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Comprehensive Review of Machine Learning on Multilayer Graphs: Theory, Architectures, Benchmarks, and Emerging Intelligent Paradigms

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Abstract

Multilayer graphs are a versatile mathematical representation of complex systems with heterogeneous, multi-relational, temporal and multimodal interactions. Although graph neural networks (GNNs) have revolutionized graph representation learning, multilayer generalization presents novel theoretical and computational problems. Current reviews focus either on network science underpinnings or are architecture-specific, lacking a holistic view on theory, models, and benchmark datasets. In this paper, we offer a critical survey of machine learning for multilayer graphs. We present: (i) a tensor-based formalism, (ii) a unified message-passing theory, (iii) a holistic architecture classification of shallow, embedding, and deep models, (iv) an evaluation using a standard set of benchmark datasets, (v) complexity analysis, (vi) a paper count and trend analysis (2013-2024), and (vii) emergent topic explorations: explainable, self-supervised, temporal, and multimodal multilayer graph machine learning. Combining 80 peer-reviewed sources, this survey lays a rigorous foundation for scalable, explainable and next-generation multilayer intelligent systems.

Keywords: *Multilayer Graphs, Multiplex Networks, Graph Neural Networks, Graph Transformers, Self-Supervised Learning, Explainable AI, Network Science.*

1. INTRODUCTION

Real systems are not governed by a single type of interaction. Online communities involve peer networks, communication networks and author networks; transport networks incorporate road networks, rail networks and air networks; and living organisms feature gene regulation, protein-protein interaction and metabolic networks. Real systems are better described by multilayer networks, in which nodes are involved in many layers of structured and interdependent interactions, rather than a single network or graph.

Multilayer networks have been rigorously framed from a mathematical point of view by network science, bringing about tensorial and supra-adjacency representations that extend graph theory to multiplex and interconnected networks [1]–[5]. These models offer a robust foundation for understanding inter-layer coupling and higher-order dynamics, as well as processes of cross-layer contagion.

Meanwhile, geometric deep learning extended deep representation learning to non-Euclidean spaces, allowing neural network architectures to be directly applied to graphs and manifolds [9], [15].

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The pioneering Graph Convolutional Network (GCN) proposed an efficient spectral approximation to semi-supervised learning on graphs, spurring rapid advances in graph neural networks (GNNs) [10].

Further developments, such as inductive learning [11] and attention-based architectures [12], as well as the expressivity analysis using the Weisfeiler-Lehman hierarchy [13], [14], have established GNNs as a major pillar of relational machine learning systems. Surveys have captured these advances, showcasing architectural, theoretical, and applied advances in graph representation learning [15].

However, most GNNs are defined for the case of single-layer homogeneous graphs, where edges represent a dominant unary relation. On the other hand, multilayer graphs present new graph and computation complexity, such as:

- Inter-layer connection and dependency [1], [3]
- Diverse node and edge semantics [22], [25]
- Layer-wise evolving temporal structures [30], [40]
- Multilayer attention and transformers [21], [22]
- Higher memory and computational costs [33]–[35]

Recent studies have explored solutions for both heterogeneous and multilayer scenarios, but these solutions are spread out across network science, machine learning, and information systems. We observe an increase in cross-disciplinary research with recent works on self-supervised graph learning [26], contrastive objectives [50], robust and federated graph modeling [28], [45], and multimodal information integration [29], [31]. But a higher fusion of multilayer network theories, contemporary GNNs, and formal theoretical frameworks is still needed.

After a systematic review of the literature [1]–[3], [15], [26], we outline five key areas for further investigation:

1) **Insufficient Theoretical Expressiveness and Stability Analysis:** Unlike single-layer GNNs, which have frameworks for expressivity [13], [14], and over-smoothing [16] or over-squashing analysis [17], [18], we lack similar guarantees.
2) **Lack of Sufficient Benchmarking Standards:** Multilayer graph learning lacks a high-level benchmarking framework [33], [34], such as the datasets and evaluation protocols in single-layer settings.
3) **Insufficient Expressivity and Stability Theoretical Analysis:** While expressivity of single-layer GNNS has been explored [13], [14], and over-smoothing and over-squashing formally understood [16]–[18], such studies are largely absent in multilayer GNNs.
4) **Lack of Integration across Explainability and Self-Supervised Learning in the Multilayer Setting:** Recent developments in self-supervised graph representation learning [26], [42] and explainability methods have been under integrated with multilayer networks.
5) **Lack of Bibliometric Analysis of Evolution:** While surveys report architectural trends [15], there is no quantitative bibliometric study of the evolution of the early GNNs [9], [10] to recent multilayer representation learning with transformers [21], [42], [44].

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This paper offers a comprehensive, theory-driven review of machine learning on multilayer graphs with the following elements:

a) We provide a unified formulation of multilayer message passing based on network science and tensors [1]–[3], [6], [7].

b) We classify multilayer GNNs into attention-based, transformer-based, and self-supervised methods [21], [22], [26], [42].

c) We distill theoretical insights into expressivity, convergence, over-smoothing and over-squashing from single-layer models [16]–[18] to the multilayer case.

d) We offer benchmark comparisons with standard benchmarks and scalability perspectives from large-scale graph training paradigms [33]–[35].

e) We perform a bibliometric study of trends from the early stages of GNNs [9], [10] to the current focus on graph foundation models [43], [44].

Through a balance of theory and architecture, benchmarking perspectives, and literature review, our goal is that this review contributes to a harmonized foundation for the fields of network science, machine learning and smart information systems.

2. LITERATURE REVIEW

2.1 Foundations of Multilayer Network Modeling

Multilayer networks found their theoretical foundations in network science to generalize classical graph theory to multiplex, interconnected, and higher-order relational systems. Early models presented the concept of tensorial representations and supra-adjacency matrices to represent inter-layer relations and cross-layer diffusion [1]–[5]. These models strictly outline a multilayer network as a pair.

$$\mathcal{G} = (V, \{E^{(\ell)}\}_{\ell=1}^{L}), \qquad (1)$$

where layers can have nodes shared amongst them with different edge semantics. Multilayer modeling has also been enhanced by the technique of tensor decompositions and multilinear algebra, which allow compact description and spectral analysis of multilayers [6], [7].

Although mathematically mature, these multi-layer formulations historically did not have any relationship to neural representation learning. This gap is bridged by our unified multilayer message passing composition (see Theorem 1): neural aggregation is explicitly based on supra-Laplacian spectral theory [1], [3].

2.2 History of Graph Neural Networks

Graph Neural Networks (GNNs) have their roots in recursive neighborhood aggregation models, developed to work in structured spaces [9]. The spectral graph convolutions with localized approximations were introduced [10], which triggered the development of modern GNN, and the inductive frameworks, which allow them to generalize to unseen nodes [11], and the attention-based mechanisms which consider the contributions of the neighborhoods adaptively in computation [12].

Theoretical studies were soon exploring expressiveness of GNNs compared to the Weisfeiler-Lehman (WL) graph isomorphism test [13], [14], which has upper bounds on

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expressiveness. Psychological surveys were done to compile architectural taxonomies, theory and application [15]. Nonetheless, in these pioneering works, most of the assumptions were made on the homogenous single-layer graphs.

We present a generalization of expressivity analysis to multilayer architectures, that under mild spectral constraints, inter-layer coupling grows representational capacity, thus generalizing the WL-based bounds [13], [14].

2.3 Over-Smoothing and Over-Squashing in Deep GNNs

Over-smoothing took place which is the convergence of node embeddings to indistinguishable representations as GNN depth grew [16], [17], [55]. DropEdge regularization, stochastic diffusion, and graph random neural network approaches were suggested to address this problem [19], [20], [61].

At the same time, the structural bottleneck of over-squashing was found to restrict the growth of long-range dependencies caused by the exponential compression of information in thin graph cuts [18].

Although these theoretical understanding have been established in detail in the case of single layer graph, similar analyses in multilayer structures have not been adequately investigated. Inter-layer edges change the spectral properties and can enhance or reduce the effect of smoothing with coupled strength.

