

Yinan Huang

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Research Interests

Graph representation learning; geometric deep learning and equivariant neural networks; machine learning for science (physics, chemistry, optimization, etc.)

Education

Duke University

USA

M.S. in Electrical and Computer Engineering (machine learning track)

2020-2023 (expected)

- GPA: 4.0/4.0

Sun Yat-Sen University

China

B.S. in Physics

2016-2020

- GPA: 4.2/5 (92/100), Class Rank: 1/83

Research Experience

Beijing Institute of General Artificial Intelligence

China

Research intern, advisor: Prof. Muhan Zhang and Prof. Jianzhu Ma

2021-2022

Equivariant graph neural networks

- Studied symmetry-awared neural networks that are equivariant under group representations, with a main focus on graph neural networks with Euclidean geometric features, i.e., 3D graphs.
- Developed an E(3) equivariant graph variational auto-encoder named 3DLinker that can simultaneously generate graphs and coordinates for drug linker design. The recovery rate and coordinate prediction attained significant improvement.

Expressive power of graph neural networks

- Studied the expressive power of Subgraph Graph neural networks (Subgraph GNNs) via cycle and path counting.
- Showed the limitation of Subgraph GNNs' counting power, which negates a previous proposition that it can count arbitrary cycles. Proposed a novel model with multiple node identifiers and theoretically prove its stronger counting ability.

Publication and Under-review

- **Yinan Huang**, Xingang Peng, Jianzhu Ma, Muhan Zhang. 3DLinker: An E(3) Equivariant Variational Autoencoder for Molecular Linker Design, ICML-2022 (long representation).
- **Yinan Huang**, Xingang Peng, Jianzhu Ma, Muhan Zhang. Boosting the Cycle Counting Power of Graph Neural Networks with I^2 -GNNs, under review.

Honors and Awards

Chinese national scholarship, Coca Cola scholarship, Wong Lo Kat scholarship

Skills

Python, Pytorch, Matlab