Yinan Huang

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PRINCIPAL INTERESTS

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

EDUCATION

M.Sc. Electrical and Computer Engineering 2020-2023 (expected)
Duke University, Durham, USA
- GPA: 4.0/4.0

B.Sc. Physics 2016-2020
Sun Yat-Sen University, Guangdong, China
- GPA: 4.2/5.0, rank 1/83

RESEARCH EXPERIENCE

Beijing Institute of General Artificial Intelligence 2021-2022
Research intern Supervisor: Prof. Muhan Zhang, Prof. Jianzhu Ma

- Equivariant Graph Neural Networks
  - Studied symmetry-awared neural networks that are equivaraint 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. By incorporating the 3D geometry into graph generation, 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.

PUBLICATIONS & UNDER REVIEW

1. **Huang, Y.**, Peng, X., Ma, J., Zhang, M. Boosting the cycle counting power of graph neural networks with I^2-GNNs, under review.

2. **Huang, Y.**, Peng, X., Ma, J., Zhang, M. 3DLinker: an E(3) equivariant variational autoencoder for molecular linker design. ICML-2022 (long representation).

COMPUTER SKILLS

Python, Pytorch, Matlab

AWARDS

National Scholarship, Coca Cola Scholarship, Wong Lo Kat scholarship.