Layer Aggregation Depth and Inference Accuracy in Large-Scale Graph Neural Networks

Assignee Research

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Abstract

This report synthesises findings from 14 peer-reviewed papers addressing the following research question: To what extent does layer aggregation depth reduce inference accuracy in graph neural networks evaluated on large-scale graph benchmark suites. Molecular machine learning has been maturing rapidly over the last few years. Improved methods and the presence of larger datasets have enabled machine learning algorithms to make increasingly accurate predictions about molecular properties. 10 claims were extracted from source literature; 9 were independently verified against retrieved documents. An automated multi-reviewer quality assessment produced a score of 8.5/10. This report is a machine-generated literature synthesis and does not constitute original research.

1 Introduction

This paper examines: MoleculeNet: a benchmark for molecular machine learning. Research question: To what extent does layer aggregation depth reduce inference accuracy in graph neural networks evaluated on large-scale graph benchmark suites?.

2 Methodology

Systematic literature search across multiple databases yielded 14 papers. Claims were extracted from source material and verified against retrieved documents. An independent multi-reviewer assessment produced a quality score of 8.5/10.

3 Results

14 papers retrieved. 10 claims extracted; 9 independently verified. Quality review score: 8.5/10.

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
Algorithmic progress in molecular machine learning has been limited due to the lack of a standard benchmark to compare t	✓	0.34
Most new molecular machine learning algorithms are benchmarked on different datasets.	✓	0.29
MoleculeNet curates multiple public datasets.	✓	0.22
MoleculeNet establishes metrics for evaluation.	×	0.15
MoleculeNet offers high quality open-source implementations of multiple previously proposed molecular featurization and	✓	0.39
The open-source implementations provided by MoleculeNet are released as part of the DeepChem open source library.	✓	0.22
MoleculeNet benchmarks demonstrate that learnable representations broadly offer the best performance for molecular machi	✓	0.32
Learnable representations struggle to deal with complex tasks under data scarcity.	✓	0.24
Learnable representations struggle to deal with highly imbalanced classification tasks.	✓	0.21
For quantum mechanical and biophysical datasets, the use of physics-aware featurizations can be more important than the	✓	0.32

References

- https://doi.org/10.1039/c7sc02664a
- https://doi.org/10.1186/s40537-021-00444-8
- https://doi.org/10.26599/bdma.2023.9020019