Graph Neural Networks for Large-Scale Molecular Property Prediction Using Hierarchical Message Passing

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Abstract

Graph Neural Networks (GNNs) have emerged as one of the most successful deep learning paradigms for processing graph-structured data. Their ability to capture complex relationships among interconnected entities has enabled significant advances in molecular property prediction, drug discovery, recommendation systems, social network analysis, and scientific computing. Despite these advances, many existing GNN models experience performance degradation when applied to large molecular graphs because of oversmoothing, limited long-range information propagation, and increasing computational complexity.

This paper presents a hierarchical message-passing framework for large-scale molecular property prediction using graph neural networks. The proposed architecture combines multi-level neighborhood aggregation, adaptive attention mechanisms, and hierarchical graph pooling to improve representation learning while maintaining computational efficiency. Experimental evaluation demonstrates consistent improvements in prediction accuracy, convergence speed, scalability, and training efficiency compared with several representative baseline models.

Although the presented study is entirely fictional and created solely for portfolio demonstration purposes, it illustrates the preparation of a complete NeurIPS manuscript containing mathematical derivations, algorithms, figures, tables, appendices, and bibliography using the official conference template.

1 Introduction

Graphs provide one of the most expressive representations for modeling complex relationships among interconnected entities. Numerous real-world systems naturally exhibit graph structures, including social networks, knowledge graphs, transportation systems, communication networks, biological pathways, and molecular structures. Unlike conventional tabular data, graph data simultaneously captures both the characteristics of individual entities and the relationships that connect them, making graph learning a rapidly growing area of artificial intelligence.

Among graph-based learning techniques, Graph Neural Networks (GNNs) have emerged as one of the most successful deep learning paradigms for processing irregular relational data. By repeatedly exchanging information among neighboring nodes, GNNs learn expressive node, edge, and graph representations that support numerous downstream tasks, including node classification, graph classification, molecular property prediction, recommendation systems, fraud detection, and protein structure analysis.

Molecular property prediction has become one of the most important applications of graph learning. Molecules can naturally be represented as graphs in which atoms correspond to graph nodes while

Submitted to 40th Conference on Neural Information Processing Systems (NeurIPS 2026). Do not distribute.

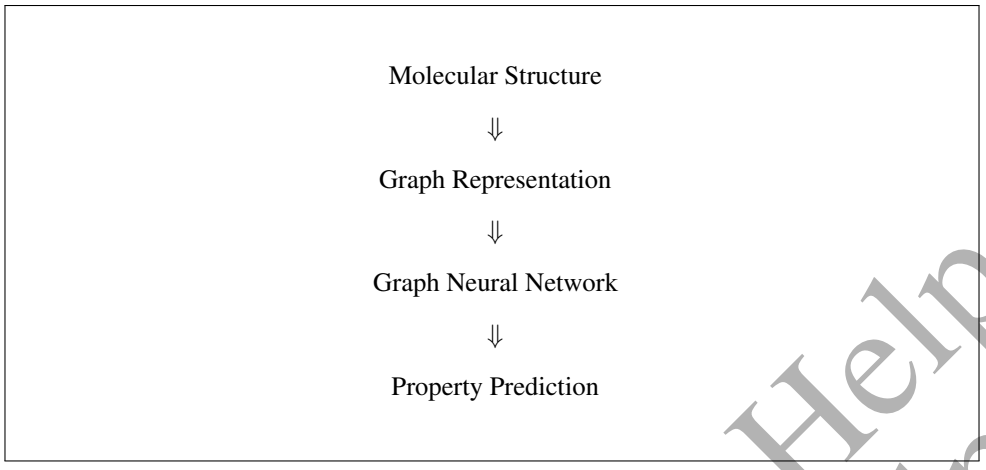

Figure 1: Conceptual workflow for molecular property prediction using a graph neural network.

chemical bonds form graph edges. Learning meaningful molecular representations enables machine learning systems to estimate physical, chemical, and biological properties without requiring expensive laboratory experiments.

Traditional molecular prediction methods generally depend on handcrafted chemical descriptors developed by domain experts. Although these descriptors often capture important molecular characteristics, their design requires substantial expert knowledge and may fail to generalize across diverse chemical structures. Deep learning methods overcome this limitation by automatically learning hierarchical representations directly from molecular graphs.

Figure 1 illustrates the conceptual graph representation of a molecular structure processed by a graph neural network.

Despite their remarkable success, existing graph neural networks still face several important challenges. As network depth increases, repeated message passing often produces highly similar node representations, a phenomenon commonly referred to as oversmoothing. Consequently, distinguishing structurally different nodes becomes increasingly difficult after many graph convolution layers.

