刘祥（BIMSA）
Title: Persistent homology: an overview
Abstract: 介绍持续同调的前世今生（历史、发展等）

刘冉（北航）
Title: Persistent path-spectral based machine learning for protein-ligand binding affinity prediction
Abstract: Molecular descriptors are essential to quantitative structure activity/property relationship (QSAR/QSPR) models and machine learning models. In this talk we will introduce our recently proposed persistent path-spectral (PPS), PPS-based molecular descriptors, and PPS-based machine learning model for the prediction of the protein-ligand binding affinity. For the graph, simplicial complex, and hypergraph representation of molecular structures and interactions, the path-Laplacian can be constructed and the derived pathspectral naturally gives a quantitative description of molecules. Further, by introducing the filtration process of the representation, the persistent path-spectral can be derived, which gives a multiscale characterization of molecules. Molecular descriptors from the persistent path-spectral attributes then are combined with the machine learning model, in particular, the gradient boosting tree, to form our PPS-ML model. We test our model on three most commonly used data sets, i.e., PDBbind-v2007, PDBbind-v2013, and PDBbind-v2016, and our model can achieve competitive results.

吴双（BIMSA）
Title: Applications of GLMY theory in metabolomic networks of complex diseases
Abstract: Human diseases involve metabolic alterations. Metabolomic profiles have served asa vital biomarker for the early identification of high-risk individuals and disease prevention. We have leveraged a statistical physics model to combine all metabolites into bidirectional, signed, and weighted interaction networks and trace how the flow of information from one metabolite to the next causes changes in health state. We integrate concepts from ecosystem theory and evolutionary game theory to model how the health state-dependent alteration of a metabolite is shaped by its intrinsic properties and through extrinsic influences from its conspecifics. We code intrinsic contributions as nodes and extrinsic contributions as edges into quantitative networks and implement GLMY homology theory to analyze and interpret the topological change of health state from symbiosis to dysbiosis. The application of this model to real data allows us to identify several hub metabolites and their interaction webs, which play a part in the formation of inflammatory bowel diseases.

王炳胥（北京大学深圳研究生院新材料学院）
题目 GLMY 理论辅助的用于材料预测和生成的机器学习框架
摘要：
高熵合金因其多样可调的活性位点所构成的广阔化学空间而在催化领域引起越来越多的关注。为了加速这一化学空间的探索，高效的深度学习模型变得至关重要。然而，在通过深度学习设计晶体材料的任务中，出现了三个主要障碍：缺乏晶体结构固有数学特征的表示，模型训练数据不足，以及由于可解释性问题导致对机器学习结果信心不足。
鉴于这些挑战，本文提出了一种基于持续 GLMY 同调的半监督预测和生成框架，由我们的 PathVAEs 提供支持。该框架旨在预测高熵合金催化剂的吸附能和设计潜力。它通过以下方

式解决这些障碍：(1) 引入一种有效的拓扑方法以提取固有特征——配体和配位特征；(2) 利用半监督学习增强模型训练；(3) 将机器学习操作与催化含义对齐。结果令人鼓舞：预测组件达到了高准确性，生成方面产生了八种高性能催化剂设计。该工作不仅提供了一种优秀的基于拓扑的特征提取方法，还为晶体材料的设计引入了一种新的研究范式。

关键词： 路径拓扑，深度学习，晶体材料，可解释性，生成框架

简历：
王炳胥是北京大学深圳研究生院新材料学院潘锋教授团队的在读博士生。他的研究工作主要集中在预测材料性质、微调结构属性以及设计新型晶体和无机小分子材料的结构，重点关注能源材料、电池材料和催化材料。研究方法涉及利用拓扑数据分析（TDA），特别是 GLMY 理论、持续同调和持续 GLMY 同调。这些技术被用于从晶体和小分子结构中提取拓扑特征，随后将这些特征与人工智能算法结合，以预测性能、优化结构设计，并开发用于材料分析和设计的专用软件。

乔子越（大湾区大学（筹））
title：Evolving Graph Machine Learning: From Stationary to Out-of-Distribution Perspectives

# Path Topology and GLMY Theory-assisted Machine Learning Framework for Material Prediction and Generation

Author(s): Bingxu Wang
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Abstract:
High-entropy alloys are attracting ever-increasing attention in the field of catalysis by virtue of the vast chemical space constituted by their diverse tunable active sites. To expedite exploration within this chemical space, a proficient deep-learning model becomes essential. However, in the task of designing crystalline materials through deep learning, three major obstacles arise: the absence of inherent mathematical features contributing to the appealing properties, insufficient training data for the model, and limited confidence in results due to interpretability issues.
In light of these challenges, this work proposes a persistent path homology-based semi-supervised prediction and generation framework, empowered by our PathVAEs. This framework aims to predict the adsorption energy and design potential for High-entropy alloy catalysts. It addresses these obstacles by (1) introducing an effective topological approach to extract intrinsic features—ligand and coordination features; (2) utilizing semi-supervised learning to enhance model training; and (3) aligning machine learning operations with catalytic implications. The results are promising: the prediction component attains high accuracy, and the generation aspect yields eight high-performance catalyst designs. This work not only offers an excellent topology-based feature extraction method but also introduces a new research paradigm for the design of crystalline materials.

Keywords:
Path topology, Deep learning, Crystalline materials, Interpretability, Generation framework

Bio(s):
Bingxu Wang is a current PhD student in Prof. Feng Pan's group at School of Advanced Materials, Peking University, Shenzhen Graduate School. His research endeavors are centered around the anticipation of properties, fine-tuning of structural attributes, and the design of novel structure of crystalline and inorganic small molecule materials with a primary emphasis on energy materials, battery materials, and catalytic materials. The research methodology involves harnessing Topological Data Analysis (TDA), specifically leveraging GLMY theory, persistent homology, and persistent GLMY homology. These techniques are employed to extract topological features from crystal and small molecule structures. Subsequently, these features are combined with artificial intelligence algorithms to predict performance, refine structural design, and develop specialized software for the analysis and design of materials.

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