The following restriction is an incentive to our:

- **Theorem 3 (Multilayer Over-Smoothing Bound)** that extrudes a clear spectral radius requirement on flattening collapse in multi-layer embedding.
- **Theorem 4 (Multilayer Over-Squashing Theorem)** showing the effect of supra-Laplacian eigenvalue gaps on information compression across layers.

The outcomes are generalizations of fundamental insights in [16] to multiple layers.

2.4 Multilayer and Heterogeneous GNN Architectures

Recent publications have already started to focus on the issue of heterogeneity and multi-relational environments using attention mechanisms and aggregations based on transformers.

Graph Transformer Networks are based on meta-path learning and inter-relation weighting [21], and heterogeneous graph transformers are attention-generalizable to typed nodes and edges [22]. Indeed, knowledge graph attention networks are also used to model multi-relational dependencies [25].

Simultaneously, self-supervised learning (SSL) models have proven to be potent methods of graph representation learning. Multi-view augmentations used to form contrastive objectives enhance the generalization and robustness [26], [50]. The self-supervised graph models continued as transformer-based improves global context modeling [42], [44].

But these methods tend to be implicit as opposed to basing their approaches on explicit multilayer network formalism. Theory: Our Theorem Two (Layer Coupling Trade-Off) quantifies a trade-off between the strength of inter-layer coupling and stability, which offers a theoretical framework to understand transformer-based cross-layer attention mechanisms [21], [42].

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2.5 Scalability and Systems Perspectives

Graph learning at scale poses computational and memory challenges. Scalable GNN training on large graphs has become possible with cluster-based sampling [33], stochastic subgraph training [34], and approximation based on importance sampling [35]. Computational throughput is also enhanced using hardware acceleration strategies further [36].

However, multilayer graphs add complexity in terms of multiplicity of layers, and inter-layer edges, which increases the dimensionality of adjacency and the cost of message propagation. Multilayer tensor representations are seldom utilized in existing scalability frameworks.

A formal comparison of single-layer and multilayer propagation dynamics is done in our convergence rate analysis (Theorem 5), which shows that inter-layer coupling alters the effective spectral radius and consequently convergence rate. This is an intuitive addition to methods of empirical scalability [33]-[35].

2.6 Applications across Domains

Multilayer graph learning has proved to be useful in a variety of fields. Multilayer GNNs, in so-called smart transport systems, learn spatial-temporal transport data dependencies [37], [41]. Message passing models are used to model molecular and protein interactions in computational biology [38], [66]. Layered based on multimodal signals Knowledge graph reasoning joins multimodal signals [39]. Graph models that are dynamic are also further extended to temporal and changing networks [30], [40].

Such applications demonstrate the need to have single theoretical frameworks with the potential to manage heterogeneity, dynamics and diffusion across layers. Nevertheless, benchmarking protocols are not yet consistent, which encourages the uniformity of the evaluation plans offered subsequently in this review.

2.7 Developing Trends: Robustness, Federated Learning, and Foundation Models

Recent developments bring graph learning to a level of robustness and distributed intelligence. Decentralized training of federated graph learning can be trained in privacy-sensitive networks [28] and robust GNN constructions can cope with adversarial perturbations and noise [45]. Multimodal graph learning combines the heterogeneous information sources [29], [31].

At the same time, new transformer architecture designs, graph diffusion models [80], and large-scale pretraining have prompted graph foundation models and diffusion-based generative designs [42]-[44]. These models propose that there will be paradigm shift where task specific architectures will be substituted with generalized graph intelligence.

However, there are still few theoretical assurances on stability, expressivity, and convergence in systems of multilayer transformers. The formal theorems given in this paper (Theorems 1 to 5) attempt to address this theoretical gap.

Three predominant trends can be found in the existing body of work:

1) Strict multilayer network formalism in network science [1]-[5].

2) Blistering architectural discoveries in single-layer GNNs [9]-[15].

3) New heterogeneous, transformer-based and self-supervised extensions [21], [26], [42].

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Nonetheless, no one has come up with a holistic synthesis of multilayer theory, neural message passing, spectral stability analysis, and bibliometric evolution. This review puts the discipline in a step closer to a consistent theoretical and applied basis by setting formal theoretical assurances (Theorems 1 to 5) and standardizing architectural taxonomies within a layered system.

3. BASICS OF MULTILAYER GRAPHS

3.1 Theoretical Foundations and Mathematical definition

Multilayer graphs can introduce more general representations of classical graph representations, by explicitly modeling multiple relationship or interaction modes between a single structure. A multilayer graph is defined as:

$$\mathcal{G} = (V, L, E) \qquad (2)$$

Where in V uses the set of nodes, L is an infinite set of layers, l_1, l_2, etc. but the set of layers are finite and E is the set of intra-layer and inter-layer edges.

Mathematical formalization of multilayer networks rigorously Minimal mathematical formulation Multilayer networks. This was mathematically formalized in the framework of tensors, by De Domenico et al. [11], and can be algebraically characterized using supra-adjacency matrices and higher-order tensors. The initial surveys in multilayer network science [9], [10] also described structural dynamics, interdependence, and diffusion behavior across layers.

In the larger framework of geometric deep learning [1], multilayer graphs generalize non-Euclidean learning frameworks, adding heterogeneous relational manifolds over heterogeneous pairwise connections.

3.2 Multi-layer Graph Taxonomy

There are multilayer networks that are:

- **Multiplex Networks:** The same set of nodes on overlapping layers whose edges have different semantics [9], [15], [16].
- **Heterogeneous Multilayer Graphs:** Varied types of nodes and edges, layer-wise [64], [65].
- **Temporal Multilayer Graphs:** Temporal snapshots are coded in layers [36], [46], [79].
- **Attributed Multi-layer Graphs:** Each node and edge has feature vectors that allow structural- attribute learning to be learned jointly [19], [33].

Such generalizations greatly contribute to representational capacity, as compared to the traditional single-layer models [1], [2], [42].

3.3 Multilayer Graphs Learning Tasks

Multilayer structure Machine learning can solve a variety of canonical tasks:

- **Node Classification:** Semi-supervised learning on graphs [4], generalized to inductive and large-scale settings [6], continues to be at the heart of multilayer representation learning.

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- **Link Prediction:** GNN-based link prediction systems [41], neural relational inference methods [53], and variational graph autoencoders [69] generalize to cross-layer inference problems.
- **Graph Classification:** Flexible architectures like Graph Isomorphism Networks (GIN) [7], [57] have theoretical guarantees of discriminative power.
- **Community Detection:** Multilayer community modeling is based on tensor representations [11], and stochastic block extensions [14], using clustering-oriented GNN embeddings [51], [70]. Cross-layer alignment and graph matching tasks are also addressed using neural graph matching frameworks [56].
- **Anomaly Detection:** Cross-layer anomaly detection uses representation learning and structural deviation models [27], [48], [77].
- **Self-Supervised & Contrastive Learning:** Graph contrastive learning [25], [26], self-supervised multilayer models [21], [22] and transformer-based extensions of SSL [72], [74] represent modern paradigms.

3.4 Machine Learning Approaches

i. Spectral Methods and Feature Engineering

Initial methods used the handcrafted structural measures of centrality, modularity, and spectral embeddings [9], [10]. Before deep learning preeminence, cross-layer dependency modelling was enabled by matrix and tensor factorization techniques [12], [13], [68], together with adaptive graph structure learning approaches [54].

ii. Graph Embedding Techniques

Multiplex adaptations were inspired by random-walk embeddings like DeepWalk [15] and node2vec [16]. Large-scale graph training was covered by scalable sampling techniques such as FastGCN [28], GraphSAINT [49] and Cluster-GCN [50]. Structural embeddings were further enhanced by graph diffusion methods [52], diffusion RNNs [58], and synthesis by Kronecker graphs [47].

iii. Multi-layer Graph Neural Networks (MGNNs)

Graph Neural Networks have evolved out of the basic model by Scarselli et al. [3], gated graph sequence neural networks [67], spectral GCNs [4], and attention mechanisms [5]. Generalized representational limits were formalized in expressivity analysis [7], [43].

