GraphTheta: A Distributed Graph Neural Network Learning System With Flexible Training Strategy

Houyi Li[*], Yongchao Liu[*], Yongyong Li[*], Bin Huang[*], Peng Zhang[*], Guowei Zhang[*], Xintan Zeng[*], Kefeng Deng[+], Wenguang Chen[*], and Changhua He[*]

[*]Ant Group, China
[+]Alibaba Group, China

Abstract

Graph neural networks (GNNs) have been demonstrated as a powerful tool for analysing non-Euclidean graph data. However, the lack of efficient distributed graph learning systems severely hinders applications of GNNs, especially when graphs are big, of high density or with highly skewed node degree distributions. In this paper, we present a new distributed graph learning system GraphTheta, which supports multiple training strategies and enables efficient and scalable learning on big graphs. GraphTheta implements both localized and globalized graph convolutions on graphs, where a new graph learning abstraction NN-TGAR is designed to bridge the gap between graph processing and graph learning frameworks. A distributed graph engine is proposed to conduct the stochastic gradient descent optimization with hybrid-parallel execution. Moreover, we add support for a new cluster-batched training strategy in addition to the conventional global-batched and mini-batched ones. We evaluate GraphTheta using a number of network data with network size ranging from small-, modest- to large-scale. Experimental results show that Graph-Theta scales almost linearly to 1,024 workers and trains an in-house developed GNN model within 26 hours on Alipay dataset of 1.4 billion nodes and 4.1 billion attributed edges. Moreover, GraphTheta also obtains better prediction results than the state-of-the-art GNN methods. To the best of our knowledge, this work represents the largest edge-attributed GNN learning task conducted on a billion-scale network in the literature.

1 Introduction

Graph neural networks (GNNs) [15] [28] have been popularly used in analyzing non-Euclidean graph data and achieved promising results in various applications, such as node classification [8], link prediction [22], recommendation [10, 32, 35] and quantum chemistry [11]. Existing GNNs can be categorized into two groups, i.e., transductive graph learning (GL) and inductive GL. From the perspective of transductive learning [8] [21], although it is easy to implement by directly learning embeddings from nodes and edges, the shortcomings of transductive learning are obvious. First, the number of parameters expands linearly with graph size, which is hard to train on big graphs. Second, it is unable to calculate embeddings for new nodes and edges that are unseen before training. These two limitations hinder the applications of transductive learning on real-world graphs. In contrast, inductive learning [16] [4] [18] [10] [32] introduces a trainable generator to compute node and edge embeddings, where the generator is often a neural network and can be trained to infer embeddings for new unseen nodes and edges.

From the perspective of inductive learning, global-batch [8] [21] and mini-batch [16] are two popular training strategies on big graphs. Global-batch performs globalized graph convolutions across an entire graph by multiplying feature matrices with graph Laplacian. It requires calculations on the entire graph, regardless of graph density. In contrast, mini-batch conducts localized convolutions on a batch of subgraphs, where a subgraph is constructed from a node with its neighbors. Typically, subgraph construction meets the challenge of size explosion, especially when the node degrees and the exploration depth are very large. Therefore, it is difficult to learn on dense graphs (dense graphs refer to graphs of high density) or sparse ones with highly skewed node degree distributions. To alleviate the challenge of mini-batch training, a number of neighbor sampling methods are proposed to reduce the size of neighbors [4, 18, 24]. However, the sampling methods often bring unstable results during inference [10].

Currently, GNNs are implemented as proof-of-concept on the basis of popular deep learning frameworks such as Tensorflow [1, 6, 27]. However, these deep learning frameworks are not specially designed for non-Euclidean graph data and thus inefficient on graphs. On the other hand, existing graph processing systems [5, 13, 26, 36] are incapable of training deep learning models on graphs. Therefore, developing a new GL system becomes urgent in industry [32] [10] [35] [25] [31].

A number of GL frameworks have been proposed based on the shared memory, such as DGL [31], Pixie [10], Pin-Sage [32] and NeuGraph [25]. These systems, however, are

restricted to the host memory size and difficult to handle big graphs. From the viewpoint of training strategy, Pixie and Pin-Sage use mini-batch, NeuGraph supports global-batch, and DGL considers both. Moreover, GPNN [23], AliGraph [35] and AGL [33] use distributed computing, but they support only one type of the training strategies. GPNN targets the global-batch node classification, but it employs a greedy trans-ductive learning method to reduce inter-node synchronization overhead. AliGraph focuses on mini-batch and constructs sub-graphs by using an independent graph storage server. AGL also targets mini-batch, but it differs from AliGraph by simply building and maintaining a subgraph for each node offline with neighbor sampling. However, such a simple solution often brings prohibitive storage overhead, hindering its appli-cations to big graphs and deep neighborhood exploration.

