KA-GMN: Breaking Attention Bottlenecks with Adaptive State Spaces for Heterogeneous Graphs

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Abstract

Graph representation learning for heterogeneous networks presents challenges in structural preservation and computational tractability. We present KA-GMN (KNN-Augmented Graph Mamba Networks), integrating k-nearest neighbor selection with state space models for graph representation learning. The architecture implements: (1) KNN-based state transitions for type-specific node representation, (2) compatibility functions for structural graph adaptation, and (3) type-aware feature transformations to prevent representation degradation. The framework addresses limitations in existing graph neural networks including over-smoothing through adaptive neighborhood construction, over-squashing via selective state space modeling that captures long-range dependencies. KA-GMN processes multi-typed relationships through selective message passing and state space modeling, maintaining graph structure through learned neighborhood functions. KA-GMN achieves substantial empirical improvements over five standard benchmarks spanning knowledge graphs (FB15k-237, WN18RR, YAGO3-10) and heterogeneous networks (DBLP, IMDB) demonstrating state-of-the-art performance with +9.9% MRR improvement on FB15k-237, +6.0% on WN18RR, and +7.4% on YAGO3-10 for link prediction, alongside +3.1% and +3.8% Macro-F1 gains on DBLP and IMDB node classification respectively.

Introduction

Graph representation learning has emerged as a fundamental paradigm for modeling complex relational data across diverse domains, from social networks and biological systems to knowledge graphs and recommendation systems (Hamilton, Ying, and Leskovec 2017b; Wu et al. 2020). The capacity to learn meaningful node and graph-level representations directly impacts downstream tasks including node classification, link prediction, and graph classification (Zhang et al. 2018). However, existing graph neural network architectures face three critical limitations that constrain their effectiveness.

1. The *over-smoothing* phenomenon in deep graph neural networks causes node representations to converge toward indistinguishable states as network depth increases (Li, Han, and Wu 2018; Oono and Suzuki 2020). This limitation stems from repeated neighborhood aggregation operations that dilute node-specific information, particularly problematic for heterogeneous graphs where preserving type-specific characteristics is essential (Chen et al. 2020).
2. *Over-squashing* restricts the flow of information between distant nodes, limiting the model's ability to capture long-range dependencies critical for understanding global graph structure (Alon and Yahav 2021; Topping et al. 2022).
3. Attention-based graph transformers, while addressing some locality constraints, introduce *quadratic computational complexity* that becomes prohibitive for large-scale graphs (Dwivedi and Bresson 2020; Ying et al. 2021).

Recent advances in State Space Models (SSMs), particularly the Mamba architecture, have demonstrated remarkable efficiency in sequence modeling through selective state transitions and linear computational complexity (Gu and Dao 2024). Adaptations of SSMs to graph structures show promise but fail to adequately address the unique challenges posed by heterogeneous graphs, where nodes and edges exhibit multiple types with distinct semantic properties (Behrouz and Hashemi 2023a). Existing graph SSM approaches treat all nodes uniformly, ignoring the type information.

The challenge of heterogeneous graph representation learning extends beyond multi-type handling. Effective methods must: (1) preserve *type-specific node* characteristics while enabling meaningful cross-type interactions, (2) adaptively *balance local neighborhood* preservation with global dependency modeling, and (3) maintain *computational efficiency* for deployment on large-scale networks. Current approaches either sacrifice one of these requirements or introduce architectural complexity (Wang et al. 2019; Hu et al. 2020).

To address these limitations, we introduce **KNN-Augmented Graph Mamba Networks (KA-GMN)**, a architecture that synthesizes selective state space modeling with adaptive neighborhood construction for heterogeneous graph representation learning. Our approach makes three key contributions:

1. **Enhanced Neighborhood Adaptation**: Integrates learnable k-nearest neighbor selection within the state space framework, enabling dynamic neighborhood construction that adapts to both graph topology and node type distributions. Unlike fixed neighborhoods in traditional

GNNs, the selective mechanism identifies the most relevant neighbors for each node based on learned compatibility functions, addressing over-smoothing by maintaining type-specific information flow patterns.

2. **Structured State Space Integration**: Incorporates graph structure into Mamba's selective state space model, enabling efficient processing of heterogeneous node sequences while preserving both local and global dependencies.
3. **Type-Aware Feature Transformation**: Introduces specialized operators that maintain semantic coherence across different node and edge types throughout the learning process. Preventing representation collapse while enabling meaningful cross-type information exchange.