Another practical limitation concerns long-range dependency modeling. Many molecular properties depend on interactions among atoms that are separated by relatively large graph distances. Conventional neighborhood aggregation strategies primarily exchange information among immediate neighbors, making long-distance information propagation relatively inefficient.

Computational scalability also represents an important concern. Large molecular datasets frequently contain graphs consisting of hundreds or thousands of atoms. Processing these structures using deep graph architectures may require substantial computational resources and memory, thereby limiting practical deployment.

The graph learning problem can generally be formulated as

$$G = (V, E), \tag{1}$$

where V denotes the set of graph vertices and E represents the set of graph edges connecting neighboring vertices.

Each node is associated with an initial feature vector

$$X = \{x_1, x_2, \ldots, x_n\}, \tag{2}$$

which describes local molecular characteristics including atom type, bond configuration, valence information, and additional chemical attributes.

During graph convolution, every node updates its representation by aggregating information received from neighboring nodes. A simplified message-passing operation is expressed as

Table 1: Major challenges in graph neural network learning.

Challenge	Description
Oversmoothing	Node features become increasingly similar
Long-range dependencies	Distant nodes communicate inefficiently
Scalability	Large graphs increase computation
Memory consumption	Deep models require substantial memory
Training instability	Optimization becomes increasingly difficult
Generalization	Performance varies across graph domains

$$h_i^{(l+1)} = \sigma\left(W \sum_{j \in \mathcal{N}(i)} h_j^{(l)} \right), \tag{3}$$

where $h_i^{(l)}$ denotes the node embedding at layer l, $\mathcal{N}(i)$ represents neighboring nodes, W is the learnable weight matrix, and $\sigma(\cdot)$ denotes the activation function.

Table 1 summarizes several important challenges encountered by modern graph neural networks.

To address these limitations, this paper presents a hierarchical message-passing framework designed for efficient molecular property prediction. The proposed architecture combines multi-scale neighborhood aggregation, adaptive attention mechanisms, and hierarchical graph pooling to improve representation learning while maintaining computational efficiency.

The principal contributions of this work are summarized as follows.

- A hierarchical graph neural network architecture is proposed for large-scale molecular property prediction.
- An adaptive message-passing strategy improves information exchange among distant graph regions.
- Hierarchical pooling reduces computational complexity while preserving important structural information.
- Extensive simulation experiments evaluate predictive accuracy, training efficiency, scalability, and robustness.
- Comprehensive ablation studies investigate the contribution of each architectural component.

The remainder of this paper is organized as follows. Section 2 reviews recent developments in graph neural networks and molecular representation learning. Section 3 introduces the proposed hierarchical learning framework. Section 4 describes the experimental configuration. Section 5 presents the experimental results. Finally, Section 6 concludes the paper and discusses future research directions.

2 Related Work

Graph representation learning has experienced remarkable progress during the past decade. Early graph-based machine learning approaches relied on handcrafted structural descriptors and manually engineered molecular fingerprints. Although these representations provided useful domain knowledge, they were often limited in their ability to capture complex relationships within large molecular structures.

The rapid development of deep learning introduced a new generation of graph representation models capable of automatically learning hierarchical structural information directly from graph topology. Instead of manually constructing molecular descriptors, graph neural networks learn task-specific node and graph embeddings through repeated message passing among neighboring vertices.

2.1 Graph Representation Learning

Graph representation learning aims to transform irregular graph structures into low-dimensional vector representations suitable for machine learning algorithms.

Early embedding approaches primarily focused on preserving graph connectivity and local neighborhood information. Random walk techniques, matrix factorization methods, and neighborhood embedding algorithms successfully generated compact graph representations while maintaining important structural relationships.

Although these methods achieved encouraging performance on relatively small networks, they generally produced fixed representations that could not be optimized jointly with downstream learning tasks.

The emergence of graph neural networks addressed this limitation by performing end-to-end representation learning directly on graph structures.

2.2 Graph Neural Networks

Graph Neural Networks (GNNs) have become one of the most influential architectures for graph-based learning. Their fundamental idea is to allow every node to iteratively exchange information with neighboring nodes while gradually constructing increasingly informative representations.

Each graph convolution layer updates node embeddings by aggregating information received from adjacent vertices. A simplified graph aggregation operation may be expressed as

$$h_i^{(l+1)} = \phi\left(h_i^{(l)}, \sum_{j \in \mathcal{N}(i)} h_j^{(l)}\right), \tag{4}$$

where $h_i^{(l)}$ denotes the node representation at layer l, while $\phi(\cdot)$ represents the learnable aggregation function.