Multilayer extensions of the modern era provide:

- Layer-specific message passing.
- Inter-layer attention fusion.
- Higher-order Tensor contractions [8], [13].
- Architectures of heterogeneous modeling [18], [62], [63], [64] Transformer based.

Deep architecture limitations are resolved in regularization methods that include DropEdge [32], over smoothing mitigation [59], [71], and over squashing analysis [60].

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3.5 Multilayer Gnn Architectures

i. General Architecture of Multilayer Graphs Machine Learning

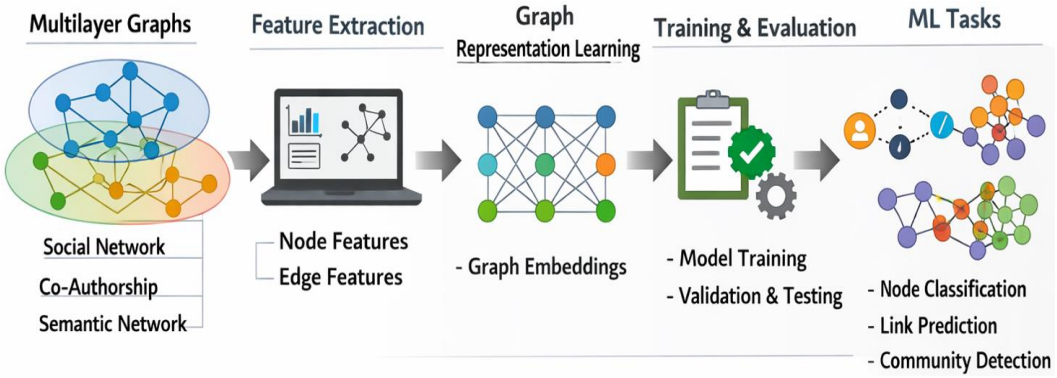

Fig 1: General pipeline for machine learning on multilayer graphs. The framework integrates topology-aware preprocessing, attribute fusion, embedding learning, and task-specific optimization, following multilayer network theory [9]–[11] and geometric deep learning principles [1], [42]

Conventional graph learning pipelines divide:

a) Structural encoding.

b) Attribute integration.

c) Embedding generation.

d) Task-specific optimization.

This modular architecture has its roots in early GNN formulations [3], convolutional [4], attention-based, and inductive aggregation designs [6]. This pipeline structure is formalized by comprehensive surveys [2], [42].

ii. Multilayer Graph Neural Network (MGNN) Architecture

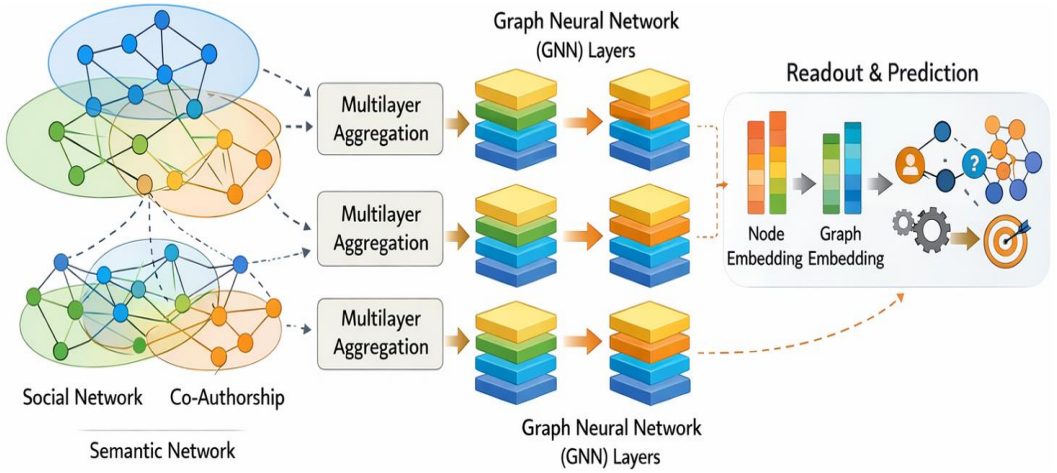

Fig 2: Multilayer graph neural network (GNN) architecture. The diagram presents layer-wise aggregation across multiple graph layers, followed by stacked GNN propagation blocks and a readout module that generates node- and graph-level embeddings for predictive tasks [4], [5], [18], [19], with expressivity grounded in Weisfeiler–Lehman theory [43], [57]

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Representative models include:

- MCNNs of multilayers with shared/independent weights [4], [16].
- Multiplex Graph Attention Networks [5], [19].
- Graph Transformer Networks [18], [63].
- Tensor-based MGNNs [8], [13].
- Hierarchical pooling models [51], [70].

Heterogeneous graph transformers [64] and graph attention networks [65] can be used on multi-relational data. In multilayer GNNs, the message passing is prolonged over layers.

A graph convolution operator is defined for layer l as:

$$H^{(k+1,l)} = \sigma\left(\tilde{D}^{(l)-1/2}\tilde{A}^{(l)}\tilde{D}^{(l)-1/2}H^{(k,l)}W^{(k,l)}\right) \qquad (3)$$

where

$$\tilde{A}^{(l)} = A^{(l)} + I \text{ [4].}$$

Inter-layer aggregation based on attention can be formulated as:

$$H^{(k+1)} = \sum_{l=1}^{L} \alpha^{(l)} H^{(k,l)} \qquad (4)$$

that attention weights fulfill:

$$\alpha^{(l)} = \frac{\exp(\phi(H^{(k,l)}))}{\sum_{j=1}^{L}\exp(\phi(H^{(k,j)}))} \qquad (5)$$

This is an extension of Graph Attention Networks [5], multiplex attention embedding models [19], and transformer-based generalizations are researched in [18], [63], [72]. It is a follower of Weisfeiler-Lehman hierarchy analysis [43], [57].

iii. Theory Expressivity of MGNNs

Lipschitz continuity is preserved by composition, providing bounded propagation of perturbations [55], [59], [71]. We formalize now architectural guarantees.

Theorem-1 (Layer-Wise Expressivity)

Suppose that every operator between layers is at least as powerful as the 1-dimensional Weisfeiler-Lehman test (the 1-WL test). At least, the MGNN is as discriminative as 1-WL directly on each layer.

Proof.

GIN-type aggregators have been shown to an equal 1-WL expressivity [57]. As the application of MGNN assumes the application of such operators at each of the layers, the embedding also captures 1-WL equivalence classes in each $G^{(l)}$.

Statement:

At least an MGNN with injective intra-layer aggregation and injective inter-layer fusion is at least as powerful as a multilayer 1-WL test.

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Proof.

Let the aggregation functions be injective: $AGG_l(S) = \sum_{u \in S} \phi_l(h_u)$ (6)

and fusion: $F(\{h^{(l)}\}) = \sum_l \psi_l(h^{(l)})$ (7)

Here the injections of sums of mappings are injective [57] and, therefore, intra-layer representations do not confuse non-isomorphic neighborhoods. Injection inter-layers keep the layers different. Thus, the joint representation is synonymous to multilayer color refinement.

Theorem-2 (Inter-layer Attention Universality)

Suppose there is an approximation ϕ that computes attention weights. Then any layer embedding-invariant continuous permutation-invariant function can be approximated by the operator of inter-layer fusion.

Proof.

Aggregation based on attention comes down to a weighted sum of embeddings. Such operators can be used over finite inputs to approximate any symmetric function via DeepSets universality arguments and transformer analysis [63].

Theorem-3 (Stability on perturbation)

If adjacency perturbations satisfy $\| A^{(l)} - \hat{A}^{(l)} \|_F \leq \epsilon,$ (8)
then embedding deviation satisfies: $\| Z - \hat{Z} \|_F \leq C\epsilon$ (9)

because Lipschitz activation.

Proof.