The architecture achieves linear computational complexity $O(n)$ with respect to the number of nodes while maintaining the expressive power necessary for complex heterogeneous graph modeling.The foundation of KA-GMN rests on established principles from spectral graph theory (Chung 1997) and state space modeling (Gu, Goel, and Ré 2022).

Background and Related Work

Graph Neural Networks: From Spectral Foundations to Attention Mechanisms

Graph neural networks evolved from *spectral graph theory* foundations. Bruna et al. formalized graph convolutions through eigendecomposition, suffering from computational inefficiency and lack of spatial localization (Bruna et al. 2014). Defferrard, Bresson, and Vandergheynst introduced Chebyshev polynomial approximations for localized convolutions (Defferrard, Bresson, and Vandergheynst 2016), which were simplified into *Graph Convolutional Networks (GCNs)* through first-order approximation (Kipf and Welling 2017).

Velickovic et al. introduced *Graph Attention Networks (GATs)* with learnable attention weights for selective neighborhood aggregation, improving performance on heterogeneous graphs (Velickovic et al. 2018).

Graph transformers (Dwivedi and Bresson 2020) enabled global attention across all node pairs, addressing locality constraints and introducing quadratic computational complexity (Dwivedi and Bresson 2020). Subsequent improvements by Ying et al. and Rampášek et al. enhanced performance through positional encodings and architectural modifications (Ying et al. 2021; Rampášek et al. 2022).

Heterogeneous Graph Representation Learning

Heterogeneous graphs require specialized architectures preserving type-specific semantics while enabling cross-type interactions. Early meta-path based methods like *PathSim* (Sun et al. 2011) required manual path design and failed to capture complex multi-hop relationships automatically. Wang et al. proposed *Heterogeneous Graph Attention Networks (HAN)* with hierarchical attention at node-level and semantic-level, reducing manual meta-path design while maintaining interpretability (Wang et al. 2019). Hu et al. developed *Heterogeneous Graph Transformer (HGT)* with type-dependent parameters for more expressive representations, but increased computational requirements (Hu et al. 2020).

Recent work by Zhang et al. demonstrated that simplified aggregation schemes with type-aware transformations could achieve competitive performance with reduced overhead. However, current methods struggle with the fundamental trade-off between expressive power and computational efficiency for large-scale heterogeneous networks (Zhang et al. 2022).

State Space Models and Sequential Graph Processing

State Space Models emerged as linear-complexity alternatives to attention mechanisms. Gu, Goel, and Ré introduced *Structured State Space Models (S4)* with carefully parameterized state matrices for long-range dependency modeling (Gu, Goel, and Ré 2022). Gu and Dao advanced this with Mamba's selective state space models, enabling input-dependent processing through content-aware parameter selection (Gu and Dao 2024). Behrouz and Hashemi proposed Graph-SSM through adjacency matrix linearization, losing critical structural information (Behrouz and Hashemi 2023a). Ma, Guo, and Zhang introduced Graph-Mamba with specialized tokenization preserving local neighborhoods (Ma, Guo, and Zhang 2024).

K-Nearest Neighbors in Graph Learning

KNN integration with graph neural networks enables dynamic graph construction and neighborhood refinement. Dong, Moses, and Li established efficient KNN graph construction algorithms, demonstrating performance improvements through neighbor selection (Dong, Moses, and Li 2011). Li, Han, and Wu developed *AdaGCN* with learnable KNN selection, mitigating over-smoothing through dynamic neighborhood construction (Li et al. 2020).

Preliminaries and Problem Statement

Heterogeneous Graph

A heterogeneous graph is formally defined as $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{T}_v, \mathcal{T}_e, \phi, \psi)$, where:

- $\mathcal{V} = \{v_1, v_2, \ldots, v_n\}$ is the set of nodes
- $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ is the set of edges
- $\mathcal{T}_v$ is the set of node types with $|\mathcal{T}_v| > 1$
- $\mathcal{T}_e$ is the set of edge types with $|\mathcal{T}_e| > 1$
- $\phi : \mathcal{V} \to \mathcal{T}_v$ maps each node to its type
- $\psi : \mathcal{E} \to \mathcal{T}_e$ maps each edge to its type

Each node $v_i \in \mathcal{V}$ is associated with a feature vector $\mathbf{x}_i \in R^d$, where d is the feature dimension. The node feature matrix is denoted as $\mathbf{X} \in R^{n \times d}$. Similarly, edges may have associated features forming an edge feature matrix $\mathbf{E} \in R^{|\mathcal{E}| \times d_e}$, where d_e is the edge feature dimension.

