Wesley Wei Qian

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Education

University of Illinois at Urbana-Champaign AUG 2017-PRESENT

Doctor of Philosophy in **Computer Science: Machine Learning & Comp. Biology/Chemistry**

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**

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

Graduate Research Assistant | UIUC AUG 2017 - PRESENT

- I work with my advisor, Jian Peng, on various problems in computational biology and chemistry with machine learning and data driven approaches. I really enjoy the science aspect our research.
- My research topics include **protein** sequence/structure modeling and design, **graph neural network** for **molecule** property prediction, reaction prediction, and conformer prediction.

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 molecule** with a team focusing on digitizing the chemical senses and the underlying technologies and theories. 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. This project is **patented** but still in work.
- 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 am working with folks in the Science / AlphaFold team on **protein** related project.

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 **mobile sensor,** and identified data quality issue causing performance issue in previous efforts. The effort also won **the first prize** for Uber's first internal machine learning poster session.
- In 2016, I designed and created a **web application** for internal mobile developer to investigate UI test failures that synchronize the test logs and videos timestamp reduce the debug time by 50%.

Undergraduate Research Assistant | Brandeis Univ. MAY 2015 - MAY 2017

- I work with Pengyu Hong on computational biology and linguistic with statistical machine learning.
- Research topics include efficient ML-based solver for graph isomorphism with application in protein structure/neural morphology as well as natural language dialogue generation for Mandarin.

Publication (* equal contribution)

- Energy-Inspired Molecular Conformation Optimization. ***ICLR*** (2022).
  - **Wesley Wei Qian***, Jiaqi Guan*, 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. ***ChemRxiv*** (2020).
  - **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

Services

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