JIAQI GUAN

Research Scientist, ByteDance
jiaqi@illinois.edu ◇ https://jiaqi.web.illinois.edu

RESEARCH INTERESTS

My research focuses on deep generative models and its applications in biology / chemistry.

I am especially interested in geometric machine learning, generative modeling, and drug / macro-biomolecule design.

EDUCATION

University of Illinois Urbana-Champaign, Urbana, IL, USA *2019.08 - 2024.05*

· Ph.D. in Computer Science. Advisor: Prof. Jian Peng.

Tsinghua University, Beijing, China *2014.08 - 2018.07*

· B.E. in Automation.

EMPLOYMENT

ByteDance AI4Science - AML, Seattle, WA 2024.06 - Now

Research Scientist

University of Illinois Urbana-Champaign, Urbana, IL 2019.09 - 2024.05

Ph.D. Research Assistant

ByteDance AI Lab, San Jose, CA 2022.05 - 2022.10, 2023.05 - 2023.08

Research Intern

Tencent AI Lab, Seattle, WA 2020.05 - 2020.08

Research Intern

PUBLICATIONS

[* indicates equal contribution]

1. LinkerNet: Fragment Poses and Linker Co-Design with 3D Equivariant Diffusion.

   Jiaqi Guan, Xingang Peng, Peiqi Jiang, Yunan Luo, Jian Peng, Jianzhu Ma.

   In Proceedings of the Neural Information Processing Systems (**NeurIPS**), 2023. (**Spotlight**).

2. DecompDiff: Diffusion Models with Decomposed Priors for Structure-Based Drug Design.

   Jiaqi Guan*, Xiangxin Zhou*, Yuwei Yang, Yu Bao, Jian Peng, Jianzhu Ma, Qiang Liu, Liang Wang, Quanquan Gu.

   In Proceedings of the International Conference on Machine Learning (**ICML**), 2023.

3. MolDiff: Addressing the Atom-Bond Inconsistency Problem in 3D Molecule Diffusion Generation.

   Xingang Peng, **Jiaqi Guan**, Qiang Liu, Jianzhu Ma.

   In Proceedings of the International Conference on Machine Learning (**ICML**), 2023.

4. 3D Equivariant Diffusion for Target-Aware Molecule Generation and Affinity Prediction.

   Jiaqi Guan*, Wesley Wei Qian*, Xingang Peng, Yufeng Su, Jian Peng, Jianzhu Ma.

   In Proceedings of the International Conference on Learning Representations (**ICLR**), 2023.

5. Pocket2Mol: Efficient Molecular Sampling Based on 3D Protein Pockets.

   Xingang Peng, Shitong Luo, **Jiaqi Guan**, Qi Xie, Jian Peng, Jianzhu Ma.

   In Proceedings of the International Conference on Machine Learning (**ICML**), 2022.

6. Equivariant Point Cloud Analysis via Learning Orientations for Message Passing.

   Shitong Luo*, Jiahan Li*, **Jiaqi Guan***, Yufeng Su, Chaoran Cheng, Jian Peng, Jianzhu Ma.

   In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (**CVPR**), 2022. (**Oral**).

7. Energy-Inspired Molecular Conformation Optimization.

   Jiaqi Guan*, Wesley Wei Qian*, Qiang Liu, Wei-Ying Ma, Jianzhu Ma, Jian Peng.

   In Proceedings of the International Conference on Learning Representations (**ICLR**), 2022.

8. A 3D Generative Model for Structure-Based Drug Design.

   Shitong Luo, **Jiaqi Guan**, Jianzhu Ma, Jian Peng.

   In Proceedings of the Neural Information Processing Systems (**NeurIPS**), 2021.

9. Generative Hybrid Representations for Activity Forecasting with No-Regret Learning.

   Jiaqi Guan, Ye Yuan, Kris M. Kitani, Nicholas Rhinehart.

   In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (**CVPR**), 2020. (**Oral**).

10. A Method for Generating Synthetic Electronic Medical Record Text.

    Jiaqi Guan, Runzhe Li, Sheng Yu, Xuegong Zhang.

    In IEEE/ACM transactions on computational biology and bioinformatics (**TCBB**), 2019.

11. Generation of Synthetic Electronic Medical Record Text.

    Jiaqi Guan, Runzhe Li, Sheng Yu, Xuegong Zhang.

    In Proceedings of IEEE International Conference on Bioinformatics and Biomedicine (**BIBM**), 2018.

12. Energy-efficient Amortized Inference with Cascaded Deep Classifiers.

    Jiaqi Guan, Yang Liu, Qiang Liu, Jian Peng.

    In Proceedings of the International Joint Conference on Artificial Intelligence (**IJCAI**), 2018.

RESEARCH EXPERIENCES

University of Illinois Urbana-Champaign, Urbana, IL *2019.09 - 2024.05*
Graduate Research Assistant. Advisor: *Prof. Jian Peng, Prof. Jianzhu Ma*

- *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.
- *PROTAC Linker Design*: fragment poses and linker co-design. Published a paper in NeurIPS 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.

ByteDance AI Lab, San Jose, CA *2022.05 - 2022.10*
Research Intern. 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 ICML 2023.

Tencent AI Lab, Seattle, WA *2020.05 - 2020.08*
Research Intern. 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.

Carnegie Mellon University, Pittsburgh, PA *2018.09 - 2019.01*
Robotics Institute Short-Term Research Scholar. 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.

TEACHING

CS 598: Principles of Generative AI	Spring 2024, Instructor: Tong Zhang
CS 440: Artificial Intelligence	Fall 2023, Instructor: Margaret Fleck
CS 598: Deep Generative and Dynamic Models	Spring 2023, Instructor: Arindam Banerjee

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

PROFESSIONAL SERVICE

Conference Reviewer	NeurIPS, ICLR, ICML, CVPR, AAAI
Journal Reviewer	Nature Computational Science