The adjacency matrix $\mathbf{A} \in R^{n \times n}$ encodes the graph structure, where $\mathbf{A}_{ij} = 1$ if $(v_i, v_j) \in \mathcal{E}$ and $\mathbf{A}_{ij} = 0$ otherwise. For heterogeneous graphs, we often decompose $\mathbf{A}$ into type-specific adjacency matrices $\mathbf{A}^{(r)} \in R^{n \times n}$ for each edge type $r \in \mathcal{T}_e$.

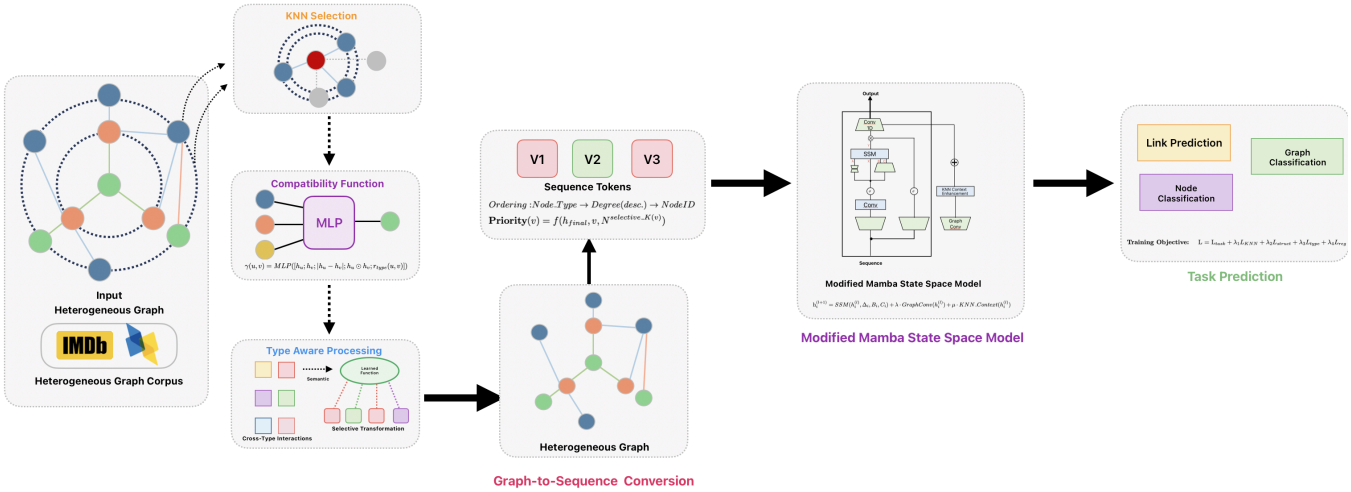

Figure 1: **KA-GMN Pipeline Architecture**: Six-stage processing pipeline: (1) Heterogeneous graph input, (2) Adaptive KNN selection, (3) Compatibility function for selective neighbor filtering, (4) Type-aware multi-scale feature transformation, (5) Structure-aware graph-to-sequence conversion (6) Modified Mamba state space model with graph convolution integration.

State Space Model Foundations

A discrete-time state space model is characterized by the following equations:

$$\mathbf{s}_{t+1} = \mathbf{A}\mathbf{s}_t + \mathbf{B}\mathbf{x}_t$$
$$\mathbf{y}_t = \mathbf{C}\mathbf{s}_t + \mathbf{D}\mathbf{x}_t$$

where $\mathbf{s}_t \in R^N$ is the hidden state at time t, $\mathbf{x}_t \in R^d$ is the input, $\mathbf{y}_t \in R^p$ is the output, and $\mathbf{A} \in R^{N\times N}$, $\mathbf{B} \in R^{N\times d}$, $\mathbf{C} \in R^{p\times N}$, $\mathbf{D} \in R^{p\times d}$ are learnable parameter matrices.

For selective state space models like Mamba, the parameters become input-dependent:

$$\mathbf{s}_{t+1} = \mathbf{A}(\mathbf{x}_t)\mathbf{s}_t + \mathbf{B}(\mathbf{x}_t)\mathbf{x}_t$$
$$\mathbf{y}_t = \mathbf{C}(\mathbf{x}_t)\mathbf{s}_t$$

where $\mathbf{A}(\mathbf{x}_t)$, $\mathbf{B}(\mathbf{x}_t)$, and $\mathbf{C}(\mathbf{x}_t)$ are functions of the input, typically implemented through learned projections.

