

Guikun Xu

AI FOR SCIENCE · MOLECULAR MACHINE LEARNING · DEEP GENERATIVE MODELS

School of Computing and Artificial Intelligence, Xipu Campus, Southwest Jiaotong University

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Education

Southwest Jiaotong University (SWJTU)

M.S. IN COMPUTER SCIENCE AND TECHNOLOGY (EXPECTED)

Chengdu, China

Sep. 2022 - Present

- **Mentors:** Professor Yan Yang and Assistant Researcher Yongquan Jiang
- **GPA:** 3.36/4
- **Main Courses:** Matrix Analysis (96.5/100); Mathematical Statistics and Multivariate Statistics (86/100); Optimization Theory and Methods (92/100); Computer Vision (85.6/100)

Southwest Petroleum University (SWPU)

B.S. IN ELECTRONIC INFORMATION SCIENCE AND TECHNOLOGY

Chengdu, China

Sep. 2018 - Jul. 2022

- **GPA:** 3.48/5.0

Reserach Experience

Reconstruction of 3D protein structures from cryo-EM images

MEGVII RESEARCH CHENGDU (AS AS INTERN)

Chengdu, China

May. 2024 - Present

- As an intern at Megvii Research Chengdu, I am engaged in a cutting-edge project focused on leveraging neural networks for the intricate task of reconstructing 3D protein structures from their cryo-electron microscopy images. cryo-EM reconstruction plays an indispensable role in biological and medical research, uncovering the intricate architecture and functionality of cellular components, thereby enriching our comprehension of the fundamental processes of life.

Deep Learning-Based Research on Molecular Conformation

SOUTHWEST JIAOTONG UNIVERSITY (SWJTU)

Chengdu, China

Sep. 2022 - Present

- Currently, I am dedicated to researching accelerated algorithms for the generation of molecular conformational ensembles. In recent years, diffusion-based algorithms for generating molecular conformational ensembles have become the mainstream approach in this field. However, the original diffusion model requires multiple steps of denoising, which significantly slows down the generation process. Therefore, the challenge lies in finding a way to accelerate the speed of the molecular conformational ensemble generation algorithm while ensuring high quality results. To address this issue, I am exploring and developing new algorithms and techniques with the aim of significantly improving the algorithm's execution speed, while maintaining high generation quality.
- Successfully, a network based on the Graph Transformer architecture has been constructed, achieving end-to-end prediction from the 2D topology of molecules to their 3D ground-state conformations, and attaining the state-of-the-art performance. In algorithm design, a novel and effective self-attention module has been proposed for 3D molecular structure modeling. This module greatly retains the practicality and elegance of the self-attention mechanism in the original Transformer network, while also exhibiting remarkable performance, making it easy to implement and quickly transfer to other molecular modeling tasks. This research achievement has been accepted by the 12th International Conference on Learning Representations (ICLR 2024) and selected as a Spotlight Presentation [Top 5%].

Publications

GTMGC: Using Graph Transformer to Predict Molecule's Ground-State Conformation

ICLR2024 (spotlight)

GUIKUN XU, YONGQUAN JIANG, PENGCHUAN LEI, YAN YANG, JIM CHEN

2024

- **Keywords:** molecular conformation prediction, molecule modeling, graph neural network, graph transformer
- **TL;DR:** We propose a Graph-Transformer network which uses a novel self-attention mechanism we developed for molecular structure modeling, achieving SOTA performance in predicting a molecule's ground-state 3D conformation from its 2D topology graph.

Skills

DL Frameworks PyTorch, TensorFlow, PaddlePaddle
Programming Python, C/C++
Languages Chinese (Native), English (CET-6 552/710)

Honors & Awards

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| 2023.10 | 2nd Class Academic Scholarship , Southwest Jiaotong University (SWJTU). | Chengdu, China |
| 2022.10 | 2nd Class Academic Scholarship , Southwest Jiaotong University (SWJTU). | Chengdu, China |
| 2021.10 | Certificate of Completion and Second Prize for Provincial-level College Students' Innovation and Entrepreneurship Training Program in 2020 , Southwest Petroleum University (SWPU). | Chengdu, China |