Yemin Yu

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Citizenship: United States

EDUCATION	**City University of Hong Kong**, Hong Kong, China

EDUCATION

City University of Hong Kong, Hong Kong, China
- Ph.D. in Computer Science — Feb 2022 – May 2025

University of Southern California, Los Angeles, CA, USA
- M.S. in Electrical Engineering, GPA:3.86/4 — Sep 2016 – Jun 2018

University of Southern California Los Angeles, CA, USA
- B.S. in Electrical Engineering, GPA:3.75/4 *Cum Laude* — Aug 2012 – Jun 2016

RESEARCH EXPERIENCE

Microsoft Research New England
- Research Intern — Jun 2023 – Sep 2023
  - Building self/weakly-supervised learning framework for image-based morphological profiling.
  - Building NLP/Geometric-based molecular structure screening/retrieval.
  - Applying LLM on information retrieval for building perturbation descriptors.

Ying Wei's Lab on AI4Science (CityU)
- Research Assistant (Supervisor: Dr. Ying Wei) — Feb 2022 –
  - Research on utilizing Language/Graph-based models (Transformers variants/GNN variants) for molecular synthesis prediction.
  - Employ Reinforcement Learning and Monte-Carlo Tree Search for path-finding in molecular synthesis route discovery.
  - Investigate the out-of-distribution (OOD) problem in molecular/reaction representation and prediction tasks and design solutions to alleviate the effect of distribution shift.

PUBLICATIONS

Active Retrosynthetic Planning Aware of Route Quality — ICLR, 2024
Yemin Yu, *Luotian Yuan, Ying Wei, Yongwei Wang, Zhihua Wang, Fei Wu**

RetroOOD: Understanding Out-of-Distribution Generalization in Retrosynthesis Prediction — AAAI, 2024
***Yemin Yu**, Luotian Yuan, Ying Wei, Hanyu Gao, Fei Wu*, Zhihua Wang, Xinhai Ye*

GRASP: Navigating Retrosynthetic Planning with Goal-driven Policy — NeurIPS, 2022
***Yemin Yu**, Ying Wei, Kun Kuang, Zhengxing Huang, Huaxiu Yao, Fei Wu**

Artificial Intelligence for Retrosynthesis Prediction — Engineering, 2022
*Yinjie Jiang, **Yemin Yu**(Co-First), Ming Kong, Yu Mei, Luotian Yuan, Zhengxing Huang, Kun Kuang, Zhihua Wang, Huaxiu Yao, James Zou, Connor W Coley*, Ying Wei**

OTHER WORK EXPERIENCE

WuXi AppTec, Shanghai, China — Jan 2021 – Feb 2022
- R&D Machine Learning Engineer - Chemical Automation
  - Built template-based/template-free single-step retrosynthesis prediction models from scratch and deployed them, including different graph/string-based classification/generative models.
  - Built different data-driven/non-data-driven models and deployed them for different multi-step retrosynthetic planning models.

DAMO Academy, Alibaba Inc., Hangzhou, China — Mar 2020 – Dec 2020
- Machine Learning Engineer Intern - Recommender System
  - Developed and deployed reinforcement learning for sequential recommendation for immersive swiping scenarios on mobile TaoBao.
  - Developed and deployed Learning2Rank on list/page-wise heavyweight ranking/re-ranking stage and re-ranking on edge devices.

Soundhound, Inc., Santa Clara, CA, USA — Oct 2018 – Dec 2019
- Machine Learning Engineer - Recommender System
  - Participated in building the Soundhound music discovery app, including Automatic Speech Recognition for queries and a recommender system for music and miscellaneous items.
  - Performed data analysis for user profiles/behaviors for better recommendations.

TECHNICAL SKILLS

Research Interests: Representation Learning in Molecules, Machine learning for Cheminformatics, Foundation Models, Natural Language Processing, Reinforcement Learning

Languages (Order in Fluency): Python, C++, MATLAB, Java