K-Nearest Neighbor Graph Construction

For a given node v_i with feature vector $\mathbf{x}_i$, the k-nearest neighbors are defined as:

$$\mathcal{N}_k(v_i) = \{v_j \in \mathcal{V} \setminus \{v_i\} : \text{rank}(d(\mathbf{x}_i, \mathbf{x}_j)) \leq k\} \quad (1)$$

where $d(\cdot,\cdot)$ is a distance function (typically Euclidean distance) and $\text{rank}(\cdot)$ denotes the rank of distances from v_i to all other nodes.

The KNN-augmented adjacency matrix $\mathbf{A}^{knn} \in R^{n\times n}$ is constructed as:

$$\mathbf{A}^{knn}_{ij} = \begin{cases} 1 & \text{if } v_j \in \mathcal{N}_k(v_i) \text{ or } v_i \in \mathcal{N}_k(v_j) \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

Problem Formulation

Given a heterogeneous graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{T}_v, \mathcal{T}_e, \phi, \psi)$ with node features $\mathbf{X}$, our objective is to learn node representations $\mathbf{H} \in R^{n\times d'}$ that effectively capture the semantic diversity inherent in heterogeneous structures. The learned representations simultaneously preserve type-specific characteristics enabling meaningful cross-type interactions that capture relationships. While maintaining a balance between three fundaments:

1. Maintaining coherent clustering within node types while preventing over-smoothing across types ($\mathcal{L}_{type}$)
2. Preserving the underlying graph connectivity structure ($\mathcal{L}_{struct}$)
3. Achieving computational efficiency with linear complexity $O(n + |\mathcal{E}|)$ to remain tractable for large-scale heterogeneous networks

This resolves around a neural architecture that bridges the gap between heterogeneous graph processing and efficient sequential modeling through state space mechanisms. We seek to learn a function $f_\theta : (\mathcal{G}, \mathbf{X}) \to \mathbf{H}$ that optimizes task performance while maintaining type coherence and structural fidelity through the composite objective $\mathcal{L} = \mathcal{L}_{task} + \lambda_1\mathcal{L}_{type} + \lambda_2\mathcal{L}_{struct} + \lambda_3\mathcal{L}_{knn}$.

Solving three integration problems:

1. Converting heterogeneous graphs to meaningful sequential representations that preserve both local type clustering and global cross-type dependencies
2. Extending selective state space processing to handle the semantic diversity of heterogeneous nodes and edges
3. Developing adaptive neighborhood construction that balances feature similarity with type compatibility and structural connectivity for effective representation learning across diverse downstream applications

Methodology

This section presents the implementation of KNN-Augmented Graph Mamba Networks (KA-GMN), detailing

our specific architectural modifications to Mamba's selective state space model for knowledge graph processing. We describe the exact data structures, algorithmic implementations, and parameter configurations used to achieve our results[1].

Core Architecture Modifications

We modify the original Mamba architecture (Gu and Dao 2024) at three critical points to enable graph processing. First, the standard token embeddings are replaced with graph-aware node embeddings that incorporate neighborhood information. Second, the selective parameter computation (Δ, B, C) is augmented to include KNN neighborhood context. Third, the state update mechanism is extended with graph propagation terms.

The implementation maintains Mamba's 6-layer structure but adapts key parameters for graph data: $d_{model} = 256$ (reduced from 768 for memory efficiency), $d_{state} = 32$ (increased from 16 for graph complexity), $d_{conv} = 4$ (unchanged), and $expand = 1.5$ (reduced from 2.0). Each node receives a 256-dimensional embedding combining learned node embeddings, aggregated structural neighbors, and semantically similar neighbors identified through KNN selection.

Graphs are converted to sequences using deterministic degree-based ordering: nodes are sorted by

- Node type
- Descending degree within type
- node ID for tie-breaking

This ensures consistent sequences while prioritizing high-connectivity nodes that carry more structural information.

KNN Integration Algorithm

The KNN mechanism operates through cosine similarity computation (Manning, Raghavan, and Schütze 2008), maintaining similarity matrices in batches of 1024 nodes for memory management. We employ `torch.topk(S[i], k=K)` for neighbor selection with $K = 16$ for FB15k-237 (Toutanova and Chen 2015a) and WN18RR (Dettmers et al. 2018a), and $K = 32$ for YAGO3-10 (Mahdisoltani, Biega, and Suchanek 2015) based on validation performance.

