Keqiang Yan

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Research Interests

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

AI for Drug and Material Discovery: predictive and generative models for molecules, materials, and proteins.

Generative Modeling: energy-based 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.

[NeurIPS 2022] **Periodic Graph Transformers for Crystal Material Property Prediction**
Keqiang Yan, Yi Liu, Yuchao Lin, and Shuiwang Ji
*Thirty-sixth Conference on Neural Information Processing Systems (**NeurIPS**), 2022*
[Paper] [Code coming soon]

We consider representation learning on periodic graphs encoding crystal materials. Different from regular graphs, periodic graphs consist of a minimum unit cell repeating itself on a regular lattice in 3D space. How to effectively encode these periodic structures poses unique challenges not present in regular graph representation learning. In addition to being E(3) invariant, periodic graph representations need to be periodic invariant. That is, the learned representations should be invariant to shifts of cell boundaries as they are artificially imposed. Furthermore, the periodic repeating patterns need to be captured explicitly as lattices of different sizes and orientations may correspond to different materials. In this work, we propose a transformer architecture, known as Matformer, for periodic graph representation learning. Our Matformer is designed to be invariant to periodicity and can capture repeating patterns explicitly. Experimental results show that our Matformer outperforms baseline methods consistently.

[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]

To facilitate graph deep learning research, we introduce DIG: Dive into Graphs, a turnkey library that provides a unified testbed for higher level, research-oriented graph deep learning tasks. Currently, we consider graph generation, self-supervised learning on graphs, explainability of graph neural networks, and deep learning on 3D graphs. For each direction, we provide unified implementations of data interfaces, common algorithms, and evaluation metrics. Altogether, DIG is an extensible, open-source, and turnkey library for researchers to develop new methods and effortlessly compare with common baselines using widely used datasets and evaluation metrics.

[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]

We consider the problem of molecular graph gen- eration using deep models. While graphs are discrete, most existing methods use continuous latent variables, resulting in inaccurate modeling of discrete graph structures. In this work, we propose GraphDF, a novel discrete latent variable model for molecular graph generation based on normalizing flow methods. We show that the use of discrete latent variables reduces computational costs and eliminates the negative effect of dequantization. Comprehensive experimental results show that GraphDF outperforms prior methods on random generation, property optimization, and constrained optimization tasks.

[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]

We note that most existing approaches for molecular graph generation fail to guarantee the intrinsic property of permutation invariance, resulting in unexpected bias in generative models. In this work, we propose GraphEBM to generate molecular graphs using energy-based models. In particular, we parameterize the energy function in a permutation invariant manner, thus making GraphEBM permutation invariant. We apply Langevin dynamics to train the energy function by approximately maximizing likelihood and generate samples with low energies. Furthermore, to generate molecules with a desirable property, we propose a simple yet effective strategy, which pushes down energies with flexible degrees according to the properties of corresponding molecules. Comprehensive experimental results on random, goal-directed, and compositional generation tasks demonstrate the effectiveness of our proposed method.

[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]

In this paper, we focus on artistic text stylization and build a novel deep neural network equipped with multitask learning and attention mechanism for text effects quality assessment. We first select stylized images from TE141K dataset and then collect the corresponding visual scores from users. Then through multitask learning, the network learns to extract features related to both style and content information. Furthermore, we employ an attention module to simulate the process of human high-level visual judgement.

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