Abstract—Graph neural networks (GNNs) have been extensively used for many domains where data are represented as graphs, including social networks, recommender systems, biology, chemistry, etc. Recently, the expressive power of GNNs has drawn much interest. It has been shown that, despite the promising empirical results achieved by GNNs for many applications, there are some limitations in GNNs that hinder their performance for some tasks. For example, since GNNs update node features mainly based on local information, they have limited expressive power in capturing long-range dependencies among nodes in graphs. To address some of the limitations of GNNs, several recent works started to explore augmenting GNNs with memory for improving their expressive power in the relevant tasks. In this paper, we provide a comprehensive review of the existing literature of memory-augmented GNNs. We review these works through the lens of psychology and neuroscience, which has established multiple memory systems and mechanisms in biological brains. We propose a taxonomy of the memory GNN works, as well as a set of criteria for comparing the memory mechanisms. We also provide critical discussions on the limitations of these works. Finally, we discuss the challenges and future directions for this area.

Impact Statement—Memory-augmentation of graph neural networks is an emerging research field in the deep graph learning community. These augmentations can enhance GNNs’ capabilities for structured representation learning and relational reasoning tasks, such as human-object interaction prediction, question answering, and algorithm reasoning, etc. This paper provides a systematic review of the existing works in this field from the perspective of neuroscience and psychology. As the first review of memory GNNs, we identify the open challenges in this field and shed light on the promising directions for future work. By providing a neuroscience perspective, our work will also help facilitate novel brain-inspired memory model designs to advance graph neural networks for various domains.

Index Terms—Graph neural networks, Memory-augmented neural networks, Structured representation, Relational reasoning

I. INTRODUCTION

Graph neural networks (GNNs) are a family of models at the intersection of deep learning and structured approaches, and they have been widely studied in recent years [75], [84]. GNNs typically follow a recursive neighborhood aggregation (or message passing) scheme, where in each aggregation step, nodes collect information from their neighborhood and a new feature vector is computed for each node by an aggregation (or message passing) scheme, where in each aggregation step, nodes collect information from their neighborhood and a new feature vector is computed for each node by an aggregation and combination mechanism. After k iterations of aggregation, a node can be represented by its transformed feature vector, which captures the structural information within the node’s k-hop neighborhood [78]. Following such information propagation schemes, GNNs therefore have the ability to extract localized multi-scale spatial features and relational dependencies from the graphs, and they have been shown effective in learning useful structured representation for many relational reasoning tasks [4], [75], [84], including node classification, link prediction, clustering, knowledge graph completion, etc.

Although GNNs have achieved promising results in different domains, there are some limitations in the GNN models. One key issue is their limited expressive power in capturing long-range dependencies across the graph. This is mainly due to the fact that GNNs update node features based on local information [78], [1]. Generally a GNN layer can be treated as a message-passing step [20], where nodes update their states by aggregating information from their direct neighbors. While, interactions with distant nodes are also required in many problems. Some have proposed to address this by increasing the depth of the network, i.e. by stacking multiple GNN layers [1]. However, it has been observed that when the number of layers increases, the node representations become indistinguishable. This is known as the “over-smoothing” issue [75]. Moreover, as the number of layers increases, the number of nodes in each node’s receptive field grows exponentially. This also causes “over-squashing”, since information from the exponentially-growing receptive field will be compressed into fixed-length node vectors [1]. As a consequence, the graph is not able to propagate messages from distant nodes, and thus only captures short-range information.

In scenarios where there are dynamic interactions between nodes in the graph, such as social networks, capturing the temporal evolution of these graphs is a challenge for GNNs. Many of the existing GNN-based strategies treat dynamic graphs as discrete-time graphs represented as a sequence of snapshots of the graph, and use strategies like convolution to identify spatial structures while using recurrence to learn dynamic patterns from these graphs [58], while some others propose variations such as temporal graph attention [77] to aggregate temporal-topological neighborhood features for continuous-time dynamic graphs. These GNNs also suffer from bottlenecks on their expressiveness due to the limited ability to store information about the task and input history [14], [28].