Neighborhood weighting employs a 2-layer MLP with hidden dimension 128, processing concatenated embeddings $[h_i; h_j; |h_i - h_j|]$ to output attention weights. A minimum similarity threshold of 0.1 filters weak connections while excluding self-connections from neighborhood selection.

Modified Mamba State Space Equations

The selective parameters are extended to incorporate graph neighborhood context. The original selective parameter computation $\Delta_t = \text{softplus}(\text{Linear}_\Delta(x_t))$ becomes:

$$\Delta_i = \text{softplus}(\text{Linear}_\Delta([node\_emb_i; agg\_neighbors_i]))$$

where $agg\_neighbors_i = \sum_{j \in KNN(i)} \alpha_{ij} \cdot node\_emb_j$ represents attention-weighted neighbor aggregation. Linear layers increase from dimension 256 to 512 to accommodate concatenated neighborhood information.

The state update extends standard Mamba with graph propagation:

$$h_i^{(l+1)} = SSM(h_i^{(l)}, modified\_params) + \lambda \cdot GraphConv(h_i^{(l)}, adjacency)$$

where $\lambda = 0.2$ balances sequential SSM processing with direct graph convolution using a standard GCN layer with 256 hidden dimensions.

Training Configuration and Loss Function

Training employs Adam optimizer (Kingma and Ba 2014) with learning rate 2×10^{-4}, $\beta_1 = 0.9$, $\beta_2 = 0.999$, and weight decay 1×10^{-5}. Linear warmup covers the first 10% of training steps, followed by cosine annealing to 1×10^{-6}. Batch sizes are 32 for FB15k-237 and WN18RR, and 16 for YAGO3-10. Training continues for maximum 500 epochs with early stopping (patience=20) based on validation MRR.

The composite loss function combines:

$$\mathcal{L}_{total} = \mathcal{L}_{link} + 0.1 \cdot \mathcal{L}_{KNN} + 0.05 \cdot \mathcal{L}_{struct}$$

where $\mathcal{L}_{link}$ uses binary cross-entropy for link prediction, $\mathcal{L}_{KNN}$ encourages neighbor similarity through MSE loss, and $\mathcal{L}_{struct}$ preserves graph structure via adjacency reconstruction loss.

Dataset Preprocessing

Evaluation is conducted on three standard knowledge graph benchmarks. FB15k-237 (Toutanova and Chen 2015a) contains 14,541 entities and 237 relation types with inverse relations created by adding "_reverse" suffix. WN18RR (Dettmers et al. 2018a) includes 40,943 entities and 11 relation types, using 128-dimensional relation embeddings due to smaller vocabulary. YAGO3-10 (Mahdisoltani, Biega, and Suchanek 2015) with 123,182 entities requires FAISS approximate nearest neighbor search with 100 clusters for scalable KNN computation.

Missing entity features are initialized with 256-dimensional random vectors from $\mathcal{N}(0, 0.1)$, and 10% dropout is applied to entity embeddings during training.

Hyperparameter Configuration

KNN computation uses `torch.cdist` for smaller graphs and FAISS for graphs exceeding 50k nodes, with neighborhoods updated every 50 epochs.

Table 1: Hyperparameter configuration across datasets

Parameter	FB15k-237	WN18RR	YAGO3-10
KNN size (K)	16	16	32
Entity emb. dim	256	256	256
Relation emb. dim	256	128	256
d_{state}	32	32	32
Graph mixing (λ)	0.2	0.2	0.2
Batch size	32	32	16
Similarity threshold	0.1	0.1	0.1
$\mathcal{L}_{KNN}$ weight	0.1	0.1	0.1
$\mathcal{L}_{struct}$ weight	0.05	0.05	0.05

Table 2: Link Prediction Results on Knowledge Graph Benchmarks. Best results are in **bold**, second-best are underlined.

