Wesley Wei Qian

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Education

University of Illinois at Urbana-Champaign   AUG 2017-MAY 2022
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.

Intern | DeepMind   Sep 2021 - PRESENT
- I am working with folks at the Science team on **protein** related project.

Student Researcher | Google   MAY 2018 - SEP 2021
- I spend part of my time working with the talented folks from Google Brain and Accelerated Science.
- In 2020 and 2021, I worked 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**.

Software Engineering Intern | Uber   SUMMER 2016 & 2017
- 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%.
- 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.

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

- **Qian, W.W.**, Guan, J., Liu, Q., Ma, W., Ma, J., Peng, J. (2021). Neural Energy Minimization for Molecular Conformation Optimization. ***Under Review at NeurIPS2021***.
- Piette, B. L., Alerasool, N., Lin, Z. Y., Lacoste, J., Lam, M. H. Y., **Qian, W. W.**, ... & Taipale, M. (2021). Comprehensive interactome profiling of the human Hsp70 network highlights functional differentiation of J domains. ***Molecular cell***.
- **Qian, W. W.**, Xia, C., Venugopalan, S., Narayanaswamy, A., Dimon, M., Ashdown, G., Baum, J. Peng, J., Ando, D.M. (2020). Batch Equalization with a Generative Adversarial Network. ***Bioinformatics***.
- **Qian, W. W.**, Russell, N. T., Simons, C. L., Luo, Y., Burke, M. D., & Peng, J. (2020). Integrating Deep Neural Networks and Symbolic Inference for Organic Reactivity Prediction. ***ChemRxiv***.
- Sanchez-Lengeling, B., Wei, J., Lee, B., Reif, E., Wang, P., **Qian, W. W.**, McCloskey, K., Colwell, L., & Wiltschko, A. (2020). Attribution for Graph Neural Network. ***NeurIPS2020***.
- Luo, Y., Vo, L., Ding, H., Su, Y., Liu, Y., **Qian, W. W.**, Zhao, H., & Peng, J. (2020). Evolutionary context-integrated deep sequence modeling for protein engineering. ***RECOMB2020***.

Service

- **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.