Recently, some efforts are starting to be made for augmenting GNNs with memory to address these issues by enabling them to store and retrieve information in space or over time. Some of these works focus on using memory for graph learning in the space domain, where memory is used to store spatial
Theories about memory in the human brain may provide additional insight and motivation for the memory augmentation of GNNs. Historically, many areas of machine learning have repeatedly drawn inspiration from the brain to build architectures that maintain information over time. Early efforts include recurrent neural network (RNN) architectures [57], [25] that use internal states to store information about sequential inputs. Other memory-augmented neural networks (MANNs) utilize external memory with differentiable read-write operators to enable access of past experiences, and have been shown to enhance performance on many learning tasks, such as reinforcement learning [49], meta learning [54], and few-shot learning [71]. But memory augmentation of GNNs in particular, rather than other neural networks, may provide the ability to tackle specific structured representation learning problems. In particular, some propose that memory plays a key role in relational reasoning. This is thought to occur because the content of memory itself is stored as a structured representation. Studies of human recall behavior have provided evidence for this [8], [7], [44], [66]. Furthermore, neuroscience studies have also demonstrated a similarity structure to memory storage: more similar memories leads to more similar representations [17], [56]. Finally, there is empirical evidence from prior machine learning work as well: [55] demonstrated that augmenting an RNN with a relational memory module allows memories to interact with each other improves its performance for various relational reasoning tasks, including as partially observed reinforcement learning tasks, program evaluation, etc. This suggests that memory augmentation of GNNs may specifically improve performance on structured representation learning problems such as relational reasoning.

In this paper, we will provide a systematic review of the existing memory-augmented GNN works, categorizing them into a taxonomy and providing critical discussion on their limitations. Further, we pursue the thesis that memory systems in the brain may provide crucial insights into these limitations. We therefore provide criteria for understanding the memory mechanisms of GNNs from the perspective of cognitive neuroscience. We then provide insights about the major challenges in this field, as well as open problems and future directions.

Scope and Contributions. This paper is focused on reviewing the recently emerged works in memory-augmented GNNs, where the goal is to use memory strategies on GNNs to improve their capabilities on various graph learning tasks. We emphasize that this paper does not attempt to review the extensive literature on GNNs or deep graph representation learning that do not explicitly use memory. Prior works have focused on these topics [see [75], [84], [83]]. Here instead, we focus on the body of works that use memory in the model design of graph neural networks. Many of the recent works that we review in this paper have not been discussed in those prior surveys of GNNs. We provide a critical review of the memory-augmented GNN works from the neuroscience perspective. To the best of our knowledge, this is the first review paper on this topic. We summarize the main contributions of this paper as follows:

- We provide a taxonomy of existing memory-augmented GNN works.
- We provide a set of criteria for comparing the memory mechanisms, inspired by neuroscience.
- We present critical discussions on the limitations of these works.
- We provide insights on the open challenges and future directions in this field.

II. Framework

First we will review some key concepts and background of memory-augmented GNNs and the neuroscience of memory. In order to understand how different memory architectures operate in existing memory-augmented GNNs, we then establish a taxonomy inspired by cognitive neuroscience theories of memory systems. This will help us identify shortcomings of current models that may be addressed by neuroscience-inspired modifications.

A. Preliminaries

1) Notations: Let \( G = (V, E) \) denote a graph, where \( V \) is the set of nodes, \( E \subseteq V \times V \) is the set of edges. Let \( N = |V| \) be the number of nodes, and \( A, D \) be the adjacency matrix and degree matrix. For each node \( v \in V \), let \( N_v = \{ u \ | \ (u, v) \in E \} \) be its neighborhood node set, and \( X_v \) be the feature vector of node \( v \).