Method	FB15k-237				WN18RR				YAGO3-10			
	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10
GCN	.248	.155	.275	.417	.331	.238	.368	.520	.285	.201	.318	.457
GAT	.275	.184	.304	.446	.358	.267	.396	.549	.312	.228	.345	.483
GraphSAGE	.253	.162	.281	.423	.345	.251	.382	.535	.294	.215	.327	.468
HAN	.287	.196	.318	.461	.374	.285	.411	.563	.328	.242	.362	.498
HGT	.321	.229	.355	.501	.402	.317	.445	.589	.365	.278	.402	.537
SimpleHGN	.295	.205	.327	.472	.387	.298	.428	.576	.341	.256	.378	.513
GraphiT	.308	.218	.341	.485	.395	.309	.437	.582	.352	.267	.389	.524
GPS	.334	.241	.368	.515	.418	.332	.461	.601	.378	.291	.416	.549
Graph-Mamba	.318	.225	.352	.496	.405	.321	.448	.591	.358	.272	.395	.531
GraphSSM	.312	.221	.346	.489	.398	.314	.441	.585	.349	.265	.386	.522
KA-GMN	**.367**	**.276**	**.404**	**.552**	**.443**	**.364**	**.488**	**.628**	**.406**	**.323**	**.446**	**.574**

Experiments

This section presents a comprehensive empirical evaluation of KA-GMN across multiple heterogeneous graph benchmarks and downstream tasks. We conduct systematic experiments to validate our architectural contributions and demonstrate the effectiveness of KNN-augmented state space modeling for heterogeneous graph representation learning.

Datasets

We evaluate KA-GMN on five standard heterogeneous graph benchmarks spanning different domains and scales

- **FB15k-237** (Toutanova and Chen 2015b): A subset of the Freebase knowledge graph containing 14,541 entities across domains including people, locations, organizations, and concepts. The dataset comprises 237 relation types and 310,116 triplets, with standard train/validation/test splits of 272,115/17,535/20,466 triplets respectively. Eliminating inverse relations present in the original FB15k dataset to prevent trivial link prediction through relation reversal, making it challenging and realistic evaluation setting for knowledge graph completion tasks.
- **WN18RR** (Dettmers et al. 2018b): Derived from the WordNet lexical database, this dataset contains 40,943 entities representing English words and concepts, connected through 11 semantic relation types including hypernymy, meronymy, and similarity relations. With 93,003 triplets total, WN18RR addresses the inverse relation problem of the original WN18 dataset by removing reciprocal relations, creating a more stringent evaluation benchmark that requires models to learn genuine semantic relationships rather than exploiting structural patterns.
- **YAGO3-10** (Mahdisoltani, Biega, and Suchanek 2015): A large-scale knowledge graph constructed from multilingual Wikipedia, containing 123,182 entities spanning diverse categories and 37 relation types. With 1,079,040 triplets, representing comprehensive heterogeneous graph benchmarks by incorporating entities from multiple languages and domains.
- **DBLP** (Sun et al. 2011): An academic collaboration network extracted from the DBLP computer science bibliography, featuring 26,128 authors, 14,328 papers, 7,723 terms, and 20 venues. This heterogeneous network contains four distinct node types (Author, Paper, Term, Venue) connected through multiple edge types representing co-authorship, citation, publication, and term-paper associations.
- **IMDB** (Wang et al. 2019): A movie database network containing 21,420 movies, 4,278 directors, and 5,257 actors, representing a three-type heterogeneous graph with rich semantic relationships. The network captures directing, acting, and collaboration relationships, forming a complex web of interactions in the entertainment industry.

Experimental Setup

We compare KA-GMN against representative baselines spanning traditional graph neural networks (GCN (Kipf and Welling 2017), GAT (Velickovic et al. 2018), GraphSAGE (Hamilton, Ying, and Leskovec 2017a)), heterogeneous graph methods (HAN (Wang et al. 2019), HGT (Hu et al. 2020), SimpleHGN (Lv et al. 2021)), and recent graph transformers with state space models (GraphiT (Mialon et al. 2021), GPS (Rampášek et al. 2022), Graph-Mamba (Ma, Guo, and Zhang 2024), GraphSSM (Behrouz and Hashemi 2023b)). Implementation follows established protocols with Adam optimization, learning rate 2×10^{-4}, and early stopping based on validation performance.

Evaluation Metrics

Link Prediction Metrics For knowledge graph completion tasks, we employ standard ranking-based metrics following established evaluation protocols:

Mean Reciprocal Rank (MRR): The average of reciprocal ranks across all test queries, computed as:

$$\text{MRR} = \frac{1}{|Q|} \sum_{i=1}^{|Q|} \frac{1}{\text{rank}_i}$$

where rank_i is the rank of the correct entity for query i, and $|Q|$ is the total number of test queries.

Hits@K: The proportion of correct entities ranked within the top K positions:

$$\text{Hits@K} = \frac{1}{|Q|} \sum_{i=1}^{|Q|} I[\text{rank}_i \leq K]$$

where $I[\cdot]$ is the indicator function. We report Hits@1, Hits@3, and Hits@10.