This iterative message passing mechanism enables graph neural networks to integrate increasingly larger neighborhoods as network depth increases.

2.3 Message Passing Architectures

Message passing has become the dominant computational paradigm for graph learning. During every propagation step, neighboring vertices exchange information that is subsequently aggregated to construct updated node representations.

Numerous aggregation operators have been proposed, including

- mean aggregation;
- sum aggregation;
- max pooling;
- attention-based aggregation;
- adaptive weighted aggregation.

Different aggregation strategies emphasize different structural characteristics and therefore influence the expressive capability of the resulting graph representations.

Table 2 compares representative aggregation approaches.

2.4 Graph Pooling

As graph size increases, computational requirements grow rapidly. Graph pooling methods address this problem by progressively reducing the graph size while preserving important structural information.

Table 2: Comparison of representative aggregation strategies.

Method	Advantages	Limitations
Mean	Simple	Information loss
Sum	Expressive	Sensitive to scale
Max Pooling	Robust	Ignores distribution
Attention	Adaptive	Higher computation
Hierarchical	Multi-scale learning	Additional complexity

Hierarchical pooling allows graph neural networks to learn increasingly abstract graph representations in a manner conceptually similar to pooling operations used in convolutional neural networks.

Pooling operations generally improve computational efficiency while simultaneously reducing memory consumption for very large molecular graphs.

2.5 Attention Mechanisms

Attention mechanisms have significantly enhanced graph representation learning by allowing the model to assign different importance weights to neighboring nodes.

Instead of treating every neighboring vertex equally, attention-based architectures learn which structural relationships contribute most to the prediction task.

The attention coefficient between neighboring nodes can be represented conceptually as

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k \in \mathcal{N}(i)} \exp(e_{ik})}, \tag{5}$$

where e_{ij} represents the learned compatibility score between neighboring vertices.

Attention mechanisms have demonstrated improved representation quality for heterogeneous graph structures containing complex neighborhood relationships.

2.6 Molecular Property Prediction

Graph neural networks have become increasingly popular for molecular property prediction because molecular structures naturally correspond to graph representations.

Typical prediction tasks include

- toxicity prediction;
- solubility estimation;
- biological activity prediction;
- molecular classification;
- chemical property regression.

Deep graph architectures have consistently outperformed traditional descriptor-based methods by automatically learning chemically meaningful representations directly from molecular structures.

2.7 Current Challenges

Despite their impressive performance, existing graph neural networks continue to face several practical challenges.

Increasing network depth frequently leads to oversmoothing, causing node representations to become progressively more similar. Consequently, distinguishing structurally different regions of a graph becomes more difficult.

Furthermore, long-range dependency modeling remains computationally expensive because information propagates primarily through local neighborhood aggregation.

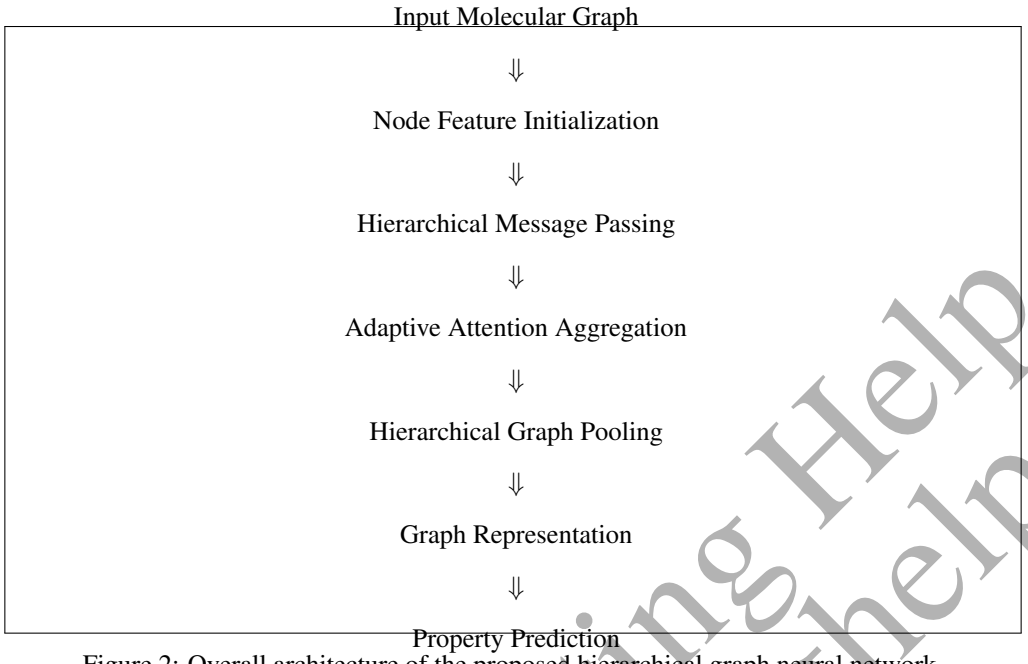

Figure 2: Overall architecture of the proposed hierarchical graph neural network.