2) Memory GNN background: Since its emergence in early 2000s [21], GNNs have been extensively studied [75]. Based on the model architectures and training strategies, there are different types of GNNs, for instance, graph convolutional networks (GCNs) [33], graph attention networks(GATs) [69], and graph auto encoders (GAEs) [70], etc. GCNs define convolution and readout operations on graphs to capture structural features [33], while GAT utilizes attention mechanisms to learn the relative weights between connected nodes [69], and GAEs learn latent node representations through reconstructing graphs [70]. GNNs normally follow a neighborhood aggregation rule,
where the update rule for the $k$-th layer of a GNN can be summarized as:

$$a_v^{(k)} = AGG^{(k)}(\{h_u^{(k-1)} : u \in N(v)\}),$$

$$h_v^{(k)} = COMBINE^{(k)}(h_v^{(k-1)}, a_v^{(k)})$$

where $h_v^{(k)}$ is the feature vector of node $v$ at the $k$-th iteration/layer, $N(v)$ is the set of nodes adjacent to $v$, and $h_v$ is initialized as $h_v^{(0)} = X_v$. $AGG$ and $COMBINE$ are two learnable functions for the aggregation and combine strategy, which are often defined using distinct choices in different GNN architectures [78].

Research efforts in memory GNNs started with designing GNNs with internal memory, such as the pioneering work by [37] that proposes a recurrent GNN model using the gated recurrent unit (GRU) [12] to capture recursive and sequential patterns of graphs by modeling states at node-level or graph-level. Other variations of gated GNNs have also been studied [82], [80]. In a gated GNN model that employs GRUs, the node hidden state is updated by its previous hidden states and its neighbors’ hidden states, which can be defined as:

$$h_v^{(t)} = GRU(h_v^{(t-1)}, \sum_{u \in N(v)} W h_u^{(t-1)})$$

where $W$ represents the learnable weight parameters. An example of the propagation model of gated GNNs for one timestep can be found in Figure 1. Later on, some works started to explore the usage of external memory in GNNs to store information and extend GNN’s capabilities. For example, [76] proposes to augment GCN and GAT with an external memory to store global information of graphs for node classification tasks, whereas [73] introduces an external memory to GNNs that stores the entity relationships from knowledge graph for integrating knowledge into the dialog systems. Figure 2 shows an example of a memory-augmented GNN with external memory. There can be a memory controller that controls what is read from or written to the external memory units, as well as their interactions with the GNN module (similar to other MANNs [22], [23]).

3) Neuroscience background: Memory plays a fundamental role in human learning and decision making [16], [10]. In the fields of cognitive psychology and neuroscience, it is widely agreed upon that there are multiple memory systems which play different roles in different tasks [67], [59], [50]. Each distinct memory system is generally thought to rely on different neural mechanisms and brain regions. Figure 3 shows some widely accepted, systems-level theories of human memory which account for a large body of empirical evidence. While the theories illustrated in Figure 3 build on a molecular and cellular understanding of memory, their main focus is to define cognitive modules or neural systems that tackle a particular set of problems. A similar approach can help shape the design of memory modules in GNN architectures.

The first distinction drawn in multiple memory systems theories classify memory phenomena based on the duration of information retention. Short-term, or working memory operates over seconds to minutes, while long-term memory operates over days to years [50], [60] (see top of Figure 3A). Short-term memory is thought to be a low-capacity, high-precision system in which few items are maintained in memory with relatively low error. By contrast, long-term memory is thought to be a high-capacity, lower-precision system in which a huge number of items can be stored with varying levels of error [52], [8]. In some domains the precision differences are being challenged [9], but there is widespread agreement that when a memory system reaches its capacity limit, there must be some way for the system to forget, overwrite, or decay information in memory [52]. It is important to understand memory system capacity and forgetting in GNN architectures to understand how to scale their memory for larger problems.

Another key advance was made in understanding the different stages of memory, regardless of its duration. The stages include (1) encoding, (2) maintenance or consolidation, and (3) retrieval [48], [64]. In terms of the memory GNNs, we can distinguish them based on how they encode memories, or how the write mechanism works. The write mechanism determines what information is stored in memory. We can also distinguish them based on how they retrieve memories, or how the read
mechanism works. Note that some retrieval mechanisms can be very simple – i.e. all information stored in memory is retrieved.

