

JIAQI GUAN

PhD candidate ◊ University of Illinois Urbana-Champaign

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RESEARCH INTERESTS

My research focuses on deep learning and its applications in computational biology / chemistry. Specifically, my research interests lie in the intersection of geometric machine learning, generative modeling, and drug / macro-biomolecule design.

EDUCATION

University of Illinois Urbana-Champaign

2019.08 - Present

- Ph.D. in Computer Science. Advisor: Prof. Jian Peng. GPA: 3.96/4.0

Tsinghua University

2014.08 - 2018.07

- Bachelor of Engineering in Automation. GPA: 89/100 (Ranking:13/135)

PUBLICATION

1. **Jiaqi Guan***, Wesley Wei Qian*, Xingang Peng, Yufeng Su, Jian Peng, Jianzhu Ma. **3D Equivariant Diffusion for Target-Aware Molecule Generation and Affinity Prediction**. ICLR 2023.
2. Xingang Peng, Shitong Luo, **Jiaqi Guan**, Qi Xie, Jian Peng, Jianzhu Ma. **Pocket2Mol: Efficient Molecular Sampling Based on 3D Protein Pockets**. ICML 2022.
3. Shitong Luo*, Jiahao Li*, **Jiaqi Guan***, Yufeng Su, Chaoran Cheng, Jian Peng, Jianzhu Ma. **Equivariant Point Cloud Analysis via Learning Orientations for Message Passing**. CVPR 2022, Oral.
4. **Jiaqi Guan***, Wesley Wei Qian*, Qiang Liu, Wei-Ying Ma, Jianzhu Ma, Jian Peng. **Energy-Inspired Molecular Conformation Optimization**. ICLR 2022.
5. Shitong Luo, **Jiaqi Guan**, Jianzhu Ma, Jian Peng. **A 3D Generative Model for Structure-Based Drug Design**. NeurIPS 2021.
6. **Jiaqi Guan**, Ye Yuan, Kris M. Kitani, Nicholas Rhinehart. **Generative Hybrid Representations for Activity Forecasting with No-Regret Learning**. CVPR 2020, Oral.
7. **Jiaqi Guan**, Yang Liu, Qiang Liu, Jian Peng. **Energy-efficient Amortized Inference with Cascaded Deep Classifiers**. The 27th International Joint Conference on Artificial Intelligence (IJCAI 2018)
8. **Jiaqi Guan**, Runzhe Li, Sheng Yu, Xuegong Zhang. **Generation of Synthetic Electronic Medical Record Text**. 2018 IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2018)
9. **Jiaqi Guan**, Runzhe Li, Sheng Yu, Xuegong Zhang. **A Method for Generating Synthetic Electronic Medical Record Text**. IEEE/ACM transactions on computational biology and bioinformatics (TCBB)

EXPERIENCE

Research Internship

2022.05 - 2022.10

ByteDance AI Lab, Remote. Advisor: *Yuwei Yang*

- Developed a new diffusion model with decomposed priors for structure-based drug design.
- Considered both atom and bond diffusion processes in the model to simultaneously generate them.
- Incorporated validity guidance in the sampling phase to improve the sample quality.
- Presented this work in a ICML 2023 submission.

Graduate Research Assistant

2019.09 - Now

Department of Computer Science, UIUC, Advisor: *Prof. Jian Peng*

- *Molecular Conformation Optimization*: develop a novel framework for deriving variants of SE(3)-equivariant neural networks from the perspective of neural energy minimization. The model shows better performance than existing baselines in molecular conformation optimization and generation.
- *Structure-Based Drug Design*: develop a 3D generative model to generate molecules that bind to specific protein binding sites. Evaluate the model based on various metrics and it shows superior performance. Several papers in this direction were accepted by NeurIPS 2021, ICML 2022, ICLR 2023.
- *Protein Loop Modeling*: develop a transformer-based graph neural network for the protein loop modeling task, especially for antibody CDR H3 loop. Lower RMSD than existing SOTA results.
- *Protein Binding Affinity Prediction*: explore various models on this task. A model based on E(n)-equivariant neural network achieve better performance than existing models.

Research Internship

2020.05 - 2020.08

Tencent AI Lab, Seattle, USA. Advisor: *Liwei Wang, Jianqiao Zhao*

- Built a large-scale Chinese dialogue generation pretrain framework.
- Focused on dialogue generation with reinforcement learning. Improved the dialogue generation performance with the dynamic self-play schema.

Short-Term Research Scholar

2018.09 - 2019.01

Robotics Institute, Carnegie Mellon University, Advisor: *Prof. Kris Kitani*

- Developed a generative model to forecast trajectory and action jointly by minimizing a symmetric cross entropy loss. The model can compute the exact probability density function.
- Implemented several baselines including condition VAE, direct cross entropy model and mixed regression and multi-label classification model.
- Proved the convexity of forward cross entropy loss mathematically and extended the model to conduct no regret online learning.
- Presented this work in CVPR 2020 paper.

Undergraduate Summer Internship

2017.06 - 2017.09

Department of Computer Science, UIUC, Advisor: *Prof. Jian Peng*

- Developed a complete algorithm about energy-efficient amortized inference on image classification task by attaching a policy model to cascaded ResNets and jointly training with REINFORCE, based on TensorFlow.
- Presented this work in paper *Energy-efficient Amortized Inference with Cascaded Deep Classifiers*.

SKILLS

Programming Languages

Python, Matlab, C/C++, C#

Framework & Tools

PyTorch, Tensorflow, Caffe, Git, ROS, OpenCV

SCHOLARSHIP & AWARDS

2018 Excellent Graduate of Department of Automation (25 of 150+)

2017 Honorable Mention, Mathematical Contest in Modeling (MCM), COMAP

2016 Tsinghua Alumni Scholarship (For excellent academic performance, top 10%)

2015 Tsinghua Alumni Scholarship (For excellent academic performance, top 10%)

2015 Tsinghua Scholarship (For excellent performance in social activities)

2015 Tsinghua University Outstanding Student Leader