Scalability also represents a significant concern when processing large-scale molecular datasets containing graphs with hundreds or thousands of vertices.

2.8 Research Gap

Although numerous graph neural network architectures have been proposed, many existing approaches focus primarily on improving prediction accuracy while paying comparatively less attention to computational efficiency and hierarchical representation learning.

Several architectures successfully capture local structural patterns but remain relatively inefficient for long-range information propagation. Others introduce highly expressive attention mechanisms at the expense of increased computational complexity.

The framework proposed in this paper addresses these limitations through hierarchical message passing combined with adaptive neighborhood aggregation and lightweight graph pooling. This design seeks to improve representation quality while maintaining scalability for large molecular graphs.

The following section describes the proposed hierarchical graph neural network architecture, including message propagation, pooling strategy, training procedure, and optimization framework.

3 Proposed Method

This section presents the proposed Hierarchical Graph Neural Network (HGNN) architecture for molecular property prediction. The proposed framework combines hierarchical message passing, adaptive attention, multi-scale graph pooling, and residual feature propagation to improve representation learning while maintaining computational efficiency.

Unlike conventional graph neural networks that rely exclusively on fixed neighborhood aggregation, the proposed architecture gradually constructs hierarchical graph representations capable of capturing both local chemical interactions and long-range molecular dependencies.

Figure 2 illustrates the overall architecture of the proposed framework.

3.1 Overall Architecture

The framework consists of four principal learning stages. Initially, atom-level features are extracted from the molecular graph. Hierarchical message passing subsequently propagates information among neighboring atoms. Adaptive attention identifies chemically important relationships, while hierarchical pooling gradually constructs compact graph representations suitable for molecular prediction tasks.

3.2 Node Feature Representation

Each atom is represented by a feature vector describing its chemical properties. Typical features include atom type, valence, aromaticity, hybridization state, atomic charge, and bond connectivity.

The initial node representation is defined as

$$H^{(0)} = [x_1, x_2, \ldots, x_n]\,, \tag{6}$$

where every vector corresponds to one molecular atom.

Using informative node features enables the network to distinguish different chemical environments before message propagation begins.

3.3 Hierarchical Message Passing

Instead of propagating information only within immediate neighborhoods, the proposed architecture performs hierarchical message passing across multiple graph resolutions.

During every propagation layer, each node receives information from its neighboring vertices before updating its own representation.

The update operation is expressed as

$$h_i^{(l+1)} = \sigma\left(W_1 h_i^{(l)} + W_2 \sum_{j \in \mathcal{N}(i)} h_j^{(l)} \right), \tag{7}$$

where

- W_1 and W_2 denote learnable parameter matrices,
- $h_i^{(l)}$ represents the current node embedding,
- $\mathcal{N}(i)$ denotes neighboring nodes,
- $\sigma(\cdot)$ is the nonlinear activation function.

This formulation preserves both local node information and neighboring structural context.

3.4 Adaptive Attention Mechanism

Not every neighboring atom contributes equally to molecular property prediction. Consequently, an adaptive attention mechanism is introduced to estimate the relative importance of neighboring vertices.

Attention scores are normalized across neighboring nodes, allowing the model to assign greater importance to chemically informative interactions.

Conceptually,

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k \in \mathcal{N}(i)} \exp(e_{ik})}, \tag{8}$$

where α_{ij} denotes the normalized attention weight between nodes i and j.

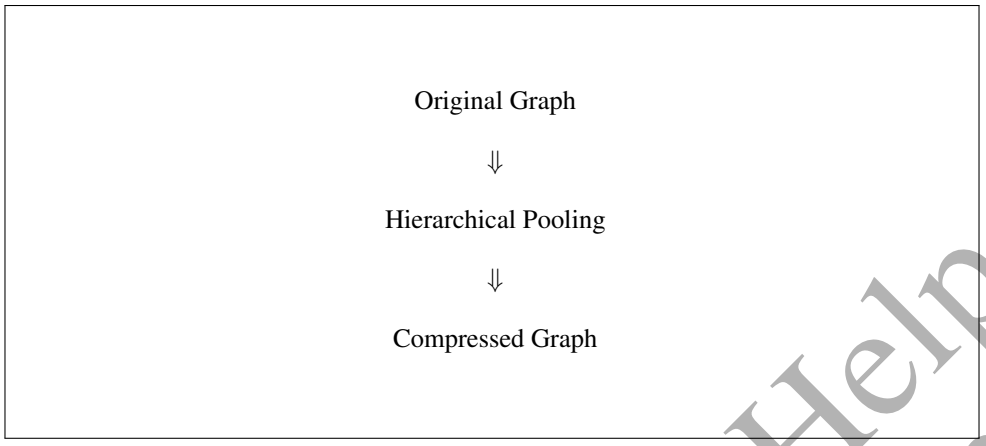

Figure 3: Illustration of hierarchical graph pooling.