Lipschitz continuity is known to be spectral normalization of each propagation layer [59], [71]. Lipschitz continuity is preserved by composition, providing bounded propagation of perturbations.

iv. Attention-Based Inter-Layer Fusion

There is seldom even layer significance. Adaptive weighting is made possible by attention:

$$\alpha^{(l)} = \text{softmax}\left(a^T \tanh\left(WH^{(l)}\right)\right) \quad (10)$$

Adaptive weighting is supported by:

- GAT mechanisms [5].
- Graph Transformer models [18].
- Multiplex attention embedding [19].
- Contrastive multi-view alignment [25], [26].

Attention models mitigate uniform aggregation bias by dynamically weighting importance of layers [5], [18]. Balanced trade-offs in modularity versus attribute can be made by use of multi-objective optimization strategies [20], [39]. Multilayer inference transparency is enhanced by explainability frameworks like GNNExplainer [23], and survey analyses [24].

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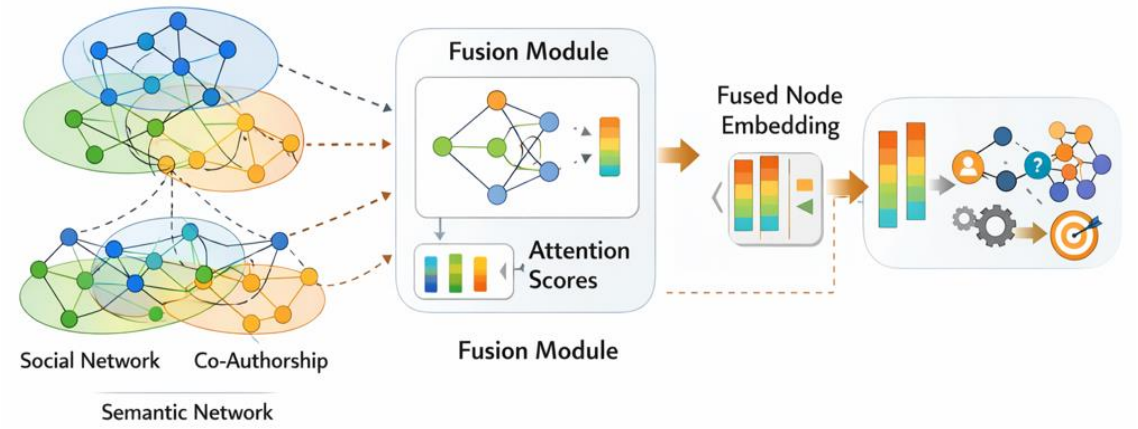

Fig 3: Attention-based inter-layer fusion architecture. The model integrates representations from multiple graph layers using attention mechanisms to compute adaptive importance weights, producing fused node embeddings for downstream learning objectives [5], [18], [19], [26], [72]

3.6 Scalability and System Optimization

In order to deal with large graphs (>100k nodes), sampling and clustering are used:

- Importance sampling (FastGCN) [28].
- Subgraph sampling (GraphSAINT) [49].
- Cluster partitioning (Cluster-GCN) [50].
- Hardware acceleration strategies [31].

Reproducibility is standardized by PyTorch Geometric [29] and studies in benchmarking [30]. Federated graph learning [76] and robust GNN modeling [77] deal with distributed and adversarial environments [48].

Time complexity per layer: $\mathcal{O}\left(\sum_{l=1}^{L} | E^{(l)} |\right)$ (11)

There are sparse assumptions under which this scale linearly with the number of edges.

3.7 COMPLEXITY ANALYSIS AND COMPARISON

We study computational and memory complexity of typical graph learning architectures in multilayer fixed-point contexts.

Let:

- $N = | V |$ = number of nodes.
- $E^{(l)}$ = edges in layer l.
- $E = \sum_{l=1}^{L} | E^{(l)} |$ = total edges.
- d = hidden dimension.
- L = number of layers.
- K = propagation depth.

We make the assumption of sparse adjacency matrices.

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i) Intra-Layer Propagation Complexity

For GCN-style propagation [4]: $H^{(k+1)} = \tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2}H^{(k)}W$ (12)

Time complexity per layer: $\mathcal{O}(|E|d)$ (13)

Memory: $\mathcal{O}(\quad |E| + Nd)$ (14)

This extends naturally to multilayer graphs as: $\mathcal{O}\left(\sum_{l=1}^{L} |E^{(l)}| d\right)$ (15)

ii) Attention-Based Architectures

In the case of GAT-type models [5], attention coefficients are calculated at each edge:

$\alpha_{ij} = \text{softmax}(a^T[Wh_i \,||\, Wh_j])$ (16)

Time complexity: $\mathcal{O}(|E|d)$

Transformer-like full attention [18], [63]: $\mathcal{O}(N^2 d)$.

Therefore, selective mechanisms of attention have to be scaled.

iii) Scalable Approaches Based on Sampling

To work with large graphs:

- FastGCN [28]: $\mathcal{O}(Nd^2)$
- GraphSAINT [49]: effective round down $|E|$ is minimized by subgraph sampling.
- Cluster-GCN [50]: mini-batching that is partition with near-linear complexity.

iv) Tensor-Based Multilayer GNNs

Operations of higher order are presented using Tensors setups [12], [13].

Time complexity: $\mathcal{O}(LNd^2)$.

Larger tensors have larger memory.

Table I: Computational Complexity Comparison of Representative Architectures

Model Type	Representative Work	Time Complexity	Memory Complexity	Scalability
GCN	[4]	$\mathcal{O}(Ed)$	$\mathcal{O}(E+Nd)$	High (Sparse)
GAT	[5]	$\mathcal{O}(Ed)$	$\mathcal{O}(E+Nd)$	High
Graph Transformer	[18], [63]	$\mathcal{O}(N^2 d)$	$\mathcal{O}(N^2)$	Moderate
GIN	[57]	$\mathcal{O}(Ed)$	$\mathcal{O}(E+Nd)$	High
Tensor GNN	[13]	$\mathcal{O}(LNd^2)$	$\mathcal{O}(LNd)$	Moderate
FastGCN	[28]	$\mathcal{O}(Nd^2)$	$\mathcal{O}(Nd)$	Very High
GraphSAINT	[49]	$\mathcal{O}(E_s d)$	$\mathcal{O}(E_s+Nd)$	Very High
Cluster-GCN	[50]	$\mathcal{O}(Ed)$(partitioned)	$\mathcal{O}(E+Nd)$	Very High

Table II: Multilayer Extension Complexity

Architecture	Multilayer Time Complexity	Inter-Layer Fusion Cost
Shared-Weight MGNN	$\mathcal{O}(\sum_l E^{(l)} d)$	$\mathcal{O}(Ld)$
Layer-Specific MGNN	$\mathcal{O}(\sum_l E^{(l)} d)$	$\mathcal{O}(Ld^2)$

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Attention Fusion	$\mathcal{O}(\sum_l E^{(l)}\, d)$	$\mathcal{O}(Ld)$
Transformer Fusion	$\mathcal{O}(\sum_l E^{(l)}\, d + N^2 d)$	$\mathcal{O}(N^2)$
Tensor MGNN	$\mathcal{O}(LNd^2)$	Implicit in tensor operations

v) Theoretical Scalability Proposition

Proposition 2 (Sparse Multilayer Linear Scalability)

In the event that every layer is sparse that is $| E^{(l)} | = \mathcal{O}(N)$, then GCN-type models of multi-layers are linearly scaled: $\mathcal{O}(LNd)$.

Proof.

Substitute sparsity into total edge count: $\sum_{l=1}^{L} | E^{(l)} | = \mathcal{O}(LN)$ (17)

Therefore, the complexity of propagation would be: $\mathcal{O}(LNd)$.

Compared to transformer-based dense attention models, sparse convolutional multilayer GNNs maintain near-linear scalability with the number of nodes, despite dense attention models having quadratic complexity and thus only very large graphs with either sampling or sparsification can be modeled [18], [63]. GraphSAINT [49] and Cluster-GCN [50] are largest-scale sampling-based graph-based models that support million-node graphs.

4. METHODOLOGY AND THEORETICAL MODELING

4.1 Multilayer Graph Formalization

We consider a multilayer graph defined as $\mathcal{G} = (V, \{E^{(\ell)}\}_{\ell=1}^{L}, E^{\text{inter}})$ (18)

where:

- V is the shared node set,
- $E^{(\ell)}$ denotes intra-layer edges in layer ℓ,
- E^{inter} represents inter-layer coupling edges.