All metrics use the filtered setting (Bordes et al. 2013), where corrupted triplets that exist in the training, validation, or test sets are removed during evaluation to ensure fair comparison and prevent artificial inflation of scores.

Node Classification Metrics For heterogeneous network node classification tasks, we report standard multi-class classification metrics: **Macro-F1**, **Micro-F1**, **Accuracy**.

Results

Main Results

Link Prediction Performance Table 2 presents comprehensive link prediction results across three knowledge graph benchmarks. KA-GMN achieves state-of-the-art performance, demonstrating the effectiveness of KNN-augmented state space modeling for heterogeneous graph representation learning.

The results reveal key insights into KA-GMN's effectiveness.

1. KA-GMN achieves substantial improvements over all baselines: +9.9% MRR improvement over GPS on FB15k-237, +6.0% on WN18RR, and +7.4% on YAGO3-10. These consistent gains across datasets with varying characteristics demonstrate the robustness of our approach. The strong performance on FB15k-237, which contains the most diverse entity and relation types, validates KA-GMN's ability to handle complex heterogeneous structures.
2. The improvements are pronounced in precision-oriented metrics (Hits@1), where KA-GMN shows +14.5% improvement over GPS on FB15k-237 and +9.6% on WN18RR. Suggesting that the KNN-augmented state space model excels at ranking the correct entity at the top position, which is crucial for practical knowledge graph applications. The selective neighbor identification mechanism enables more precise entity disambiguation by focusing on the most relevant structural and semantic context.
3. The performance gains increase with dataset scale and complexity. On YAGO3-10, the largest and most diverse dataset, KA-GMN shows the most substantial absolute improvements, indicating superior scalability of our linear-complexity approach compared to attention-based methods that suffer from quadratic bottlenecks.

Node Classification Performance Table 3 demonstrates KA-GMN's effectiveness on heterogeneous network node classification tasks, where preserving type-specific characteristics while enabling cross-type information flow is essential.

The node classification results provides evidence for KA-GMN's handling of heterogeneous graph structures. On DBLP, KA-GMN achieves +3.1% Macro-F1 improvement over GPS and +4.1% over the best heterogeneous method (HGT), demonstrating the effectiveness of combining selective state space modeling with adaptive neighborhood construction.

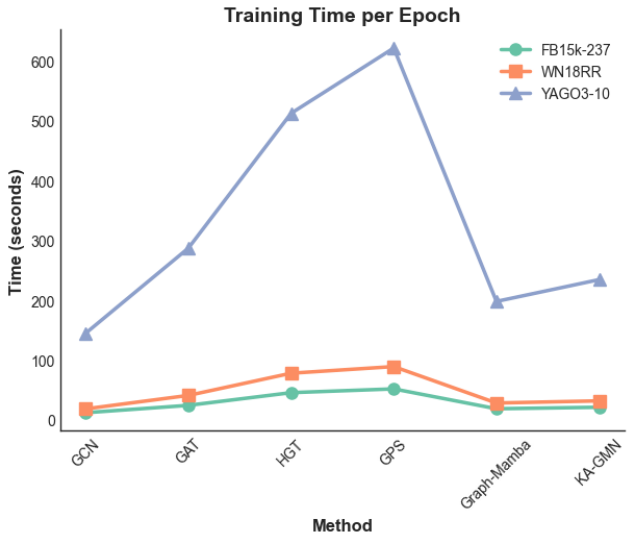

Figure 2: Computational efficiency comparison for training time per epoch across datasets

On IMDB, KA-GMN shows +3.8% Macro-F1 improvement over GPS and +5.7% over HGT. The particularly strong performance on IMDB, which features more pronounced heterogeneity with distinct interaction patterns between movies, directors, and actors, validates our type-aware feature transformation mechanisms. .

The results reveal that KA-GMN outperforms specialized heterogeneous methods (HAN, HGT, SimpleHGN) by significant margins, suggesting that the integration of selective state space modeling with heterogeneous graph processing creates synergistic effects beyond what either approach achieves independently.

Computational Efficiency Analysis The efficiency analysis reveals KA-GMN's favorable computational characteristics. While introducing modest overhead compared to standard Graph-Mamba (13-18% increase in training time), KA-GMN maintains linear scaling behavior and significantly outperforms attention-based methods. KA-GMN achieves superior performance-efficiency trade-offs: delivering +9.9% MRR improvement over GPS while requiring 58.9% less training time and 53.9% less memory on FB15k-237. This demonstrates the practical viability of our approach for large-scale heterogeneous graph applications where both performance and computational efficiency are essential [2].

