

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

Founding Staff Research Engineer / Manager | Osmo

Sep 2022 - Present

- ▶ I am leading the machine learning team responsible for the data collection strategy and model development behind fragrance molecule discovery and [scent teleportation](#).
- ▶ I stood up the ML infra. and port TensorFlow implementation to PyTorch post [Google](#) spin out.
- ▶ I drove the development of a new molecule intensity model from molecule sample preparation, annotation protocol, data plumbing, model development, prospective validation, to deployment.

Student Researcher | Google

May 2018 - Sep 2022

- ▶ I spent part of my Ph.D. working with the talented folks from Google Brain and Accelerated Science.
- ▶ Between 2020 to 2022, I worked on receptor binding, transfer learning, and metabolic activity related to odorant molecules with a team focusing on digitizing smell. I led/participated in one [utility patent](#) and four publications highlighted in [various news outlets](#). Our team's discovery eventually led to the spinout of [Osmo](#), backed by Google Venture, Lux Capital, and other investors with \$60M.
- ▶ In 2019, I 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 various genome construction and filed as a [utility patent](#).
- ▶ In 2018, I 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. I also 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 video timestamps to reduce the debug time by 50%.

Publication (*equal contribution)

- ▶ **A Principal Odor Map Unifies Diverse Tasks in Human Olfactory Perception**
Science (2023)
 - Brian K. Lee*, Emily E Mayhew*, Benjamin Sanchez-Lengeling, Jennifer N. Wei, **Wesley W. Qian**, Kelsie Little, Matthew Andres, Britney B. Nguyen, Theresa Moloy, Jacob Yasonik, Jane K. Parker, Richard C. Gerkin, Joel D. Mainland, Alexander B. Wiltschko
- ▶ **Metabolic activity organizes olfactory representations**
eLife (2023)
 - **Wesley W. Qian**, Jennifer N. Wei, Benjamin Sanchez-Lengeling, Brian K. Lee, Yunan Luo, Marnix Vlot, Koen Dechering, Jian Peng, Richard C. Gerkin, Alexander B. Wiltschko
- ▶ **3D Equivariant Diffusion for Target-Aware Molecule Generation and Affinity Prediction**
ICLR (2023)
 - Jiaqi Guan*, **Wesley W. Qian***, Xingang Peng, Yufeng Su, Jian Peng, Jianzhu Ma
- ▶ **A central chaperone-like role for 14-3-3 proteins in human cells**
Molecular Cell (2023)
 - Dmitri Segal, Stefan Maier, Giovanni J Mastromarco, **Wesley W. Qian**, Syed Nabeel-Shah, Hyunmin Lee, Gaelen Moore, Jessica Lacoste, Brett Larsen, Zhen-Yuan Lin, Abeeshan Selvabaskaran, Karen Liu, Craig Smibert, Zhaolei Zhang, Jack Greenblatt, Jian Peng, Hyun O Lee, Anne-Claude Gingras, Mikko Taipale
- ▶ **Pervasive mislocalization of pathogenic coding variants underlying human disorders**
Under Review (2023)
 - Jessica Lacoste, Marzieh Haghighi, Shahan Haider, Zhen-Yuan Lin, Dmitri Segal, Chloe Reno, **Wesley W. Qian**, Xueting Xiong, Hamdah Shafqat-Abbasi, Pearl V Ryder, Rebecca Senft, Beth A Cimini, Frederick P Roth, Michael Calderwood, David Hill, Marc Vidal, S Stephen Yi, Nidhi Sahni, Jian Peng, Anne-Claude Gingras, Shantanu Singh, Anne E Carpenter, Mikko Taipale
- ▶ **A deep learning and digital archaeology approach for mosquito repellent discovery**
Under Review (2022)
 - Jennifer N. Wei*, Marnix Vlot*, Benjamin Sanchez-Lengeling, Brian K. Lee, Luuk Berning, Martijn W. Vos, Rob W.M. Henderson, **Wesley W. Qian**, D. Michael Ando, Kurt M. Groetsch, Richard C. Gerkin, Alexander B. Wiltschko, Koen J. Dechering
- ▶ **Energy-Inspired Molecular Conformation Optimization**
ICLR (2022)
 - Jiaqi Guan*, **Wesley W. Qian***, Qiang Liu, Wei-Ying Ma, Jianzhu Ma, Jian Peng
- ▶ **Integrating Deep Neural Networks and Symbolic Inference for Organic Reactivity Prediction**
ACS National Meeting (2021)
 - **Wesley W. Qian***, Nathan T. Russell*, Claire L. W. Simons, Yunan Luo, Martin D. Burke, 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 W. 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 W. Qian**, Stephanie Tran, Brett Larsen, Eric Campos, Jian Peng, Anne-Claude Gingras, Mikko Taipale
- ▶ **Batch Equalization with a Generative Adversarial Network**
Bioinformatics (2020)
 - **Wesley W. Qian**, Cassandra Xia, Subhashini Venugopalan, Arunachalam Narayanaswamy, Michelle Dimon, George W. Ashdown, Jake Baum, Jian Peng, D Michael Ando
- ▶ **Evaluating Attribution for Graph Neural Networks**
NeurIPS (2020)
 - Benjamin Sanchez-Lengeling, Jennifer Wei, Brian Lee, Emily Reif, Peter Wang, **Wesley W. Qian**, Kevin McCloskey, Lucy Colwell, Alexander B. Wiltschko
- ▶ **Evolutionary context-integrated deep sequence modeling for protein engineering**
RECOMB (2020)
 - Yunan Luo, Lam Vo, Hantian Ding, Yufeng Su, Yang Liu, **Wesley W. Qian**, Huimin Zhao, Jian Peng

Services

- ▶ **Program Committee** for ICML - ML Interpretability for Scientific Discovery Workshop 2020
- ▶ **Reviewer** for ICML (2024), ICLR (2024), NeurIPS (2023), LoG (2022 & 2023), RECOMB (2021), ISMB (2019 & 2020)