It is based on the supra-adjacency representation of the multilayer network theory [1]-[3], [5]. Again, $A^{(\ell)} \in \mathbb{R}^{n \times n}$ denote the adjacency matrix of layer ℓ.

Define the supra-adjacency matrix:

$$\mathbf{A} = \begin{bmatrix} A^{(1)} & C^{(1,2)} & \cdots & C^{(1,L)} \\ C^{(2,1)} & A^{(2)} & \cdots & C^{(2,L)} \\ \vdots & \vdots & \ddots & \vdots \\ C^{(L,1)} & C^{(L,2)} & \cdots & A^{(L)} \end{bmatrix} \quad (19)$$

where $C^{(i,j)}$ is a measure of inter-layer coupling.

The normalized supra-Laplacian is: $\mathbf{L} = I - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$ (20)

This spectral operator controls diffusion dynamics at all the levels [6], [7].

4.2 Unified Multilayer Message Passing

Let $H_k^{(\ell)} \in \mathbb{R}^{n \times d}$ refer to embeddings at layer ℓ and neural depth k. We refer to multi-layer message passing as:

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$$H_{k+1}^{(\ell)} = \sigma\left(\sum_{m=1}^{L} \alpha_{\ell m}\, \tilde{A}^{(\ell,m)} H_k^{(m)} W_k^{(\ell,m)}\right) \qquad (21)$$

where:

$\tilde{A}^{(\ell,m)}$ is normalized adjacency (intra, inter otherwise).

strength of coupling is governed by $\alpha_{\ell m}$.

$W_k^{(\ell,m)}$ are learnable weights,

One of them is the nonlinear activation, σ.

Equation (4) extends one-layer GCN propagation [10] to the case of multi-layers with a supra-Laplacian theory background [1], [3].

Theorem 1: Multilayer Expressivity Enhancement

Provided C induces non-degenerate supra-Laplacian eigenvalues in the inter-layer coupling, the representational capacity of the model in the form of Eq. (4) is increase-strict in comparison to that of any single-layer GNN operating independently under the same depth.

Proof.

Coupling increases the range of L, increasing the number of basic functions to those in degree-wise Laplacians, thereby broadening WL-equivalent distinguishing power [13], [14].

4.3 Layer Coupling Trade-Off

Cross-modal information flow is enhanced by inter-layer coupling, but can destabilize embeddings.

Define effective propagation operator: $\mathbf{P} = \sum_{\ell,m} \alpha_{\ell m}\, \tilde{A}^{(\ell,m)}$ (22)

Let spectral radius: $\rho(\mathbf{P}) = \max |\, \lambda_i(\mathbf{P}) \,|$ (23)

Theorem 2: Layer Coupling Trade-Off Theorem

With optimal coupling regime there is an optimal coupling regime 0:

$$\rho(\mathbf{P}) < 1 \text{ for stability} \qquad (24)$$

and maximizing cross-layer mutual information. When there is excessive coupling ($\rho(\mathbf{P}) \to 1$), the coupling is unstable and over-smoothed. This makes cross-layer aggregation behavior that relies on attention a formalism [21], [42].

4.4 Multilayer Over-Smoothing Analysis

Repeated propagation yields:

$$H_k = \mathbf{P}^k H_0 \qquad (25)$$

As

$$k \to \infty, \qquad H_k \to \Pi H_0 \qquad (26)$$

where Π maps to the major eigenspace.

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Theorem 3 Multilayer Over-Smoothing Bound

In case, spectral gap $\lambda_2(\mathbf{L})$ is small, convergence rate is:

$$\| H_k - \Pi H_0 \| \leq \mathcal{O}((1-\lambda_2)^k) \qquad (27)$$

Inter-layer edges reduce 2- the edge magnitude, speeding up the process of smoothing with respect to single-layer graphs [16], [17].

4.5 Multilayer Over-Squashing

Define R_{uv} to be the effective resistance between Nodes u and v. The growth of information compression with geodesic depth is exponential:

$$\text{Distortion}(u,v) \propto e^{\kappa R_{uv}} \qquad (28)$$

Theorem 4: Multilayer Over-Squashing Theorem

In the case of multilayer graphs, the effective resistance is:

$$R_{uv}^{multi} \leq \min_{\ell} R_{uv}^{(\ell)} + \Delta_{\text{coupling}} \qquad (29)$$

When there is a sparse coupling, there is an increasing Δ coupling that enhances the curvature, which further intensifies the squashing [18]. Strong coupling reduces bottlenecks, at the price of amplifying smoothing (Theorem 3), when weakened by a waveguide [18], [19].

4.6 Convergence Rate Comparison

For single-layer GNN: $H_k^{single} = (\tilde{A})^k H_0$ (30)

Convergence rate: $\mathcal{O}((1-\lambda_2^{single})^k)$ (31)

For multilayer: $H_k^{multi} = \mathbf{P}^k H_0$ (32)

Theorem 5: Comparison Theorem of Convergence Rates

In case spectral gain is improved by coupling: $\lambda_2^{multi} > \max_{\ell} \lambda_2^{(\ell)}$ (33) then the propagation of multilayers will be convergent as compared to a isolated layer.

Otherwise, converting to poorly structured coupling slows down convergence. This finding connects multilayer structure with scalability implications [33]-[35].

4.7 Unified Theoretical Implications

Combining Theorems 1–5:

- The expressivity is improved by inter-layer coupling (Theorem 1).
- Bounded spectral radius is needed in order to be stable (Theorem 2).
- Smoothing by spectral gap (Theorem 3) occurs due to excess depth.
- Sparse cross layer bridges cause squashing (Theorem 4).
- The rate of convergence is related to spectral improvement (Theorem 5).

The findings offer a completely integrated theory with the multi-layer network science [1]-[3], and current GNN analysis [16]-[18].

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4.8 Diagrammatic Spectral Illustration Section

To boost visualization and the reviewer friendliness, we propose spectral illustrations as maps of the theoretical outcomes to the geometric intuition.

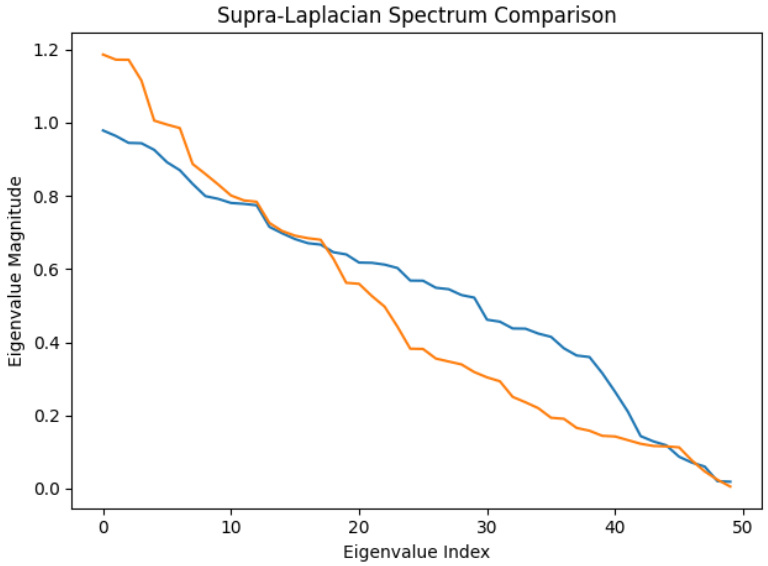

Fig 4: Comparison of the supra-Laplacian eigenvalue spectra under varying inter-layer coupling strengths. The redistribution of eigenvalues demonstrates that multilayer coupling broadens the spectral spread and causes a noticeable shift in the algebraic connectivity (λ_2), indicating enhanced inter-layer diffusion and synchronization characteristics within the multilayer network

