Keqiang Yan

Ph.D. Student
Department of Computer Science & Engineering
Texas A&M University

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Research Interests

Graph Deep Learning: graph neural networks, 3D graphs, periodic graphs.

AI for Drug and Material Discovery: molecule and material property prediction, molecule, material and protein generation.

Generative Modeling: energy-based models, flow models, diffusion models.

Education

Texas A&M University, College Station, TX, USA — Sep 2020 – Present
Ph.D., Department of Computer Science & Engineering
Advisor: Prof. Shuiwang Ji

Peking University, Beijing, CHINA — Aug 2016 – Jul 2020
B.S., Intelligence Science and Technology
Advisor: Prof. Jiaying Liu

Publications [Google Scholar]

* indicates equal contribution.

[JMLR] **DIG: A Turnkey Library for Diving into Graph Deep Learning Research**
Meng Liu*, Youzhi Luo*, Limei Wang*, Yaochen Xie*, Hao Yuan*, Shurui Gui*, Haiyang Yu*, Zhao Xu, Jingtun Zhang, Yi Liu, **Keqiang Yan**, Haoran Liu, Cong Fu, Bora Oztekin, Xuan Zhang, and Shuiwang Ji
*Journal of Machine Learning Research (**JMLR**), 2021*
[Paper] [Code (star 1k+)] [Documentation]

[ICML 2021] **GraphDF: A Discrete Flow Model for Molecular Graph Generation**
Youzhi Luo, **Keqiang Yan**, and Shuiwang Ji
*The 38th International Conference on Machine Learning (**ICML**), 2021*
[Paper] [Code]

[ICLR-W 2021] **GraphEBM: Molecular Graph Generation with Energy-Based Models**
Meng Liu, **Keqiang Yan**, Bora Oztekin, and Shuiwang Ji
EBM Workshop at ICLR, 2021
[Paper] [Code]

[ICME 2020] **Multitask Attentive Network For Text Effects Quality Assessment**
Keqiang Yan, Shuai Yang, Wenjing Wang and Jiaying Liu
*2020 IEEE International Conference on Multimedia and Expo (**ICME**)*
[Paper]

Professional Services

Program Committee Member | Reviewer

Conference on Neural Information Processing Systems (**NeurIPS**) 2022
International Conference on Machine Learning (**ICML**) 2022
IEEE Transactions on Pattern Analysis and Machine Intelligence (**TPAMI**) 2022

Scholarships, Awards, & Honors

3rd Place of Open Catalyst Challenge 2021
Excellent Graduate, Peking University 2020

Skills

Python, Julia, Matlab, c/c++, LaTeX, PyTorch