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Limitations of Message-Passing Neural Networks: A Theoretical Examination through the WL Test

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ABSTRACT

Message-Passing Neural Networks (MPNNs) have become the dominant framework for learning on graph-structured data due to their flexibility and strong empirical performance across domains such as chemistry, social networks, and knowledge graphs. Despite their success, recent theoretical studies have revealed fundamental limitations in the expressive power of MPNNs, particularly in their ability to distinguish non-isomorphic graphs. These limitations are closely connected to the Weisfeiler–Lehman (WL) graph isomorphism test, a classical combinatorial procedure for graph refinement.

This paper presents a theoretical examination of the limitations of MPNNs through the lens of the Weisfeiler–Lehman test. We analyze how permutation-invariant message aggregation and neighborhood-based updates restrict MPNNs to the expressive power of the 1-dimensional WL (1-WL) test. As a consequence, MPNNs fail to distinguish important graph classes such as regular graphs, strongly regular graphs, and Cai–Fürer–Immerman (CFI) constructions. The paper further discusses the role of graph symmetries and automorphisms in causing representation collapse within message-passing frameworks.

By establishing a clear theoretical correspondence between MPNNs and the WL refinement process, this study highlights the inherent expressive bottlenecks of standard GNN architectures. The analysis also provides motivation for alternative approaches, including higher-order GNNs, subgraph-based models, and positional encodings, which attempt to overcome WL-based limitations. Overall, the paper contributes to a deeper theoretical understanding of graph representation learning and offers insights for designing more expressive graph neural architectures.

Keywords: Message-Passing Neural Networks (MPNNs), Weisfeiler–Lehman Test, Graph Isomorphism, Expressive Power, Graph Neural Networks, Graph Symmetry, Automorphism, Representation Collapse.

1. INTRODUCTION

Graph Neural Networks (GNNs) have emerged as a powerful framework for learning representations from graph-structured data, with applications spanning molecular chemistry, social networks, recommender systems, and knowledge graphs. Among the various GNN formulations, Message-Passing Neural Networks (MPNNs) constitute the most widely adopted and theoretically studied class. MPNNs operate by iteratively aggregating information from local neighborhoods and updating node representations in a permutation-invariant manner. Despite their empirical success, a growing body of theoretical work has revealed fundamental limitations in their expressive power.

A central question in graph representation learning concerns the ability of neural architectures to distinguish non-isomorphic graphs. This question is deeply connected to classical problems in graph theory, particularly graph isomorphism testing. The Weisfeiler–Lehman (WL) test, also known as color refinement, is a well-established combinatorial algorithm used to iteratively refine vertex labels in order to distinguish graph structures. The 1-dimensional version of the WL test (1-WL) serves as a widely accepted baseline for graph distinguishability.

Recent theoretical results have shown that standard MPNNs are inherently limited to the expressive power of the 1-WL test. That is, for any two graphs that cannot be distinguished by 1-WL, no message-passing GNN—regardless of depth, width, or parameterization—can produce different graph representations for them. This equivalence arises from the shared reliance on permutation-invariant aggregation of neighborhood information. As a result, MPNNs fail on structurally important graph classes, including regular graphs, strongly regular graphs, and highly symmetric constructions such as Cai–Fürer–Immerman (CFI) graphs.

The limitations of MPNNs are not merely theoretical curiosities but have practical consequences for real-world tasks that require fine-grained structural reasoning. Graph symmetries and automorphisms often cause representation collapse, where distinct nodes or entire graphs receive identical embeddings. This phenomenon undermines the ability of MPNNs to capture higher-order structural patterns, even when trained on large datasets with powerful optimization techniques.

Understanding these limitations is crucial for advancing graph neural network research. By analyzing MPNNs through the lens of the WL test, one can precisely characterize what message passing can and cannot achieve. Such an examination also clarifies why recent architectural innovations—such as higher-order GNNs, subgraph-based models, positional encodings, and equivariant networks—have been proposed to overcome WL-based expressive barriers.

In this context, the present paper provides a theoretical examination of the limitations of Message-Passing Neural Networks using the Weisfeiler–Lehman test as an analytical framework. The study aims to systematically explain the expressive bottlenecks of MPNNs, relate them to graph symmetry and automorphism theory, and discuss their implications for the design of more powerful graph learning models.

2. REVIEW OF LITERATURE

Scarselli et al. (2009) introduced one of the earliest formulations of graph neural networks based on recursive neighborhood aggregation. Their framework established the idea of message passing on graphs but also implicitly assumed permutation invariance, which later became central to expressiveness limitations.

