JIAQI (ALEX) HAN

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Homepage | Github | Google Scholar

EDUCATION

Tsinghua University Beijing, China
B. Eng in Computer Science Sep. 2017 – July 2021

- GPA: 3.82/4.00 (ranked top 5%); admitted on basis of national college admissions exam (ranked 4/180,000)
- Selected awards: First Place in Open Catalyst 2022 Competition, Outstanding Graduate of Beijing (top 3%), Academic Excellence Award 2018 & 2019
- Research interests: Graph neural networks - theories and applications; AI4Science – molecular and protein modeling, 3D geometric models, physics-inspired model designs.

PUBLICATIONS

1. **Jiaqi Han**, Wenbing Huang, Hengbo Ma, Jiachen Li, Joshua B. Tenenbaum, and Chuang Gan. "Learning Physical Dynamics with Subequivariant Graph Neural Networks". *Advances in Neural Information Processing Systems (NeurIPS 2022)*
2. **Jiaqi Han**, Wenbing Huang, Tingyang Xu, Yu Rong. "Equivariant Graph Hierarchy-Based Neural Networks". *Advances in Neural Information Processing Systems (NeurIPS 2022)*
3. Wenbing Huang*, **Jiaqi Han***, Yu Rong, Tingyang Xu, Fuchun Sun, and Junzhou Huang. "Equivariant Graph Mechanics Networks with Constraints". *International Conference on Learning Representations (ICLR 2022)*
4. Rui Jiao, **Jiaqi Han**, Wenbing Huang, Yu Rong, and Yang Liu. "Energy-Motivated Equivariant Pretraining for 3D Molecular Graphs". *AAAI Conference on Artificial Intelligence (AAAI 2023)*
5. **Jiaqi Han**, Wenbing Huang, Yu Rong, Tingyang Xu, Fuchun Sun, and Junzhou Huang. "Structure-Aware DropEdge Towards Deep Graph Convolutional Networks". Conditional Acceptance. *IEEE Transactions on Neural Networks and Learning Systems (TNNLS)*
6. Zhihan Li, Youjian Zhao, **Jiaqi Han**, Ya Su, Rui Jiao, Xidao Wen, and Dan Pei. "Multivariate Time Series Anomaly Detection using Hierarchical Inter-Metrc and Temporal Embedding". *The 27th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD 2021)*
7. **Jiaqi Han**, Yu Rong, Tingyang Xu, and Wenbing Huang. "Geometrically Equivariant Graph Neural Networks: A Survey". *arXiv preprint 2202.07230.*
8. **Jiaqi Han**, Wenbing Huang, Yu Rong, Jun Wang, and Peilin Zhao. "Multi-task Parameter Passing Networks". Under Review.

RESEARCH EXPERIENCE

Tencent AI Lab, Machine Learning Center Shenzhen, China
Research Intern to Dr. Yu Rong, Prof. Junzhou Huang, and Prof. Wenbing Huang Feb. 2020 – Present
Geometric Graph Neural Networks for Science

- Investigated injecting equivariance (symmetry constraint) in modeling constrained physical and biochemical systems like molecules, as well as for larger and hierarchical systems like proteins.
- The designed models improved the molecular dynamics simulation precision by up to 26% and protein dynamics simulation by 20%, verifying the efficacy of the proposed equivariant GNN in modeling complex systems of different scales.
- Two first author papers accepted to ICLR 2022 and NeurIPS 2022.
- Selected into Tencent Rhino Bird Elite Program 2020.

MIT, CSAIL Cambridge, United States
Research Assistant to Dr. Chuang Gan and Prof. Joshua B. Tenenbaum Mar. 2022 – June 2022
Modeling Physical interactions with Proper Symmetry as Prior

- Designed a particle-based GNN that considers physical symmetry of the system with external forces.
- Demonstrated model is 3x more data-efficient and generalizable on physical scene simulation tasks.
- First author paper accepted to NeurIPS 2022.

Tsinghua University, Institute of AI Industry Research (AIR) Beijing, China
Research Assistant to Prof. Wenbing Huang Sep. 2021 – Feb. 2022
Geometrically Equivariant Graph Neural Networks: Survey and Applications

- Surveyed recent advances in geometrically equivariant GNNs; First author paper available on arXiv.
- Proposed a novel 3D pretraining framework for molecular graphs, equipped with an energy-based representation model. The pretraining framework is also theoretically guaranteed to meet the symmetry constraint by leveraging the Riemann-Gaussian distribution.
- Second author Paper on 3D molecular pretraining accepted to AAAI 2023.

University of Chicago, Department of Computer Science Chicago, United States
Research Assistant to Prof. Yuxin Chen July 2020 – Sep. 2020
Multi-fidelity Bayesian Optimization for Physical PDE Solvers

- Studied multi-fidelity Bayesian Optimization in combinatorial setting to bring down the simulation cost of finding proper parameter configuration of physical simulations.
- Implemented a toolkit that achieved the goal by cutting down the cost by half over existing approaches.

Tsinghua University, Netman Lab Beijing, China
Research Assistant to Prof. Dan Pei June 2019 – Jan. 2020
Anomaly Detection on Multivariate Time Series

- Developed a novel framework for anomaly detection and interpretation of multivariate time series data. The method takes a two-view modeling approach with both inter-metric and temporal embeddings. The framework has been deployed in a network company and received positive feedbacks.
- Paper accepted to KDD 2021.

AWARDS AND HONORS

- NeurIPS'22 Open Catalyst Challenge 2022, received first place and invited to give speech 2022
- Outstanding Graduate of Tsinghua University (top 5%) 2021
- Outstanding Graduate of Beijing (top 3%) 2021
- Academic Excellence Award, Tsinghua University (top 3%) 2019
- Academic Excellence Award, Tsinghua University (top 3%) 2018
- Outstanding Freshman Award, Tsinghua University (top 5%) 2017

ADDITIONAL INFORMATION

Professional Service

- Serve as reviewer for ICML 2022, KDD 2022, NeurIPS 2022

Other Interests

- Piano: Proficient with amateur level-10 national certificate.

Computer and Language Skills

- Coding language: Proficient in Python, C++, Java.
- Deep learning framework: PyTorch, PyG (PyTorch Geometric), DGL (Deep Graph Library), TensorFlow.
- Biochemistry library: RDKit, MDAnalysis.
- Languages: Chinese (native), English (proficient)