Wenhao Yu

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Education

The Chinese University of Hong Kong (CUHK), HKSAR, China — Sep. 2024 – Present

Ph.D. Candidate in Computer Science & Engineering (CSE)

Beihang University (BUAA), Beijing, China — Jul. 2020 – Jul. 2024

B.S. in Artificial Intelligence. Grading rank at 10%.

Publications

Shengyin Sun*; **Wenhao Yu***; Yuxiang Ren; Weitao Du; Liwei Liu; Xuecang Zhang; Ying Hu; Chen Ma. DiffRetro: Retrosynthesis Prediction with Dual Graph Enhanced Molecular Representation and Diffusion Generation. *The 39th Annual AAAI Conference on Artificial Intelligence*(AAAI 2025).

Research Experience

Huawei Central Research(2012 Lab) — Jul. 2023 – May. 2024

Internship Graph Deep Learning and Applications in Science

Task: Participate in graph analysis, graph mining, graph learning, graph combination optimization. Specifically, AI4EDA, AI4Sci.

1. Molecular Graph Rethosynthesis with Equivariant Diffusion Model(**Retrosynthesis, Graph Embedding& Diffusion. Paper & patent submitted**): We first proposed using dual-graph embedding to improve the performance of edge-/graph-level prediction. Additionally, we first use equivariant diffusion model to generate reactants from synthons.
2. Motif-based Self-Supervised Learning on Molecular Protein Prediction(**NAS, Graph SSL**): The frequent presence of these motifs in a graph implies the semantic information it possesses. We propose the ideas of the controller, which select propagation scope for each node in a molecule.

Center for Machine Learning Research, Peking University — May. 2024 – Aug. 2024

Summer Internship AI for Science.

Task: Transition state search is key in chemistry for elucidating reaction mechanisms and exploring reaction networks. We are devoted in improving the transition state prediction accuracy with flow matching method, which is also meaningful for simulating the whole chemical reaction process.

Beihang University ACT Lab Intern — Jul. 2022 – May. 2023

Internship Graph Deep Learning

- Classic methods like GCN, Sage, node2vec, deepwalk etc.
- Graph Self-Supervised Learning, Graph Contrast Learning, Learning on Heterophily Graph, HyperGraph Diffusion, Adversal Attacks on Graph and Graph Scalability.
- Usage of Pytorch, PyG, DGL. Additionally, I verify and modify several codes of papers with respect to Learning on heterophilous graph, graph self-supervised learnings.

Honors and Awards

Grand Prize, Subject Competition Scholarship — 2022

1st Prize, National Undergraduate Mathematics Contest (non-mathematical major) — Nov. 2021 & Sep. 2022

2nd Provincial Prize, High School Mathematics Joint Competition — 2018 & 2019

Good Rating(10%), High School Student Summer Camp of Tsinghua University — 2019