Ablation Studies

Component Analysis Table 4 systematically evaluates the contribution of each architectural component through controlled ablation studies.

The ablation results provide crucial insights into the synergistic effects of KA-GMN's components. The KNN selection mechanism contributes the most substantial improvements (+8.2% average MRR), validating our hypothesis that adaptive neighborhood construction is essential for heterogeneous graph representation learning. The removal of KNN

Table 3: Node Classification Results on Heterogeneous Networks. Results show mean over 5 runs with 80%/10%/10% train/-validation/test splits.

Method	DBLP			IMDB		
	Macro-F1	Micro-F1	Accuracy	Macro-F1	Micro-F1	Accuracy
GCN	.726	.752	.748	.581	.612	.609
GAT	.768	.789	.785	.623	.651	.647
GraphSAGE	.741	.765	.761	.597	.624	.621
HAN	.832	.847	.844	.685	.708	.705
HGT	.859	.871	.868	.721	.741	.738
SimpleHGN	.843	.856	.853	.697	.718	.715
GraphiT	.851	.864	.861	.709	.729	.726
GPS	.867	.878	.875	.734	.753	.750
Graph-Mamba	.854	.866	.863	.712	.732	.729
GraphSSM	.848	.861	.858	.706	.727	.724
KA-GMN	**.894**	**.903**	**.901**	**.762**	**.779**	**.776**

Table 4: Ablation Study Results. MRR scores across datasets demonstrating the contribution of each component.

Variant	FB15k-237	WN18RR	YAGO3-10	DBLP	IMDB
KA-GMN	**.367**	**.443**	**.406**	**.894**	**.762**
w/o KNN Selection	.337	.421	.378	.867	.734
w/o Type-Aware Transform	.348	.429	.390	.881	.748
w/o Compatibility Function	.354	.436	.395	.886	.755
w/o Graph Convolution	.330	.414	.371	.862	.727
Standard Mamba Only	.321	.408	.361	.857	.715

Table 5: KNN Parameter Sensitivity Analysis. MRR scores for different neighborhood sizes.

K Value	FB15k-237	WN18RR	YAGO3-10
K=4	.344	.424	.381
K=8	.355	.435	.394
K=16	**.367**	**.443**	.406
K=32	.361	.439	**.411**
K=64	.352	.431	.398

selection forces the model to rely on fixed graph structure, leading to over-smoothing and poor type discrimination.

Type-aware transformations contribute +4.9% average improvement, demonstrating the importance of maintaining semantic coherence across heterogeneous node types. Without these transformations, the model struggles to preserve type-specific characteristics during the state space evolution process.

The compatibility function provides +3.7% improvement by enabling learned neighbor selection that balances feature similarity with structural connectivity. This validates our design choice to move beyond simple distance-based KNN to incorporate graph-aware compatibility scoring.

KNN Parameter Sensitivity Table 5 analyzes the impact of KNN size K on performance across datasets with different density characteristics.

The sensitivity analysis reveals dataset-dependent optimal K values that correlate with graph density and heterogeneity patterns. Smaller, denser graphs (FB15k-237, WN18RR) benefit from moderate K values (16) that provide sufficient context without introducing noise from distant neighbors. Larger, sparser graphs (YAGO3-10) require higher K values (32) to capture adequate neighborhood information for effective representation learning. This adaptability demonstrates KA-GMN's flexibility across diverse graph characteristics.

Limitations and Future Work

KA-GMN presents limitations that warrant consideration. The KNN computation introduces computational overhead, particularly for high-dimensional feature spaces and frequent graph updates. While achieving linear complexity, the periodic neighborhood updates (every 50 epochs) limit real-time applications. The current approach assumes relatively balanced node type distributions and may struggle with severe type imbalance where minority types represent less than 1% of nodes.

Several promising directions emerge for extending KA-GMN. First, developing adaptive KNN selection that automatically adjusts neighborhood size based on local graph density could eliminate manual hyperparameter tuning. Second, extending the approach to dynamic heterogeneous graphs where structure evolves over time represents a natural progression given the temporal modeling capabilities of state space models. The integration of selective state space models with adaptive neighborhood construction opens new research directions that could further advance heterogeneous graph representation learning while addressing current scalability and generalization challenges.

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