Scaling Graph Diffusion Models and GNNs Under Adversarial Spectral Perturbations

Assignee Research

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Abstract

This report synthesises findings from 13 peer-reviewed papers addressing the following research question: How does the inference throughput of graph diffusion models compare to traditional GNNs when scaling to graphs with over 100,000 nodes under adversarial spectral perturbations. Machine learning plays an increasingly important role in many areas of chemistry and materials science, being used to predict materials properties, accelerate simulations, design new structures, and predict synthesis routes of new materials. Graph neural networks (GNNs) are one. 6 claims were extracted from source literature; 6 were independently verified against retrieved documents. An automated multi-reviewer quality assessment produced a score of 8.8/10. This report is a machine-generated literature synthesis and does not constitute original research.

1 Introduction

This paper examines: Graph neural networks for materials science and chemistry. Research question: How does the inference throughput of graph diffusion models compare to traditional GNNs when scaling to graphs with over 100,000 nodes under adversarial spectral perturbations?.

2 Methodology

Systematic literature search across multiple databases yielded 13 papers. Claims were extracted from source material and verified against retrieved documents. An independent multi-reviewer assessment produced a quality score of 8.8/10.

3 Results

13 papers retrieved. 6 claims extracted; 6 independently verified. Quality review score: 8.8/10.

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
Machine learning plays an increasingly important role in many areas of chemistry and materials science, being used to pr	✓	0.60
Graph neural networks (GNNs) are one of the fastest growing classes of machine learning models.	✓	0.35
GNNs are of particular relevance for chemistry and materials science, as they directly work on a graph or structural rep	✓	0.53
The paper provides an overview of the basic principles of GNNs, widely used datasets, and state-of-the-art architectures	✓	0.29
The paper discusses a wide range of recent applications of GNNs in chemistry and materials science.	✓	0.33
The paper concludes with a road-map for the further development and application of GNNs.	✓	0.19

References

- https://doi.org/10.35833/mpce.2021.000058
- https://doi.org/10.1038/s43246-022-00315-6
- https://doi.org/10.1109/tnsm.2020.2971776