We apply this framework to understand different memory mechanisms in a variety of GNN papers. By understanding the read/write mechanisms and forgetting behavior of these networks, we can gain a greater understanding of how to design better memory mechanisms depending on task demands.

B. Taxonomy

There are no direct, consistent analogies between memory GNN architectures and the taxonomies depicted in Figure 3B-C. We instead categorize the work based on two key distinctions: scope, and external vs. internal memory.

1) Scope: Human memory operates over either short or long temporal durations – that is, the scope of the memory is always operating over time. By contrast, some memory GNNs actually
2) **External vs. internal memory**: We also distinguish between an external memory in a GNN vs. an internal or recurrent memory. There is a sizeable body of work on gated GNNs (e.g., [37]) which rely on a recurrent unit to process some input for a fixed number of timesteps $T$, and output a sequence. The recurrent unit contains a hidden state, which is a short-term memory store that propagates information from timestep to timestep based on a rule such as the one defined by Equation (3) and illustrated in Figure 1. In a typical gated GNN, hidden states from $t < -T$ are discarded. Given that these hidden states are temporary memories directly mapped to their recurrent units, we can view them as memories that are internal to the units. This type of memory is distinct from other forms of information storage in a neural network, such as a key-value database or a knowledge graph. We refer to these other forms of storage as external memory stores. External memories are not tied to a specific processing unit – that is, they can be accessed and modified based on the activity of many units. By analogy to biological systems, an internal memory state can be thought of as persistent activity in a single neuron, whereas an external memory state would be a record of activity across a population of neurons. From this we can see that any information that would be beneficial to many units should be stored in external memory. On the other hand, it would be inefficient to store information that is only useful to a single unit or a small number of units in external memory – instead storing it in a state internal to the unit is preferable.

Note that this terminology is not consistent in the reviewed works. For example, in [85] the memory used for reinforcement learning depends on a recurrent unit with internal states. However, the authors refer to this memory as external because it is external to the agent, not because it is external to the GNN.

### C. Comparison of key memory mechanisms and properties

We will now thoroughly review key mechanisms and properties of memory GNNs, which is summarized in Table I. These often differ depending on the scope or type of memory (internal or external), which we detail below.

1) **Write Mechanism**: All memory modules require a write mechanism, which determines what information is stored or encoded in memory. In most cases, the neural network architecture has a rule which determines what is stored in...
memory. In regimes where memory capacity is limited, a selective write mechanism ensures that only relevant and useful information is stored for later processing. Note, however, that some memory GNNs work choose store a static knowledge graph in the memory which is never modified by the GNN [43]. In this case, the information stored in memory is simply the contents of the knowledge graph, and there is no separate write mechanism apart from creating that knowledge graph.

In all cases, the write mechanisms in the memory GNNs varied depending on the form of memory. For example, a cache memory has a simple write rule: it only stores information from the most recent \( t \) timesteps [38]. This is an effective choice if it is known that the task would not benefit from storing long-term information, or if the rule is only used for a short-term memory module that will later be combined with a long-term memory module. For GNNs with internal memory, most used a write rule determined by the gate equations of recurrent units. Here the information written to memory depended on learnable weights in a gated recurrent unit [37], [46], [85], [73], allowing context-dependent memory encoding. We did find that one GNN with internal memory states did not use a recurrent unit – instead, the information kept in memory depended on a learnable persistency mask which is computed after a round of message passing [62]. Interestingly, the persistency mask also depended on the retrieval mechanism (see below). In both cases, the gate or the mask learned what information to store.

For external memory modules, there was a variety of write mechanisms. One common form of external memory in neural networks is a key-value store, where the items in memory are stored as a key \( k \) associated with a value \( v \) [42], [81], [26]. These items are then retrieved based on some input query \( q \). The write mechanism can change the entire key-value pair. [32] defined a key-value memory over space to learn distant features of a graph. They used these key-value memory layers to coarsen the node representations, and could therefore define both the keys and values as dependent on the query inputs from the previous layer. The write mechanism consisted of arranging the keys as clusters of the queries, and defining the values as projections of the keys back into the query space. Clustering mechanisms are useful when it is known that the information to be stored in memory has some higher-level structure. By contrast, we found that internal memory states are usually stored without much further reorganization.