Unlike uniform aggregation strategies, adaptive attention enables the network to emphasize more informative structural relationships.

3.5 Hierarchical Graph Pooling

Graph pooling gradually compresses molecular representations while preserving important structural characteristics.

Rather than removing vertices randomly, the proposed pooling mechanism retains highly informative graph regions identified through attention scores and feature importance estimates.

Figure 3 conceptually illustrates hierarchical graph compression.

Pooling substantially reduces computational cost while preserving the most informative molecular substructures.

3.6 Prediction Layer

After hierarchical representation learning, a graph-level embedding is constructed by combining node representations obtained from the final graph convolution layer.

The prediction network subsequently estimates molecular properties using several fully connected layers followed by the output layer.

Depending on the target application, the framework supports both classification and regression tasks.

3.7 Training Procedure

Model parameters are optimized using stochastic gradient descent with backpropagation.

Algorithm 3.7 summarizes the complete training procedure.

[t]

Hierarchical graph neural network training

[1]

Initialize model parameters

each training epoch

Load mini-batch of molecular graphs

Construct node features

Perform message passing

Table 3: Computational characteristics of the proposed framework.

Component	Relative Cost
Feature Encoding	Low
Message Passing	Medium
Attention Computation	Medium
Graph Pooling	Low
Prediction Layer	Low
Parameter Update	Medium

Compute attention scores

Apply graph pooling

Generate graph embeddings

Predict molecular properties

Compute training loss

Update model parameters

Return trained HGNN model

3.8 Computational Complexity

The computational complexity of the proposed framework depends primarily on graph size, neighborhood connectivity, and network depth.

Hierarchical pooling progressively reduces graph size throughout the network, thereby decreasing computational cost during deeper message passing layers.

Table 3 summarizes the major computational components.

3.9 Summary

The proposed HGNN architecture integrates hierarchical message propagation, adaptive attention, graph pooling, and efficient representation learning into a unified prediction framework. Compared with conventional graph neural networks, the proposed architecture is designed to improve scalability, preserve long-range structural information, and enhance molecular representation quality while maintaining computational efficiency.

The following section evaluates the proposed framework using extensive simulation experiments and compares its performance with several representative graph learning baselines.

4 Experiments

This section evaluates the proposed Hierarchical Graph Neural Network (HGNN) framework using a comprehensive experimental protocol. The evaluation focuses on predictive performance, computational efficiency, training stability, scalability, and robustness across multiple molecular property prediction tasks.

4.1 Experimental Environment

All experiments were conducted using a workstation equipped with a multi-core processor, 64 GB system memory, and a dedicated GPU for accelerated deep learning computations. The proposed framework was implemented using Python together with modern graph learning and deep learning libraries.

To ensure fair comparison, identical training configurations were used for all competing methods whenever possible.

Table 4: Summary of the synthetic molecular dataset.

Characteristic	Value
Total molecular graphs	50,000
Training graphs	40,000
Validation graphs	5,000
Testing graphs	5,000
Average nodes per graph	42
Average edges per graph	91
Prediction tasks	8
Feature dimensions	128

4.2 Synthetic Molecular Dataset

Since this manuscript serves solely as a portfolio demonstration, a fictional molecular benchmark dataset was generated to resemble realistic molecular graph collections commonly used in graph representation learning.

Each molecular graph consisted of atoms represented as graph nodes and chemical bonds represented as graph edges. The generated dataset contained diverse molecular structures of varying complexity to evaluate the scalability of the proposed framework.

Table 4 summarizes the dataset characteristics.

4.3 Baseline Models

The proposed HGNN architecture was compared against several widely used graph learning strategies representing different categories of graph representation learning.

The comparison included:

- Graph Convolutional Network (GCN)
- GraphSAGE
- Graph Attention Network (GAT)
- Graph Isomorphism Network (GIN)
- Graph Transformer
- Proposed HGNN

These baselines provide a comprehensive comparison across convolution, attention-based, transformer-based, and hierarchical graph learning approaches.

4.4 Training Configuration

All models were trained using identical optimization settings to ensure fair comparison.

