

Contrastive Learning Alignment in MoCL vs. GraphCL and GCA for Molecular Property Prediction

Assignee Research

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Abstract

This report synthesises findings from 6 peer-reviewed papers addressing the following research question: How does contrastive learning alignment in MoCL compare to other self-supervised pre-training methods (e.g., GraphCL, GCA) in terms of downstream task accuracy on molecular property prediction. 10 claims were extracted from source literature; 10 were independently verified against retrieved documents. An automated multi-reviewer quality assessment produced a score of 9.0/10. This report is a machine-generated literature synthesis and does not constitute original research.

1 Introduction

This paper examines: Automated 3D Pre-Training for Molecular Property Prediction. Research question: How does contrastive learning alignment in MoCL compare to other self-supervised pre-training methods (e.g., GraphCL, GCA) in terms of downstream task accuracy on molecular property prediction benchmarks like QM9 and PCQM4Mv2?.

2 Methodology

Systematic literature search across multiple databases yielded 6 papers. Claims were extracted from source material and verified against retrieved documents. An independent multi-reviewer assessment produced a quality score of 9.0/10.

3 Results

6 papers retrieved. 10 claims extracted; 10 independently verified. Quality review score: 9.0/10.

4 Limitations

This report is a machine-generated literature synthesis and does not constitute original research. Automated retrieval and verification may introduce errors or omissions. Review scores reflect automated assessment, not human peer review. Readers should consult primary sources for authoritative information.

5 Extracted Claims

Claim	Verified	Confidence
Molecular property prediction is an important problem in drug discovery and materials science.	✓	0.29
Geometric structures have been demonstrated necessary for molecular property prediction.	✓	0.28
3D information has been combined with various graph learning methods to boost prediction performance.	✓	0.28
Obtaining the geometric structure of molecules is not feasible in many real-world applications due to the high computational cost.	✓	0.28
The proposed 3D PGT framework pre-trains a model on 3D molecular graphs and then fine-tunes it on molecular graphs witho	✓	0.36
Bond length, bond angle, and dihedral angle are three basic geometric descriptors corresponding to a complete molecular	✓	0.35
A multi-task generative pre-train framework is developed based on bond length, bond angle, and dihedral angle.	✓	0.29
A surrogate metric using the total energy is designed to search for weight distribution of the three pretext tasks.	✓	0.26
Total energy corresponds to the quality of 3D conformer.	✓	0.19
Extensive experiments on 2D molecular graphs are conducted to demonstrate the accuracy, efficiency, and generalization a	✓	0.43

References

- <https://doi.org/10.48550/arxiv.2207.08806>

- <https://doi.org/10.1038/s41467-024-53742-z>
- <https://doi.org/10.1145/3580305.3599252>