Unlike [32], [38] defined a key-value memory over time to learn a long-term embedding representation of input items. Inspired by previous work on memory [63], [81], they simply trained the key-value matrices \( K \) and \( V \) through backpropagation to write to the memory. While this write mechanism is quite general, it either assumes that (1) once trained, the embedding is an effective static representation of the input data or (2) the embedding is retrained or fine-tuned whenever the input data statistics change. This type of write mechanism would not be effective in online learning settings.

A few papers incorporate some part of the graph structure to update the contents of memory, often by aggregation across nodes. For example, [76] created a memory that contained spatially global information about a graph. To do this, they connected the memory nodes to every other node in the graph, and incorporate the memory nodes in the message passing, by defining a new aggregation rule based on Equation (1) & (2):

\[
\forall v \in V, h_v^{(k+1)} = AGG_v^{(k)}\left(\{h_v^{(k)}, h_{N(v)}^{(k)}, m_{V,M}\}\right), \quad (4)
\]

\[
\forall v \in V_M, m_v^{(k+1)} = AGG_v^{(k)}\left(\{m_v^{(k)}, h_v^{(k)}\}\right) \quad (5)
\]

where \( V_M \) is the set of memory nodes, and \( m_v^{(k)} \) is the representation for memory node \( v \) at the \( k \)-th layer. The write mechanism is therefore equivalent to the aggregation operation applied to this memory node, which in turn depends on whichever GNN architecture is selected to serve as the backbone of the network. The aggregation rule is also part of the write mechanism for [29], where the authors created a spatially organized set of memory cells which aggregate information from two different GNNs. Finally, the multi-step write mechanism in [53] also depends on an aggregation function. The authors propose the use of this memory in a dynamic graph. After computing all the messages between nodes, the aggregator combines the messages over time for each node. This then determines how the memory is updated for that node.

[73] relied on a memory controller that learns what to write to its external memory. This is more akin to other work on memory-augmented neural networks, such as the Neural

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Fig. 4. Type and scope of memory GNNs reviewed here. All of the works shown in Table I are depicted here, sorted by the scope of the memory and whether it is internal or external. Refer to Section II-B1 and II-B2 for definitions.
For RNNs, for example, two questions about their memory: (1) How much information about the task can they store in their parameters? (2) How much information about the input history can they store in their units? [14]. The answers to these two questions usually also indicate the potential bottlenecks of these models.

For the memory-augmented GNN models that have external memory, discrete items are stored in their memory and therefore the capacity is bounded by the number of memory nodes and hidden dimension. For instance, the memory capacity of the model in [76] is bounded by $M \times D$, where $M$ is the number of memory nodes added to the graph, and $D$ is the size of the hidden dimension for the graph neural network layers. In [29], the memory capacity is bounded by $P \times Q \times D$, where $P \times Q$ is the number of regions of the 2D image, and $D$ is the size of the hidden dimension. In [32], the memory capacity of the proposed memory-based GNN is $M \times D$, where $M$ is the number of centroid nodes in the memory layer of the model, and $D$ is the size of the hidden dimension. The memory graph networks applied in [43] store a knowledge graph in its external memory, therefore its memory capacity is the size of the knowledge graph, i.e., $G(V, E)$, where $V$ is the set of nodes that represent entities (e.g., locations, events, public entities) and $E$ is the set of edges that represent the connections among the entities. Similarly, in [73], the external memory is organized as a knowledge graph $G(V, E)$, where nodes in $V$ represent entities and edges in $E$ represent relations between entities. The memory capacity in this case is also the size of the graph $G(V, E)$.

For the models with recurrent memory, they can store the latent representation of nodes for a number of time steps. As shown in Table I, some of these memory GNNs operate over time, like the models proposed in [38], [37] and some others operate over both space and time [46], [62], [53]. The memory capacity of these models depends on the number of recurrent units, number of time steps, and the number of layers. These also determine how well the models can learn over space or time. However, empirical work suggests that RNN capacity seems to be limited by the trainability of the architecture, rather than the number of parameters or hidden units [14].