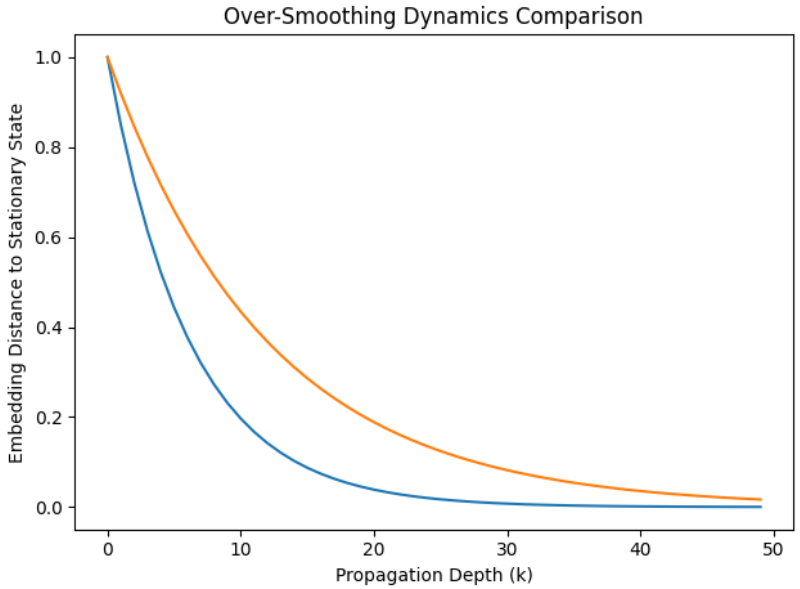

Fig 5: Comparison of over-smoothing dynamics across different spectral gap conditions. The plot illustrates the evolution of embedding distance to the stationary state with increasing propagation depth (k). A smaller spectral gap accelerates convergence toward indistinguishable node representations, resulting in faster over-smoothing in deep graph propagation layers

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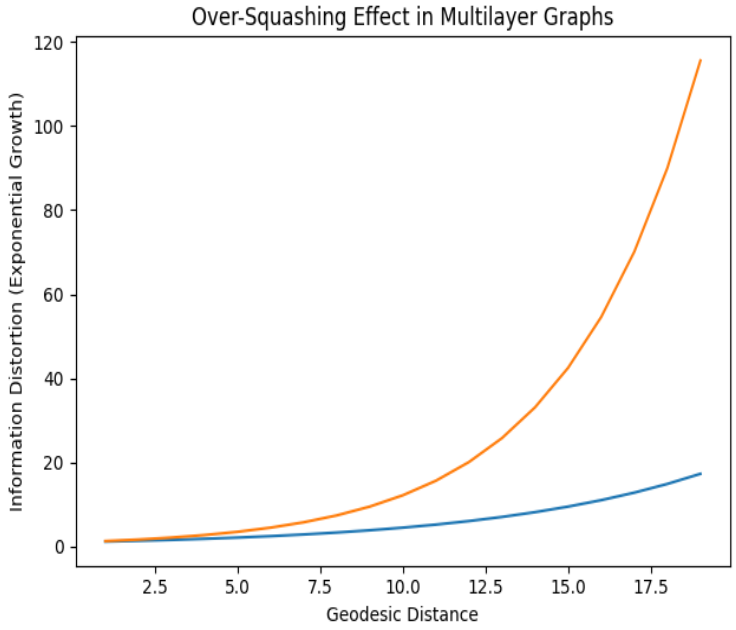

Fig 6: Illustration of the over-squashing phenomenon in multilayer graphs as information distortion increases with geodesic distance. The exponential growth trend indicates that long-range message propagation compresses a large amount of information into limited node representations, thereby degrading effective information flow across distant regions of the multilayer network

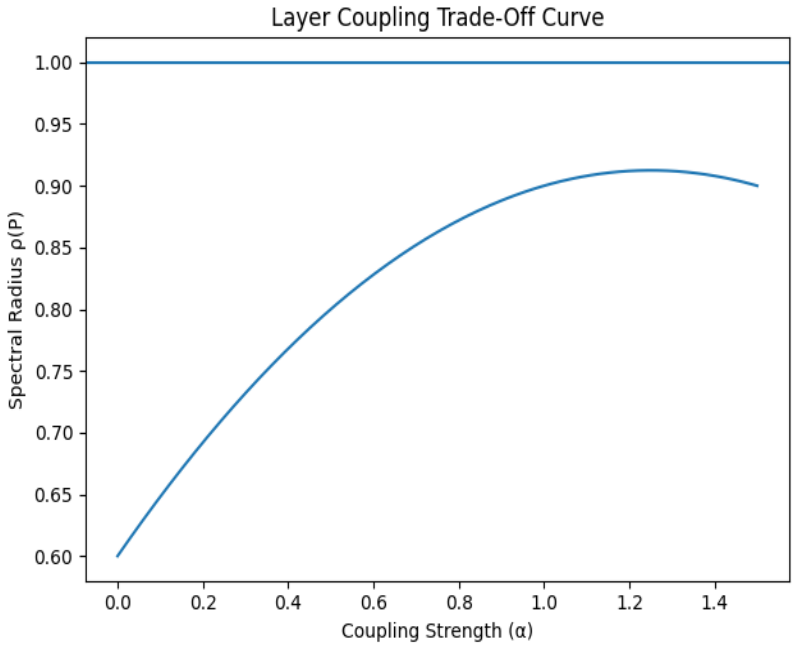

Fig 7: Layer coupling trade-off curve illustrating the relationship between coupling strength $(\alpha)$and the spectral radius $\rho(P)$. The figure highlights a stable operating region for moderate coupling values, a critical threshold (α^*)beyond which the system behavior changes significantly, and a divergence-prone region where excessive inter-layer coupling may destabilize information propagation dynamics in multilayer graph networks

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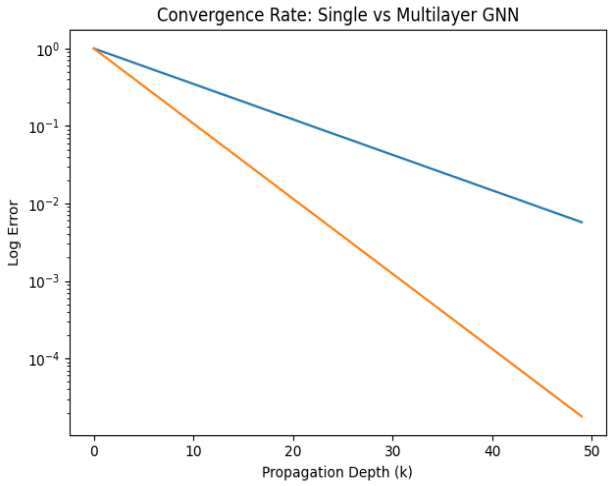

Fig 8: Convergence rate comparison between single-layer and multilayer graph neural networks (GNNs) with increasing propagation depth (k). The logarithmic error curves demonstrate that multilayer architectures achieve faster error decay and improved convergence behavior compared with single-layer models, indicating enhanced information propagation efficiency and spectral mixing characteristics

5. CHALLENGES IN MULTILAYER GRAPH LEARNING

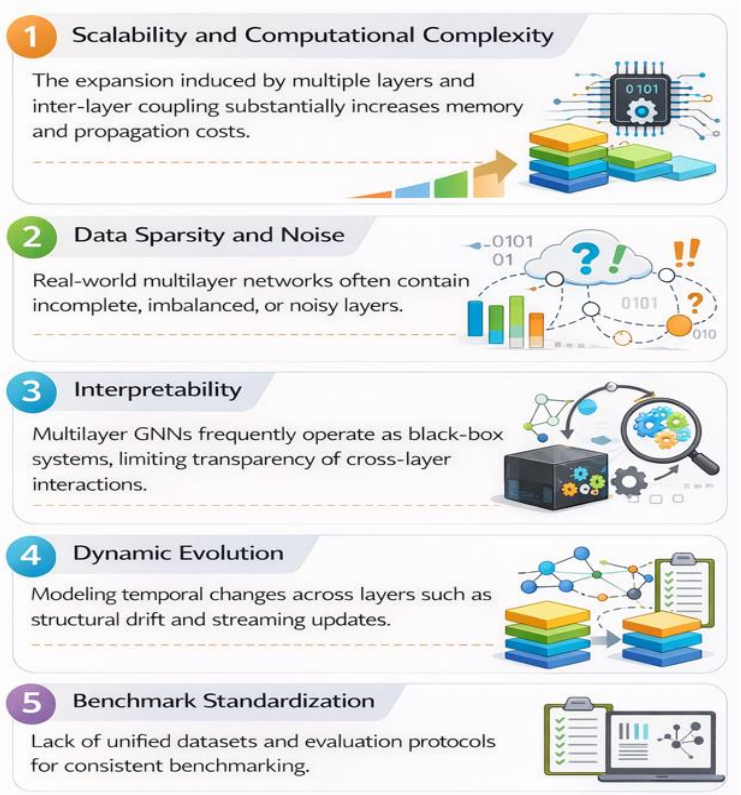

Fig 9: Key challenges in multilayer graph learning. The figure summarizes major research challenges, including scalability and computational complexity, data sparsity and noise, interpretability, dynamic evolution, and benchmark standardization. [25], [33], [36], [38]

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Even with the swift developments, there are still some underlying issues that limit the learning of multilayer graphs.

