



## Education

### University of Illinois Urbana Champaign

AUG 2017 - AUG 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

SEP 2013 - MAY 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 time 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. A utility patent has been filed and the manuscript for the work is in preparation.
- ▶ 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 Science / AlphaFold team on **protein-related** projects.

### 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