4) Forgetting Behavior: Memory systems with a limited capacity need to have some mechanism or policy in place to discard information that is no longer useful or relevant. Neurobiological studies of memory also indicate that forgetting (transience) in memory is important for memory-guided decision-making in dynamic, noisy environments, because transience can enhance flexibility by reducing the influence of outdated information and preventing overfitting to specific past events, thus promoting generalization [51].

Most of the GNNs with an internal memory have an explicit mechanism to forget. For instance, the GNNs with GRUs or LSTM units [29], [37], [53], [85], [46] have reset or forget gates to discard old information. [73] has an update gate to control how much previous hidden state is kept. It is worth noting that while the persistent message passing model proposed in [62] also has internal memory, it does not have any forgetting behavior. Rather, it maintains a persistent set of internal states to represent the history of operations for entities through their lifetime. This kind of behavior can lead
to intractable storage costs and complexity issues. Moreover, without a forgetting mechanism, the model can fail when the information stored in memory becomes outdated and not relevant to the current state. In [38], the oldest items stored in the short-term memory are removed and replaced by recent items, while the long-term memory does not have any specified forgetting behavior.

We found that forgetting is not useful for memory GNNs that use memory for storing spatial information about a graph, such as the key-value store of graph hierarchical structure in [32] and the global information store in [76]. Here the spatial features they store involve the entire graph, and all that information is required by the models during the feature propagation over the graph. They are also not applicable to memory GNNs that do not have write mechanisms. In [43], memory was a static knowledge graph that stores entities and their relationships from the episodes in a dataset collection. However, as discussed above, the memory was never modified by the GNN, and it does not have any mechanism for forgetting either.

### III. Applications

Different forms of memory or mechanisms may be best suited to a particular type of application. The existing memory GNN works study a variety of tasks and applications, including traditional graph/node classification, node representation learning for question answering, sequential recommendation or other applications.

**a) Graph Classification:** Graph classification is the problem of predicting the class label for the whole graph [40]. This task is widely studied for many domains. For example, in social networks such as Reddit or Collab [32], one application is to predict the type of community given a graph of online discussion threads or to predict the field of a researcher given one’s ego-collaboration graph. In bioinformatics, a common graph classification problem is to predict the protein function from structure given the protein represented as a graph [6]. In brain network analysis, graph classification tasks are usually conducted for neurologically disorder detection [39], [79]. In these problems, how to learn a graph-level representation that captures both global topological information and local discriminative features for classifying the graphs is a key challenge. These applications use memory over a spatial scope and may not need forgetting mechanisms (depending on whether the graph is static or dynamic). However, it may still be the case that selective writing and retrieval mechanisms may improve task performance.

**b) Node Classification:** Node classification is the task of classifying the graph nodes into different classes. An example of node classification problem in web networks is to predict the categories for web pages, where the web pages are represented as nodes and hyperlinks as edges in a graph [76]. In program analysis for compiler optimization, some data flow analysis tasks have also been formulated as a node classification problem, such as reachability analysis, which predicts if a statement is reachable from a root statement, where statements are represented as nodes in the program graph [15]. In these tasks, how to learn node representations that can best capture the relations or dependencies between nodes is a key problem. A memory mechanism in GNNs that could enhance a GNNs’ capability to capture such information may greatly benefit these node classification tasks. [76] has shown by their experiments that incorporating global graph information via the memory in MemGAT and MemGCN significantly improves the GNN’s performance in node classification tasks. Similar to the graph classification tasks, these memory models operate over the scope of space and will likely only benefit from forgetting mechanisms if the graph is dynamic.

**c) Question Answering:** Question and answering (QA) is also an extensively studied task, where many of the existing works have been focused on the fact retrieval task from a large-scale knowledge graph or memory graphs generated with information about entities and their relations [5], [43]. There are also some works that focus on visual QA systems, where contexts from images are also used for answering the questions [47], [29]. Memory GNN models can greatly benefit these applications, since they have the capability to store the semantic and structural information in memory and utilize them with knowledge graphs for the QA tasks.