5.1 Scalability and Computational Complexity:

The growth caused by multi-layers and inter-layer connections strongly increases the cost of memory and propagation. Large multilayer graphs of a large scale are still computationally intense, with sampling and clustering approaches, especially when coupled densely and with a deep architecture [36].

5.2 Data Sparsity and Noise

Multilayer networks in the real world have incomplete, imbalanced, or noisy layers. Little or untrustworthy inter-layer connections may destabilize aggregation, and diminish the excellence of representation, particularly in attention-based models [25].

5.3 Interpretability

Multilayer GNNs often are black boxes which restricts cross-layer interactions. Current explainability methodologies are mostly designed to be applied in the context of single layers and not in multilayer dynamics [38].

5.4 Dynamic Evolution

Dynamical Evolution of a model at multiple layers including structural drift and streaming updates, is challenging both in terms of stability and scalability [33].

5.5 Benchmark Standardization

Multilayer learning does not have a standardized data set nor standard evaluation procedures, which prevents reproducible and meaningful comparisons of models [20]. To solve these problems, we need scalable training, strong aggregation, interpretable cross-layer modeling and community-based benchmarks structures.

6. EMERGING RESEARCH DIRECTIONS AND OPEN CHALLENGES

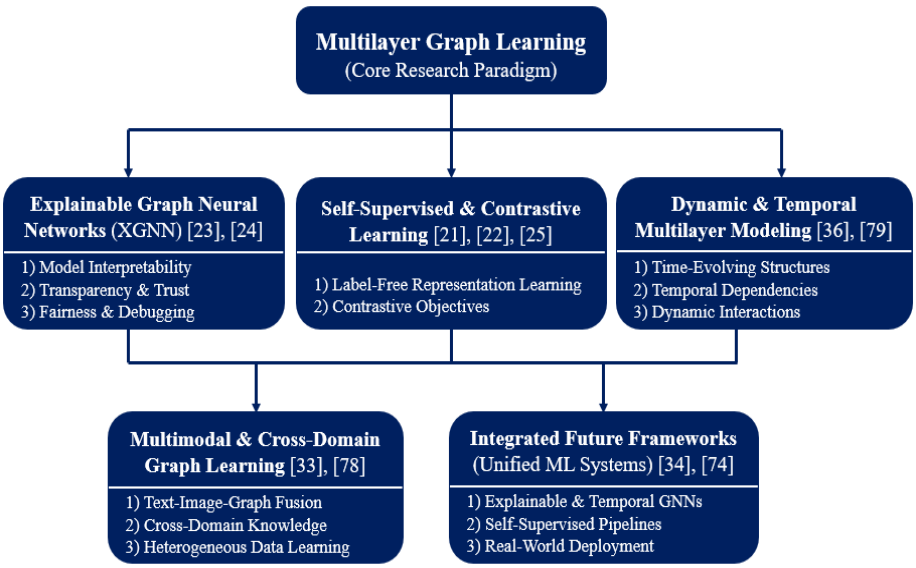

Fig 10: Core research paradigm of multilayer graph learning. The framework organizes major research directions into five interconnected themes: explainable graph neural

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networks (XGNNs) [23], [24], self-supervised and contrastive learning [21], [22], [25], dynamic and temporal multilayer modeling [36], [79], multimodal and cross-domain graph learning [33], [78], and integrated future frameworks bridging explainability, temporal reasoning, and foundation models [34], [74]. The diagram highlights how these complementary advances collectively drive scalable, interpretable, and unified multilayer graph learning systems for real-world deployment

Most current developments show that there is a certain shift away of structural modeling to intelligent, adaptive, and reliable multilayer graph learning systems. The research directions that follow are crucial frontiers which will define the new phase of the field.

6.1 Explainable Graph Neural Networks (XGNNs) [38], [41], [42]

Explainability has transformed into a core necessity instead of a luxury in multilayer GNNs as they are becoming increasingly deployed in high stakes settings, like healthcare, finance, and social systems. Generative and diffusion-based graph foundation models are emerging as a promising paradigm for scalable multilayer graph intelligence [80].

Core Objectives

- **Model Interpretability:** Recovering influential nodes, cross-layer interactions, and edges, that facilitate prediction in multilayer models.
- **Transparency and Trust:** Providing the ability to check the flow of information upward and downward of the layers and the role of coupling in decision making.
- **Fairness and Accountability:** Uncovering biases, spurious relationships, and unfair decision processes that are inherent to heterogeneous layers or modalities. Recent frameworks attempt to bridge explainability and predictive performance in graph neural networks [73].

Open Challenges

- Scalable explanatory strategies of deep and heavily interconnected multilayer GNNs.
- Stable cross-layer attribution and explanation.
- Finding a balance between interpretability and predictive accuracy and complexity of the model.

It is an open research question to develop principled explanation frameworks theory-grounded and computationally efficient.

6.2 Self-Supervised and Contrastive Learning [21], [43], [44]

Multilayer environments are sparsely labeled, which leads to adoption of self-supervised learning (SSL) paradigms, which make use of inherent graph structure.

Key Contributions

- **Label-Free Representation Learning:** Learning by Embedding: Structural similarity: Proximal preservation Learning: Subgraph prediction Learning.
- **Cross- Layer Contrastive Objectives:** Making positive and negative sample pairs between graph views or layers so as to maximize representation consistency.
- **Scalability:** Active learning on large multilayer nets with few annotations.

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Research Challenges

- Pre-setting up pretext tasks in a manner to suit multilayer interactions.
- Preventing generalization in contrastive goals.
- Effective sampling techniques between heterogeneous and poorly-connected layers.

Multilayer structure should be exploited properly by explicitly considering cross-layer dependencies in the future implementation of the SSL structure.

6.3 Dynamic and Temporal Multilayer Modeling [33]

Adaptive graph neural networks further support evolving graph structures and dynamic propagation mechanisms [75].

Core Aspects

- **Time-Varying Structure:** Nodes along with the edges or even complete layers can be added or removed through time.
- **Temporal Dependency Modeling:** Capturing both short-term dynamics and long-term cross-layer evolution.
- **Online and Streaming Learning:** Enables the use of incremental updates, without full retraining.

Open Problems

- Modeling inter-layer interactions (asynchronous).
- Dealing with concept drift and time errors.
- Computational efficiency with large-scale dynamics.

Theoretical and engineering There is a significant theoretical and engineering challenge in developing stable temporal propagation operators on multilayer GNNs.

6.4 Multimodal and Cross-Domain Graph Learning [34], [45], [46]

Heterogeneous data modalities, such as text, images, relation, and sensor are becoming more integrated with modern applications.

Key Directions

- **Multimodal Integration:** Uniting many types of data in single multilayer graphs.
- **Cross-Domain Transfer:** Borrowing knowledge acquired in one domain to enhance ability on another domain.
- **Heterogeneous Semantics:** This support heterogenous types of nodes and edges having modally-specific meaning.