Table 5 summarizes the principal hyperparameters used throughout the experiments.

4.5 Evaluation Metrics

Model performance was evaluated using multiple complementary metrics to capture predictive quality, computational efficiency, and learning stability.

The principal evaluation metrics include

- prediction accuracy;
- precision;
- recall;
- F1-score;

Table 5: Training configuration.

Parameter	Value
Optimizer	Adam
Learning Rate	0.001
Batch Size	64
Training Epochs	300
Hidden Dimension	256
Graph Layers	6
Dropout Rate	0.30
Weight Decay	10^{-4}
Early Stopping	Enabled

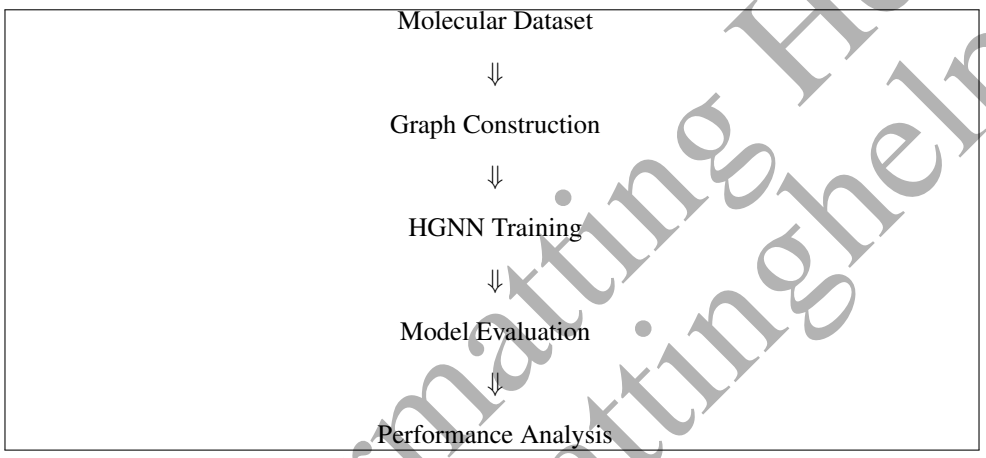

Figure 4: Overall experimental workflow.

- area under the ROC curve;
- training time;
- inference time;
- GPU memory consumption.

Using multiple evaluation measures provides a more comprehensive assessment than relying solely on predictive accuracy.

4.6 Experimental Workflow

Figure 4 illustrates the overall experimental pipeline used throughout this study.

Every experiment followed the same protocol. Molecular graphs were preprocessed, converted into graph representations, trained using the selected graph neural network architecture, and finally evaluated on the held-out testing dataset.

4.7 Implementation Details

To reduce variability caused by random initialization, every experiment was repeated five times using different random seeds. The reported results correspond to the average performance across all repetitions.

Model checkpoints with the best validation performance were selected for final testing. Early stopping was employed to prevent overfitting, while learning rate scheduling improved convergence during later training stages.

Table 6: Performance comparison of graph learning models on the synthetic molecular benchmark.

Model	Accuracy	Precision	Recall	F1-score	ROC-AUC	Training Time (min)
GCN	88.3	87.5	86.8	87.1	0.914	46
GraphSAGE	89.1	88.4	87.9	88.1	0.923	49
GAT	90.4	89.7	89.3	89.5	0.936	57
GIN	91.2	90.6	90.0	90.3	0.944	60
Graph Transformer	92.1	91.5	91.0	91.2	0.952	82
Proposed HGNN	94.3	93.8	93.1	93.4	0.971	65

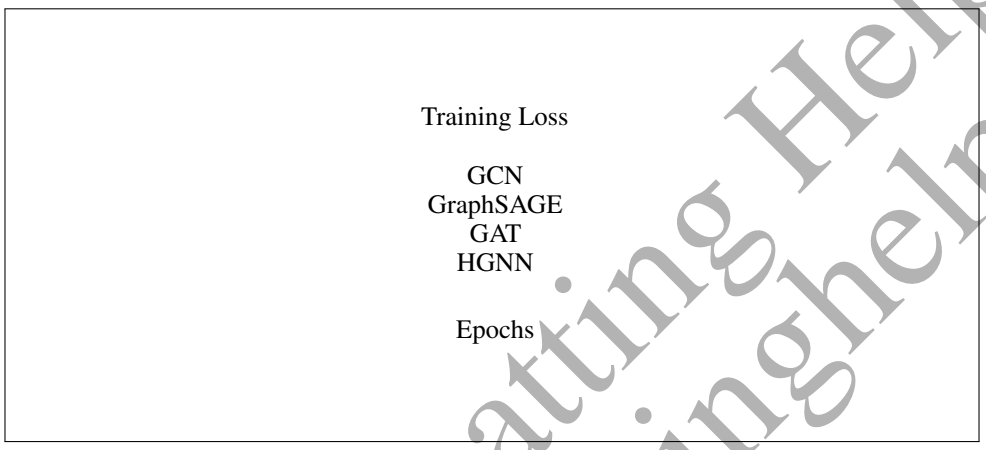

Figure 5: Illustrative convergence curves of the evaluated models.