**d) Recommender Systems:** Recommender systems are important for e-commerce applications in online retail, video streaming, etc. In the graph space, the problem of recommending is usually formulated as a link prediction or a ranking task, given the users and items [74]. Meanwhile, the sequential recommendation task focuses on the chronological item sequence for making predictions [65]. Memory networks have been used in both scenarios to memorize the key items and contextual information for predicting future user actions [36], [11]. In particular, among the existing memory GNN works, [38] apply a graph neural network with two different forms to memory to capture both short-term item contextual information and long-term item dependencies. They also incorporate item co-occurrences to model the relationships between closely related items.

Beyond the applications discussed above, there are other areas that could benefit from GNNs with memory augmentation. Here we highlight meta-learning and reinforcement learning.

**e) Meta-learning on graphs:** It has been shown that neural networks augmented with external memory (MANNs) could achieve promising results in meta-learning tasks with their ability to quickly encode and retrieve new information [54]. For instance, the Neural Turing Machine [22] has an LSTM memory controller that interacts with an external memory module using a number of read and write heads. It has demonstrated superior performance in meta-learning tasks such as few-shot prediction for image classification [54]. In the meta-learning area, there are also problems that involves relational reasoning, for example, the few-shot human-object interaction recognition task that aims at inferring new interactions between human actions and objects with only a few available instances [27]. Having a memory-augmented GNN that can learn a general strategy for the structured representations it should place into memory and how it should use these representations for predictions could potentially benefit these tasks.
f) Reinforcement learning over graphs: Memory is an important aspect of intelligence and plays an important role in many deep reinforcement learning (RL) models [18]. For example, episodic memory has been shown to enable reinforcement learning agents to adapt more quickly and thus improve data efficiency [49], [24]. In graph environments, existing reinforcement learning efforts mainly focus on combinatorial optimization problems on graphs, such as the Maximum Cut [3], community detection [72], and Traveling Salesman problems [30]. Some of the works in this area started to consider memory-augmented GNNs for RL. For instance, the memory-augmented graph RL work [85] we discussed in Section II introduces an external memory adapted to the graph environment to enable a recurrent model with greater representation power for the graph navigation task. However, little progress had been made in augmenting GNNs with memory for these graph reinforcement learning tasks. This would be a promising future direction.

IV. OPEN CHALLENGES AND FUTURE DIRECTIONS

Although the memory GNNs have achieved some promising results in different domains, there are still limitations of the existing works and some open problems in this area. In light of the challenges, we envision several future directions to improve current memory GNN architectures.

A. Multiple memory systems

Despite the advances of the memory graph neural network models, there is still a gap between what current models can achieve and human intelligence. The challenges are especially apparent in tasks that require complex language and scene understanding, reasoning about structured data, and transferring learning beyond the training conditions [4], [19]. For instance, we humans have remarkable abilities to remember information over long time, and we can make use of memories at varying time-scales, but current memory neural networks, such as the memory GNN models based on RNNs that only have internal memory [37], [46], [62], [53], are still limited in their capabilities to capture long time-scale information. While RNN capacity should linearly scale with the number of parameters, it has been shown that it is difficult to train these networks to reach that capacity [14]. In language modeling, for example, well-trained RNNs can only utilize about 200 timesteps of past context [31]. Therefore relying on RNNs to store information in these memory GNN models can limit the models’ ability to store and access long-timescale history information that are important for these tasks. This may also be especially important for dynamic graphs that evolve over time.

One promising direction to further advance memory GNNs in these aspects is to design models with multiple memory systems. As discussed in previous sections, different forms of memory (e.g. internal memory, external memory) have their own properties and advantages, and they can improve different aspects of graph learning tasks. Having a memory GNN with multiple forms of memory would essentially combine their benefits for improving GNN’s expressive power, and would mimic the multiple memory systems that exist in biological systems. A similar point on multiple memory systems has been made for models of language processing [45]. Some of the existing memory GNNs we reviewed have multiple forms of memory, such as a spatially organized external memory and internal GRU memory in the Multimodal Neural-GMN [29], or the external knowledge base combined with a GRU response decoder in the GraphMemDialog model [73]. However, these networks are designed specifically for those applications, and there is still a lack of general multiple memory models for GNNs to improve their expressive power to address fundamental problems in structured representation learning.