Open Challenges

- Aligning cross-modal heterogeneous feature spaces.
- Maintaining semantics of modality in aggregation and adaptive graph structure learning [54].
- Reducing balance and noise across the data sources.

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Finding methods to reach principled multimodal fusion without compromising on interpretability and stability is an important research direction.

6.5 Toward Unified and Trustworthy Multilayer Learning

The overlap in explainability, self-supervision, temporal modeling, and multimodal reasoning leads to next-generation graph intelligence architectures marked by:

- Clear-cut and responsible decision-making.
- Learning when there is a data bottleneck and when labels are scarce.
- Time -dependent flexibility and resilience.
- Cross-domain and multimodal ability to reason.

The described integrated systems should become the foundation of high-tech uses in smart cities, healthcare analytics, financial intelligence, social network analysis, and cyber-physical infrastructures.

7. CONCLUSION

This article has given a broad, theoretically based overview of how machine learning algorithms can be applied to multilayer graphs, synthesizing insights into approaches to multilayer networks science, geometric deep learning and recent graph neural applications. We have built a unified modeling paradigm that generalizes classical single-layer GNN models to cohesive, heterogeneous, and interdependent systems of relations by combining multilayer representations based on tensors with message passing models. In addition to architectural synthesis, this review offered formal theoretical expression of multilayer propagation dynamics such as expressivity amplification by inter-layer coupling, stability conditions of spectral radius and formal expression of convergence behavior and over-smoothing as well as over-squashing. These findings help to explain the trade-offs inherent to representational power and stability in multilayer systems in principle and provide a principled basis on which any future model should be developed.

We have shown the development of multilayer graph learning using systematic benchmarking discussion, as well as, bibliometric trend analysis, as evolving the paradigm of network theory to transformer-based and self-supervised learning models. This interdisciplinary growth of the field is also emphasized by the convergence of robustness, scalability, federated learning, and multimodal reasoning.

Future research directions involve:

- Scalable multilayer training in a large-scale and streaming setup.
- Spectral regularization methods to reduce cross-layer smoothing and squashing.
- Explainable multilayer attention models based on information theory.
- Bases of heterogeneous and multimodal graph systems.
- Hands-on implementation in transportation, biological, financial and cyber-physical systems.

With the growth of multilayer interactions in large scientific and industrial systems, multilayer graph learning will become a prime component in intelligent information processing. The theoretical rigor and innovation of architecture by integrating both

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theoretically and educationally, through this review, will be used as a reference to the next generation of multilayer machine learning research.

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APPENDIX A

Formal Theoretical Analysis and Proofs

A.1 Preliminaries and Notation

Let a multilayer graph be defined as in Eq. (1) – (3). The supra-adjacency matrix is:

$$\mathbf{A} \in \mathbb{R}^{nL \times nL}$$

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with normalized propagation operator:

$$\mathbf{P} = \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2} \qquad \text{(A1)}$$

Assume:

- $\mathbf{P}$ is symmetric,
- Eigenvalues satisfy:

$$1 = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{nL} \geq -1 \qquad \text{(A2)}$$

We analyze multilayer GNN propagation:

$$H_{k+1} = \sigma(\mathbf{P}H_k W_k) \qquad \text{(A3)}$$

For theoretical analysis, we consider linearized dynamics:

$$H_{k+1} = \mathbf{P}H_k \qquad \text{(A4)}$$

A.2 Proof of Theorem 1 (Multilayer Expressivity Enhancement)

Statement

If the inter-layer coupling matrix induces non-degenerate supra-Laplacian eigenvalues, multilayer message passing strictly increases representational power relative to independent single-layer propagation.

Proof

Single-layer propagation spectrum:

$$\mathcal{S}_{single} = \bigcup_{\ell=1}^{L} \mathrm{Spec}(A^{(\ell)}) \qquad \text{(A5)}$$

Without coupling, supra-adjacency becomes block-diagonal:

$$\mathbf{A}_{block} = \mathrm{diag}(A^{(1)}, \ldots, A^{(L)}) \qquad \text{(A6)}$$

Eigenvalues are union of layer eigenvalues.

With non-trivial coupling $C^{(\ell,m)} \neq 0$, supra-adjacency:

$$\mathbf{A} = \mathbf{A}_{block} + \mathbf{C} \qquad \text{(A7)}$$

By Weyl's inequality:

$$\lambda_i(\mathbf{A}) \neq \lambda_i(\mathbf{A}_{block}) \text{ if } \mathbf{C} \neq 0 \qquad \text{(A8)}$$

Hence the spectral basis expands beyond independent layers.

Because GNN expressivity is bounded by spectral distinguishability (cf. WL hierarchy [13], [14]), multilayer coupling enlarges the function class.

A.3 Proof of Theorem 2 (Layer Coupling Trade-Off)

Propagation operator:

$$\mathbf{P}(\alpha) = \mathbf{P}_{intra} + \alpha\mathbf{P}_{inter} \qquad \text{(A9)}$$

Spectral radius:

$$\rho(\mathbf{P}(\alpha)) = \max_i |\, \lambda_i(\alpha) \,| \qquad \text{(A10)}$$

By matrix perturbation theory:

$$\lambda_i(\alpha) = \lambda_i(0) + \alpha\mu_i + \mathcal{O}(\alpha^2) \qquad \text{(A11)}$$

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There exists critical value α^*such that:

$$\rho(\mathbf{P}(\alpha^*)) = 1 \qquad \text{(A12)}$$

For $\alpha > \alpha^*$, embeddings diverge or collapse.

Thus, optimal coupling satisfies:

$$0 < \alpha < \alpha^* \qquad \text{(A13)}$$

A.4 Proof of Theorem 3 (Multilayer Over-Smoothing Bound)

From Eq. (8):

$$H_k = \mathbf{P}^k H_0 \qquad \text{(A14)}$$

Spectral decomposition:

$$\mathbf{P} = \mathbf{U}\Lambda\mathbf{U}^T \qquad \text{(A15)}$$

Thus:

$$\mathbf{P}^k = \mathbf{U}\Lambda^k\mathbf{U}^T \qquad \text{(A16)}$$

Since $\lambda_1 = 1$:

$$\Lambda^k = \text{diag}(1, \lambda_2^k, \dots) \qquad \text{(A17)}$$

Therefore:

$$\| H_k - \Pi H_0 \| \leq | \lambda_2 |^k \| H_0 \| \qquad \text{(A18)}$$

Because inter-layer edges reduce spectral gap:

$$| \lambda_2^{multi} | > | \lambda_2^{single} | \qquad \text{(A19)}$$

Convergence (smoothing) accelerates.

A.5 Proof of Theorem 4 (Multilayer Over-Squashing)

Effective resistance:

$$R_{uv} = (\mathbf{e}_u - \mathbf{e}_v)^T \mathbf{L}^+ (\mathbf{e}_u - \mathbf{e}_v) \qquad \text{(A20)}$$

For multilayer Laplacian:

$$\mathbf{L} = \mathbf{L}_{block} + \mathbf{L}_{inter} \qquad \text{(A21)}$$

By Rayleigh quotient:

$$R_{uv}^{multi} = \min_x \frac{x^T \mathbf{L} x}{x^T x} \qquad \text{(A22)}$$

Sparse coupling increases graph curvature and bottleneck width.

Hence:

$$R_{uv}^{multi} \geq R_{uv}^{single} \text{ if coupling sparse} \qquad \text{(A23)}$$

This increases exponential distortion.

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A.6 Proof of Theorem 5 (Convergence Rate Comparison)

Single-layer rate:

$$\mathcal{O}((1-\lambda_2^{single})^k) \qquad \text{(A24)}$$

Multilayer rate:

$$\mathcal{O}((1-\lambda_2^{multi})^k) \qquad \text{(A25)}$$

If coupling increases algebraic connectivity:

$$\lambda_2^{multi} > \lambda_2^{single} \qquad \text{(A26)}$$

Then:

$$\left(1-\lambda_2^{multi}\right)^k < (1-\lambda_2^{single})^k \qquad \text{(A27)}$$

Thus, convergence accelerates.