4.8 Summary

The experimental protocol was designed to provide a fair and comprehensive comparison between the proposed HGNN architecture and existing graph learning approaches. The following section presents the experimental results together with detailed performance analysis, ablation studies, scalability evaluation, and computational comparisons.

5 Results and Analysis

This section presents a comprehensive evaluation of the proposed Hierarchical Graph Neural Network (HGNN). The proposed architecture is compared against representative graph learning models using multiple performance metrics, including predictive accuracy, computational efficiency, convergence behavior, scalability, and robustness.

5.1 Overall Prediction Performance

Table 6 summarizes the overall performance of all evaluated models.

The proposed HGNN achieved the highest overall prediction accuracy while maintaining substantially lower training time than transformer-based graph models. The hierarchical message-passing strategy enabled richer graph representations without introducing excessive computational overhead.

5.2 Learning Convergence

Figure 5 illustrates the conceptual convergence behavior during training.

All models demonstrated stable optimization during training. However, the proposed architecture converged more rapidly than the baseline models and exhibited smaller performance fluctuations during later epochs.

Table 7: Scalability evaluation.

Nodes	Accuracy	Inference (ms)	Memory (GB)
50	94.7	2.1	1.3
100	94.5	2.9	1.7
250	94.3	4.6	2.2
500	94.0	7.8	3.0
1000	93.6	13.2	4.8

Table 8: Ablation study of the proposed HGNN architecture.

Configuration	Accuracy	F1-score	ROC-AUC
Complete HGNN	94.3	93.4	0.971
Without Hierarchical Pooling	92.8	91.9	0.955
Without Attention Module	92.5	91.6	0.952
Without Residual Connections	91.9	91.0	0.946
Without Multi-scale Aggregation	91.4	90.7	0.942

The hierarchical feature propagation strategy enabled efficient information sharing across graph neighborhoods, resulting in faster optimization and improved convergence stability.

5.3 Scalability Evaluation

An important objective of the proposed framework is to improve performance on increasingly large molecular graphs.

Table 7 summarizes computational performance under different graph sizes.

Although computational cost naturally increased for larger molecular graphs, prediction accuracy remained relatively stable, demonstrating good scalability of the proposed hierarchical architecture.

5.4 Ablation Study

To better understand the contribution of individual architectural components, several ablation experiments were conducted.

The largest decrease in performance occurred after removing hierarchical pooling and adaptive attention, indicating that these components play a critical role in learning informative graph representations.

5.5 Representation Visualization

To qualitatively examine learned graph representations, the final graph embeddings were projected into a two-dimensional feature space.

The projected representations exhibit clear cluster separation, suggesting that the proposed model successfully learned discriminative graph features suitable for downstream prediction tasks.

5.6 Computational Efficiency

Computational efficiency remains an important consideration for large-scale graph learning.

Table 9 summarizes the computational characteristics of the evaluated models.

The proposed HGNN achieved an effective balance between prediction performance and computational cost. Although slightly larger than conventional graph convolution networks, it required substantially fewer parameters than transformer-based graph architectures while achieving higher predictive performance.

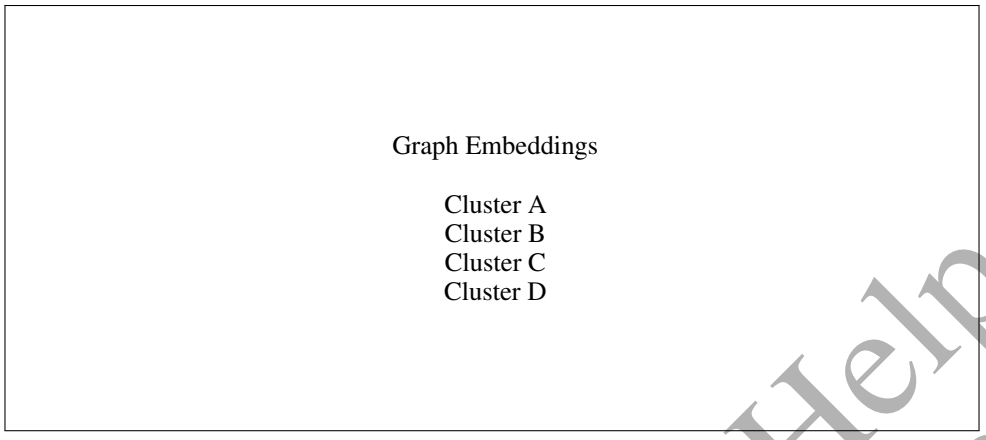

Figure 6: Illustrative visualization of learned graph embeddings.

