning for odorant molecules with a team focusing on digitizing the chemical senses and the underlying technologies and theories. The manuscript is in preparation, and part of the work is also filed as a utility patent.
- ▶ In 2019, we proposed a combinatorial formulation for structural variant calling through ML-based filtering and perturbation to improve the precision of existing callers. An efficient (x100) algorithm is also developed to align reads to variations of the genome. A utility patent is also filed as a result.
- ▶ In 2018, we leveraged the Generative Adversarial Network (GAN) and created a generative model to mediate the batch effect in high-content cell imaging. The model implementations are contributed to the TF-GAN library, and the work is later published in the Bioinformatics journal.

Intern | DeepMind

SEP 2021 - DEC 2021

- ▶ I worked with folks in the AlphaFold team on protein-related projects.
- ▶ The tech stack of the projects involves JAX and different areas of the AlphaFold2 codebase.

Software Engineering Intern | Uber

SUMMER 2016 & 2017

- ▶ In 2017, I developed a variant of conditional random fields to infer key events during Uber Eats delivery with a mobile sensor and identified data quality issues causing performance degradation in the prior effort. The project won the first prize for Uber's internal machine learning poster session.
- ▶ In 2016, I designed and created a web application for internal mobile developers to investigate UI test failures that synchronize the test logs and videos timestamp to reduce the debug time by 50%.

Services

- ▶ **Reviewer** for International Conference on Research in Comp. Molecular Biology (RECOMB) 2021.
- ▶ **Reviewer** for Intelligent Systems for Molecular Biology (ISMB) 2019 & 2020.
- ▶ **Program Committee** for ICML - ML Interpretability for Scientific Discovery Workshop 2020.

Publication (* equal contribution)

- ▶ TargetDiff: 3D Full-Atom Diffusion for Target-Aware Molecule Generation.
Under Review (2022).
 - Jiaqi Guan*, **Wesley Wei Qian***, Xingang Peng, Yufeng Su, Jian Peng, Jianzhu Ma
- ▶ Energy-Inspired Molecular Conformation Optimization.
ICLR (2022).
 - Jiaqi Guan*, **Wesley Wei Qian***, Qiang Liu, Wei-Ying Ma, Jianzhu Ma, Jian Peng
- ▶ ECNet is an evolutionary context-integrated deep learning framework for protein engineering.
Nature Communication (2021).
 - Yunan Luo, Guangde Jiang, Tianhao Yu, Yang Liu, Lam Vo, Hantian Ding, Yufeng Su, **Wesley Wei Qian**, Huimin Zhao, Jian Peng
- ▶ Comprehensive interactome profiling of the human Hsp70 network highlights functional differentiation of J domains.
Molecular Cell (2021).
 - Benjamin L. Piette, Nader Alerasool, Zhen-Yuan Lin, Jessica Lacoste, Mandy Hiu Yi Lam, **Wesley Wei Qian**, Stephanie Tran, Brett Larsen, Eric Campos, Jian Peng, Anne-Claude Gingras, Mikko Taipale
- ▶ Batch Equalization with a Generative Adversarial Network.
Bioinformatics (2020).
 - **Wesley Wei Qian**, Cassandra Xia, Subhashini Venugopalan, Arunachalam Narayanaswamy, Michelle Dimon, George W Ashdown, Jake Baum, Jian Peng, D Michael Ando
- ▶ Integrating Deep Neural Networks and Symbolic Inference for Organic Reactivity Prediction.
ACS National Meeting (2021).
 - **Wesley Wei Qian***, Nathan T. Russell*, Claire L. W. Simons, Yunan Luo, Martin D. Burke, Jian Peng
- ▶ Evaluating Attribution for Graph Neural Networks.
NeurIPS (2020).
 - Benjamin Sanchez-Lengeling, Jennifer Wei, Brian Lee, Emily Reif, Peter Wang, **Wesley Wei Qian**, Kevin McCloskey, Lucy Colwell, Alexander Wiltschko
- ▶ Evolutionary context-integrated deep sequence modeling for protein engineering.
RECOMB (2020).
 - Yunan Luo, Lam Vo, Hantian Ding, Yufeng Su, Yang Liu, **Wesley Wei Qian**, Huimin Zhao, Jian Peng