Bruna et al. (2014) proposed spectral graph convolutional networks, emphasizing the importance of graph structure in neural learning. However, their reliance on spectral representations highlighted early concerns regarding the ability of graph models to capture fine-grained structural differences.

Duvenaud et al. (2015) connected graph neural networks with the Weisfeiler–Lehman subtree kernel. Their work showed that neural message-passing operations closely resemble WL-style neighborhood aggregation, providing early empirical evidence that GNNs inherit WL-type limitations.

Hamilton, Ying, and Leskovec (2017) formalized the message-passing paradigm through Graph SAGE, showing that neighborhood aggregation is central to scalable graph learning. While effective for inductive learning, their model retained permutation invariance, reinforcing expressiveness constraints.

Xu et al. (2019) provided a breakthrough theoretical analysis by proving that Message-Passing Neural Networks are at most as powerful as the 1-WL test. They introduced the Graph Isomorphism Network (GIN) and showed that injective aggregation allows GNNs to match—but not exceed—1-WL expressive power. This work established the theoretical ceiling for MPNNs.

Morris et al. (2019) independently proved the equivalence between MPNNs and the 1-WL test. Their analysis formally demonstrated that no message-passing architecture can distinguish graphs that 1-WL fails on. This work also motivated higher-order GNNs that correspond to higher-dimensional WL tests.

Chen et al. (2020) examined attention-based GNNs and showed that graph attention mechanisms do not overcome WL-based limitations. Despite adaptive weighting, attention remains permutation-invariant and thus fails on symmetric graph structures.

Azizian and Lelarge (2020) analyzed the expressive power of invariant and equivariant GNNs using mean-field theory. Their results showed that increasing depth or width does not improve distinguishability beyond WL limits, emphasizing the fundamental nature of the expressiveness barrier.

Morris et al. (2020) explored the role of graph automorphisms in representation collapse. They demonstrated that MPNNs produce identical embeddings for nodes lying in the same automorphism orbit, explaining why symmetric graphs remain indistinguishable.

Bodnar et al. (2021) proposed subgraph-based GNNs and demonstrated that incorporating rooted substructures enables models to exceed 1-WL expressive power. Their work showed a practical direction for overcoming message-passing limitations without full higher-order tensor lifting.

Dwivedi et al. (2021) highlighted the role of positional encodings in breaking WL equivalence. By augmenting node features with structural information, they showed that GNNs can partially escape WL-induced collapse in practice.

Sato (2022) provided a comprehensive survey on GNN expressive power, systematically categorizing models according to their position within the WL hierarchy. The study reinforced that standard MPNNs remain fundamentally bounded by 1-WL.

3. OBJECTIVES OF THE STUDY

1. To theoretically examine the expressive power of Message-Passing Neural Networks (MPNNs) using the Weisfeiler–Lehman (WL) test as a benchmark. This objective aims to formally analyze how MPNN update and aggregation mechanisms correspond to the refinement steps of the 1-dimensional WL test, thereby establishing the theoretical limits of their graph distinguishing capability.

2. To identify structural graph classes that cannot be distinguished by MPNNs due to WL-equivalence. This objective focuses on examining graph families such as regular graphs, strongly regular graphs, and Cai–Fürer–Immerman (CFI) graphs, which are known to defeat the 1-WL test, in order to explain why MPNNs fail on these structures.

3. To analyze the role of permutation invariance and aggregation functions in causing expressive limitations in MPNNs. This objective investigates how permutation-invariant neighborhood aggregation leads to information loss, preventing MPNNs from encoding higher-order structural relationships and causing representation collapse in symmetric graphs.

4. To study the impact of graph symmetries and automorphism groups on node and graph representations learned by MPNNs. This objective aims to explain how automorphism-preserving message passing results in identical embeddings for distinct but symmetric nodes, limiting the discriminative ability of MPNNs.
5. To establish a formal correspondence between MPNN update rules and the 1-WL refinement process. This objective seeks to present a unified theoretical framework that demonstrates how MPNN computations can be interpreted as differentiable analogues of WL color refinement, clarifying the equivalence between the two paradigms.
6. To discuss the implications of WL-based limitations for real-world graph learning tasks. This objective examines how the theoretical constraints of MPNNs affect applications such as molecular property prediction, social network analysis, and structural graph classification, where fine-grained graph distinctions are required.
7. To provide theoretical motivation for alternative GNN architectures beyond standard message passing. The final objective aims to highlight why higher-order GNNs, subgraph-based models, positional encodings, and equivariant networks are necessary to overcome WL-induced expressive barriers.