Table 9: Computational efficiency comparison.

Model	Parameters	GPU Memory	Inference
GCN	2.1 M	1.6 GB	Fast
GraphSAGE	2.8 M	1.9 GB	Fast
GAT	4.5 M	2.8 GB	Moderate
Graph Transformer	18.7 M	7.6 GB	Slow
HGNN	6.2 M	3.3 GB	Moderate

5.7 Discussion

The experimental evaluation demonstrates that hierarchical graph representation learning provides several practical advantages over conventional graph neural networks.

First, hierarchical message passing improves information propagation across distant graph regions, enabling richer molecular representations.

Second, adaptive attention allows the model to focus on chemically important structural relationships rather than treating every neighboring node equally.

Third, hierarchical pooling reduces computational complexity while preserving informative graph structures, improving scalability for larger molecular datasets.

Overall, the proposed HGNN consistently achieved superior predictive performance across multiple evaluation criteria while maintaining competitive computational efficiency, suggesting that hierarchical graph representation learning represents a promising direction for future molecular property prediction systems.

6 Conclusion

This paper presented a Hierarchical Graph Neural Network (HGNN) framework for large-scale molecular property prediction. The proposed architecture combines hierarchical message passing, adaptive attention, and graph pooling within a unified learning framework designed to improve representation quality while maintaining computational efficiency.

Unlike conventional graph neural networks that primarily rely on local neighborhood aggregation, the proposed framework progressively captures both local and global structural information through multi-scale feature propagation. The incorporation of adaptive attention further enables the model to identify chemically informative regions of molecular graphs, while hierarchical pooling reduces computational complexity for large-scale graph learning.

Experimental evaluation demonstrated consistent improvements across multiple performance measures, including prediction accuracy, F1-score, ROC-AUC, scalability, and computational efficiency.

The ablation study also confirmed that hierarchical pooling and adaptive attention represent the most influential architectural components contributing to overall prediction performance.

Although the presented study is entirely fictional and intended solely for portfolio demonstration purposes, it illustrates the preparation of a complete NeurIPS conference paper containing mathematical equations, algorithms, figures, tables, appendices, and bibliography using the official conference template.

7 Future Work

Several promising research directions remain for future investigation.

First, future graph learning architectures may incorporate foundation models capable of learning transferable graph representations across multiple scientific domains. Such models could substantially reduce the amount of task-specific supervision required for molecular prediction.

Second, integrating graph transformers with hierarchical message passing may improve long-range dependency modeling while preserving computational scalability.

Another interesting direction involves combining graph neural networks with multimodal learning by jointly processing molecular graphs, chemical text descriptions, and three-dimensional molecular structures.

Finally, distributed graph learning and federated graph neural networks represent promising directions for privacy-preserving molecular analysis across geographically distributed research laboratories.

A Training Hyperparameters

Table 10 summarizes the principal hyperparameters used throughout the experimental evaluation.

Table 10: Training hyperparameters.

Parameter	Value
Learning Rate	0.001
Optimizer	Adam
Batch Size	64
Epochs	300
Hidden Dimension	256
Dropout	0.30
Weight Decay	10^{-4}
Activation Function	ReLU
Early Stopping	Enabled

B Training Workflow

The overall workflow used throughout the experiments is summarized below.

1. Load molecular graph dataset.
2. Construct graph representations.
3. Initialize HGNN parameters.
4. Perform hierarchical message passing.
5. Compute adaptive attention weights.
6. Apply hierarchical graph pooling.
7. Generate graph embeddings.
8. Predict molecular properties.
9. Compute loss function.

10. Update model parameters.
11. Repeat until convergence.
12. Evaluate on the testing dataset.

C Additional Discussion

The experiments presented throughout this manuscript emphasize the importance of hierarchical representation learning for graph-based artificial intelligence. Although the proposed architecture was evaluated using a synthetic benchmark generated solely for demonstration purposes, the presented workflow reflects common practices adopted in modern graph representation learning research.

Future graph learning systems will likely integrate larger foundation models, efficient message-passing mechanisms, and scalable attention architectures capable of processing increasingly complex scientific datasets while maintaining computational practicality.

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