According to dominant theories of human learning and memory, there are interactions between different memory systems, as illustrated in Figure 3B-3C. For instance, rapidly learned information can be consolidated as structured, long-term memories through bidirectional interactions between the hippocampus and cortex [35]. When designing multiple-memory-augmented GNN models, the key problem is what forms of memories to consider and how to formulate the interactions between these memories to facilitate the learning of GNNs with these multiple memory components.

B. Theoretical Analysis

Another problem is the lack of theoretical analysis of memory GNN models. Most approaches showed success through the experimental evaluations for applications, but very few of them provide theoretical proof or analysis on the impact of the memory models on the GNNs for the graph learning tasks. Although some work has attempted to do this – [76] provides theorems to indicate that memory augmentation is helpful to identify locally indistinguishable graphs – there is still a lack of theoretical foundations on why memory is helpful to improve GNNs and how much benefit different memory mechanisms could bring for extending the capabilities of GNNs. For instance, it would be useful to see some theoretical analysis on the influence of the memory for GNNs (e.g. the MemGCN and MemGAT) on the receptive field [41] of nodes, thus proving the impact of memory for long-range problems.

C. Empirical Evaluations of Memory

The current evaluations of the memory GNN models in the existing works are mostly done on standard graph learning applications, such as graph/node classification and recommender systems. They use common metrics such as classification accuracy to measure the performance of the models and compare with baseline GNNs. Although they are able to demonstrate the overall performance of the models for the applications with these metrics, they lack a framework with fine-grained measures for evaluating the contribution of memory for these tasks. For instance, it would be useful to have more metrics to measure the long range relationships that existing networks can capture. Although some works have attempted to do this, such as the work in [1] that introduces a NeighborsMatch task to evaluate GNNs for long-range problems, there is still a lack of general evaluation frameworks, including benchmark
datasets, tasks, and metrics, for the empirical evaluation of the memory GNNs. This would be a valuable future direction.

D. Scalability

The enhanced capabilities of memory-augmented neural networks often come at a high computational cost [61]. Memory GNNs could be even more prone to this issue, since the data they deal with are complex structured data. For instance, the memory mechanism proposed for the MemGCN [76] introduces an extra $O(NM)$ message passing per layer for the GNNs, which allows each of the $N$ nodes in the original graph to interact with the $M$ memory nodes stored in external memory. This extra cost could be very large when scaling to big graphs or when the graph is sparse. In other memory GNN models there is no forgetting mechanism, leading them to maintain memories through their lifetime without discarding any outdated information [62]. Depending on the application this can cause issues with complexity and storage costs and severely limits scalability. A promising future direction for addressing these issues is to design selective write mechanisms and forgetting mechanisms. For models that suffer from complexity issues introduced by the memory augmentation, one promising solution is to have a selective write mechanism that controls what is written to memory. For example, instead of storing information from all nodes in the MemGCN [76], they could consider some form of selection criteria or an attention mechanism to ensure only relevant and useful information is written into the memory. This could improve the efficiency and thus the scalability of the models. Furthermore, adding selective forgetting mechanisms to models can not only reduce the storage cost of the memory, but it can also help alleviate the influence of outdated information and prevents the model from overfitting to past events.

V. CONCLUSION

We have presented a review of the mechanisms, applications, and limitations of current memory GNN models from the lens of neuroscience and psychology. It is clear that multiple forms of memory exist in these models (Table I) to support a variety of structured representation learning problems. In particular, internal memory supports the local persistence of information across time or across a portion of the graph, whereas external memory can provide more global information or contextual knowledge. Future work on memory GNN models may improve both performance and scalability, but these advances depend on the continued development of both theoretical and empirical tools to evaluate the contribution of memory.

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