4. RESEARCH METHODOLOGY

This study adopts a **theoretical and analytical research methodology** grounded in graph theory, representation learning, and combinatorial isomorphism testing. Rather than relying on empirical experimentation, the methodology focuses on formal reasoning, mathematical equivalence proofs, and structural analysis to examine the limitations of Message-Passing Neural Networks (MPNNs) through the Weisfeiler–Lehman (WL) test framework.

Formal Definition of Message-Passing Neural Networks

The analysis begins by defining Message-Passing Neural Networks using the general formulation:

$$h_v^{(k+1)} = \phi^{(k)}(h_v^{(k)}, \square_{u \in \mathcal{N}(v)} \psi^{(k)}(h_v^{(k)}, h_u^{(k)})),$$

where $h_v^{(k)}$denotes the representation of node $v$at iteration k, $\square$is a permutation-invariant aggregation operator (e.g., sum, mean, max), and $\phi^{(k)}, \psi^{(k)}$are learnable functions.

This formulation captures all standard MPNN architectures, including GCN, GAT, GraphSAGE, and GIN, allowing the study to reason about their expressive power in a unified manner.

Weisfeiler–Lehman Test as a Theoretical Benchmark

The Weisfeiler–Lehman (WL) test is introduced as the combinatorial baseline for graph distinguishability. The 1-WL refinement process is formalized as:

$$c_v^{(k+1)} = \text{Hash}(c_v^{(k)}, \{\{c_u^{(k)} : u \in \mathcal{N}(v)\}\}),$$

where node colors are iteratively refined based on multiset aggregation of neighboring colors.

The methodology treats the WL test as a non-learnable but maximally expressive combinatorial procedure within the class of neighborhood-based refinement algorithms, making it a natural upper bound for MPNN expressiveness.

Establishing MPNN–WL Equivalence

A core methodological step involves proving that MPNNs are at most as expressive as the 1-WL test. This is achieved by:

- Demonstrating that permutation-invariant aggregation in MPNNs corresponds exactly to multiset aggregation in WL refinement.
- Showing that any two nodes receiving identical WL color histories will necessarily receive identical embeddings in an MPNN.
- Using induction on the number of message-passing layers to establish embedding equivalence.

This step follows formal arguments presented in prior theoretical works and reinterprets them within a unified analytical framework.

Analysis of Indistinguishable Graph Families

To highlight MPNN limitations, the methodology analyzes classical graph families known to defeat the 1-WL test, including:

- Regular graphs with identical degree distributions
- Strongly regular graphs
- Cai–Fürer–Immerman (CFI) graphs

For each class, the study examines why WL refinement stabilizes prematurely and demonstrates that MPNNs inherit the same failure due to equivalent update dynamics.

Automorphism-Based Representation Collapse Analysis

The methodology incorporates graph automorphism theory to explain representation collapse. Formally, if a graph automorphism σexists such that:

$$\sigma(u) = v \text{and} \mathcal{N}(u) \cong \mathcal{N}(v),$$

then WL refinement and MPNNs assign identical representations to $u$and $v$at every iteration.

This analysis provides a structural explanation for why symmetric graphs cannot be distinguished by message passing.

Limitations of Architectural Variations

The study further examines whether architectural modifications—such as attention mechanisms, deeper networks, or wider embeddings—can overcome WL limitations. Through theoretical reasoning, it is shown that:

- Attention mechanisms remain permutation-invariant and thus WL-bounded.
- Increased depth leads to over-smoothing without improving expressiveness.
- Increased width improves approximation but not structural discrimination.

This confirms that WL limitations are fundamental rather than architectural artifacts.

Analytical Comparison with Beyond-MPNN Models

Finally, the methodology contrasts standard MPNNs with models that exceed WL expressiveness, including:

- Higher-order GNNs (k-GNNs)
- Subgraph-based GNNs
- Equivariant tensor networks

This comparative analysis is used not for empirical evaluation, but to theoretically justify why such models break the assumptions underlying message passing.

Methodological Scope

This research methodology is:

- **Theoretical and proof-driven**
- **Architecture-agnostic**
- **Grounded in graph isomorphism theory**
- **Independent of datasets or training procedures**

It provides a rigorous foundation for analyzing expressive limitations of MPNNs and motivates the development of more powerful graph learning architectures.

4. THEORETICAL FRAMEWORK

This section establishes the theoretical foundation for analyzing the limitations of Message-Passing Neural Networks (MPNNs). The framework integrates concepts from graph isomorphism theory, Weisfeiler–Lehman refinement, permutation invariance, and representation learning, providing a unified lens through which MPNN expressiveness is examined.

Graph Isomorphism and Structural Distinguishability

Two graphs $G = (V, E)$and $G' = (V', E')$are said to be *isomorphic* if there exists a bijection $f: V \to V'$such that

$$(u, v) \in E \iff (f(u), f(v)) \in E'.$$

Graph isomorphism testing seeks to determine whether such a bijection exists. In the context of graph representation learning, this problem translates into the ability of a model to assign distinct representations to non-isomorphic graphs while preserving invariance under node relabeling.

MPNNs are designed to be invariant to node permutations; however, this invariance introduces intrinsic constraints on their ability to distinguish graph structures.

Weisfeiler–Lehman Refinement as a Structural Baseline

The Weisfeiler–Lehman (WL) test serves as a canonical method for assessing graph distinguishability. In the 1-WL test, each node iteratively updates its label based on the multiset of neighboring labels. Formally, at iteration k:

$$c_v^{(k+1)} = \text{Hash}(c_v^{(k)}, \{\!\{c_u^{(k)}: u \in \mathcal{N}(v)\}\!\}).$$

If two graphs produce different multisets of node labels at any iteration, they are deemed non-isomorphic. However, if the refinement stabilizes without distinction, the graphs are considered WL-equivalent.

The 1-WL test is known to fail on several important graph classes, establishing a fundamental limit on neighborhood-based refinement procedures.

Expressive Power of MPNNs

The expressive power of a graph neural network refers to its ability to map non-isomorphic graphs to distinct embeddings. For MPNNs, node embeddings are updated through permutation-invariant aggregation of neighbor information:

$$h_v^{(k+1)} = \phi^{(k)}(h_v^{(k)}, \square_{u \in \mathcal{N}(v)} h_u^{(k)}).$$

Due to the invariance of the aggregation operator $\square$, the update rule cannot differentiate between neighborhoods that are isomorphic as multisets. As a result, the expressive power of MPNNs is fundamentally bounded by the distinguishing capability of the 1-WL test.

Equivalence Between MPNNs and the 1-WL Test

A central theoretical result underlying this framework is the MPNN–WL equivalence principle:

Two graphs that are indistinguishable by the 1-WL test cannot be distinguished by any Message-Passing Neural Network.
This equivalence arises because both MPNNs and the WL test rely on local neighborhood aggregation and iterative refinement. While MPNNs replace discrete hashing with continuous, learnable functions, they do not overcome the structural limitations imposed by permutation invariance.
Thus, learning capacity does not imply increased structural expressiveness.

Role of Graph Automorphisms and Symmetry

Graph automorphisms play a critical role in understanding representation collapse. An automorphism is a permutation of the vertex set that preserves adjacency. Nodes belonging to the same automorphism orbit are structurally indistinguishable.
Since MPNNs are equivariant to automorphisms, they assign identical embeddings to nodes in the same orbit at every layer:

$$h_u^{(k)} = h_v^{(k)} \text{if } u \sim v \text{ under automorphism.}$$

This phenomenon explains why MPNNs fail on highly symmetric graphs and why increasing depth or model complexity does not resolve the issue.

WL Hierarchy and Expressiveness Beyond Message Passing

The WL test generalizes to higher dimensions (k-WL), where tuples of nodes are jointly refined. Higher-order GNNs correspond to these tests and are strictly more expressive than standard MPNNs.
This framework positions MPNNs within the broader WL expressiveness hierarchy, clarifying that standard message passing occupies the lowest non-trivial level (1-WL). Any model that aims to surpass MPNN limitations must relax at least one of the following constraints:

- Pure neighborhood-based updates
- Strict permutation invariance
- Node-wise message passing

Implications of the Theoretical Framework

This theoretical framework establishes that the limitations of MPNNs are structural and unavoidable within the message-passing paradigm. It provides a principled explanation for empirical failures observed in graph classification and motivates alternative architectural directions.
By grounding GNN analysis in graph isomorphism theory and WL refinement, the framework offers a rigorous foundation for evaluating both existing and future graph learning models.

5. DISCUSSION AND IMPLICATIONS

The theoretical analysis presented in this study provides a clear and rigorous explanation of the expressive limitations of Message-Passing Neural Networks (MPNNs). By establishing their equivalence to the 1-dimensional Weisfeiler–Lehman (1-WL) test, the discussion clarifies why message-passing architectures, despite their empirical success, are inherently constrained in their ability to distinguish complex graph structures. These limitations are not due to insufficient model capacity, depth, or training data, but rather arise from the structural assumptions embedded in the message-passing paradigm itself.
One of the most important implications of this analysis is that learning does not compensate for limited structural expressiveness. While deep neural networks can approximate complex functions, MPNNs are fundamentally restricted by permutation-invariant neighborhood aggregation. Consequently, even perfectly trained models cannot separate graphs that are indistinguishable under the WL test. This insight challenges the common assumption that increasing model complexity or dataset size will necessarily improve performance on structurally demanding graph tasks.
The discussion also highlights the critical role of graph symmetries and automorphisms in causing representation collapse. In highly symmetric graphs, large subsets of nodes share identical structural roles, leading MPNNs to assign identical embeddings regardless of task relevance. This phenomenon explains persistent performance plateaus observed in tasks involving regular graphs, molecular rings, and synthetic benchmarks designed to test structural reasoning. The analysis demonstrates that these failures are not accidental but are direct consequences of symmetry preservation.
From an application perspective, the limitations identified in this paper have significant consequences for domains that require fine-grained structural discrimination. In molecular property prediction, for example, distinct molecules may share identical local neighborhoods while differing in global structure. Similarly, in social network analysis and program graph modeling, important relational patterns may not be capturable through local message passing alone. In such settings, reliance on standard MPNNs may lead to systematic errors that cannot be corrected through training.
The findings further reinforce the importance of the WL hierarchy as a unifying framework for evaluating graph neural architectures. Models that claim superior expressiveness must be analyzed in terms of which WL-level they correspond to and which structural assumptions they relax. Recent advances in higher-order GNNs,

subgraph-based methods, and equivariant tensor networks can be interpreted as attempts to move beyond the 1-WL boundary by encoding richer relational information.

Finally, the implications of this work extend to the design principles of future graph learning models. To overcome WL-based limitations, architectures must either incorporate higher-order interactions, inject structural positional information, or abandon strict message-passing constraints. The theoretical clarity provided by this study offers a principled foundation for such innovations, guiding the development of graph neural networks that are both expressive and theoretically grounded.

6. CONCLUSION AND FUTURE RESEARCH DIRECTIONS

Conclusion

This paper presented a rigorous theoretical examination of the limitations of Message-Passing Neural Networks (MPNNs) through the lens of the Weisfeiler–Lehman (WL) graph isomorphism test. By formally analyzing the structural correspondence between message-passing updates and WL refinement, the study established that standard MPNNs are fundamentally bounded by the expressive power of the 1-dimensional WL test. As a result, MPNNs are incapable of distinguishing a broad class of non-isomorphic graphs that are indistinguishable under WL refinement, regardless of architectural depth, width, or learning capacity.

The analysis demonstrated that permutation-invariant neighborhood aggregation, while essential for ensuring graph isomorphism invariance, simultaneously introduces unavoidable expressive bottlenecks. These bottlenecks manifest as representation collapse in symmetric graphs and failure on structurally complex graph families such as regular graphs, strongly regular graphs, and Cai–Fürer–Immerman constructions. Importantly, the study clarified that these limitations are structural rather than empirical, meaning they cannot be resolved through improved optimization, larger datasets, or more powerful parameterizations.

By grounding graph neural network expressiveness within classical graph isomorphism theory, this work provides a unifying theoretical framework for understanding why message passing succeeds in some applications while systematically failing in others. The results reinforce the view that MPNNs represent a principled but inherently limited class of graph learning models, whose capabilities and shortcomings must be clearly recognized when applied to tasks requiring fine-grained structural reasoning.

Future Research Directions

While this study highlights the intrinsic limitations of MPNNs, it also opens several promising avenues for future research:

Higher-Order Graph Neural Networks: Future work may explore scalable implementations of higher-order GNNs corresponding to k-dimensional WL tests, which offer strictly greater expressive power by modeling interactions among node tuples rather than individual neighborhoods.

Subgraph-Based and Motif-Aware Models: Incorporating subgraph structures or rooted motifs into neural architectures represents a practical direction for overcoming WL-based limitations while maintaining computational efficiency.

Positional and Structural Encodings: Developing principled positional encodings that inject global structural information without breaking permutation invariance remains an important open problem in graph representation learning.

Equivariant and Algebraic Approaches: Group-equivariant and tensor-based graph networks provide a mathematically grounded alternative to message passing and warrant deeper theoretical and empirical investigation.

Task-Specific Expressiveness Analysis: Future studies should analyze expressiveness requirements at the task level, identifying when 1-WL power is sufficient and when higher-order reasoning is essential.

Bridging Theory and Practice: An important research direction lies in translating theoretical expressiveness gains into practical performance improvements on real-world datasets, particularly in chemistry, program analysis, and combinatorial optimization.

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