In fact, existing mini-batch based distributed methods use a data-parallel execution, where each worker takes a batch of subgraphs, and performs the forward and gradient compu-tation independently. Unfortunately, these methods severely limit the system scalability in processing highly skewed node degree distribution such as power-law, as well as the depth of neighborhood exploration. On one hand, there are often a number of high-degree nodes in a highly skewed graph, where a worker may be short of memory space to fully store a subgraph. For example, in Alipay dataset, the degree of a node easily reaches hundreds of thousands. On the other hand, a deep neighborhood exploration often results in explosion of a subgraph. In Alipay dataset, a batch of subgraphs obtained from a two-hop neighborhood exploration with only 0.002% nodes can generate a large size of 4.3% nodes of the entire graph. If the neighborhood exploration reaches 0.05%, the batch of subgraphs reaches up to 34% of the entire graph. In this way, one training step of this mini-batch will include 1/3 nodes in the forward and backward computation.

In this paper, we aim to develop a new parallel and dis-tributed graph learning system GraphTheta to address the following key challenges: (*i*) supporting both dense graphs and highly skewed sparse graphs, (*ii*) allowing to explore new training strategies in addition to the existing mini-batch and global-batch methods, and (*iii*) enabling deep neighborhood exploration w/o neighbor sampling. To validate the perfor-mance of our system, we conduct experiments using different GNNs on various networks. The results show that compared with the state-of-the-art methods, GraphTheta yields compara-ble and even better prediction results. Moreover, GraphTheta scales almost linearly to 1,024 workers in our application en-vironment, and trains an in-house developed GNN model on Alipay dataset of 1.4 billion nodes and 4.1 billion attributed edges within 26 hours on 1,024 workers. Our technical con-tributions are summarized as follows:

- We present a new GL abstraction NN-TGAR, which en-ables user-friendly programming (supporting distributed training as well) and bridges the gap between graph pro-cessing systems and popular deep learning frameworks.

- To alleviate the redundant calculation among batches, we implement to support a new type of training strategy, i.e. cluster-batched training [7], which performs graph convolution on a cluster of nodes and can be taken as a generalization of existing mini- or global-batch strategy.

- A new distributed graph training engine is developed with gradient propagation. The engine implements a new hybrid-parallel execution. Compared to existing data-parallel executions, the new engine can easily scale up to big dense/sparse graphs as well as deep neighborhood exploration.

2 Preliminary

2.1 Notations

A graph can be defined as $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$, where $\mathcal{V}$ and $\mathcal{E}$ are nodes and edges respectively. For simplicity, we define $N = |\mathcal{V}|$ and $M = |\mathcal{E}|$. Each node $v_i \in \mathcal{V}$ is associated with a feature vector $\boldsymbol{h}_i^0$, and each edge $e(i, j) \in \mathcal{E}$ has a feature vector $\boldsymbol{e}_{i,j}$, a weight value $a_{i,j}$. To represent the structure of $\mathcal{G}$, we use an adjacency matrix $\boldsymbol{A} \in \mathbb{R}^{N \times N}$, where $A(i, j) = a_{i,j}$ if there exists an edge between nodes i and j, otherwise 0.

Algorithm 1 MPGNN under different training strategies

1: Partition graph $\mathcal{G}$ into P non-intersect subgraphs, denoted as $\mathcal{G} = \bigcup \{\mathcal{G}_1, \mathcal{G}_2, ..., \mathcal{G}_P\}$.
2: $\mathcal{G}_p \leftarrow \mathcal{G}_p \cup N_K(\mathcal{G}_p) \ \forall p \in [1, P]$
3: **for** each $r \in [1, St]$ **do**
4:     Pick γ subgraphs randomly, $\mathcal{B}_r \leftarrow \bigcup_\gamma \{\mathcal{G}_i\}$
5:     **for** each $k \in [1, K]$ **do**
6:         $\boldsymbol{n}_i^k \leftarrow Proj_k(\boldsymbol{h}_i^{k-1} | \boldsymbol{W}_k) \ \forall v_i \in \mathcal{B}_r$
7:         $\boldsymbol{m}_{j \to i}^k \leftarrow Prop_k\left(\boldsymbol{n}_j^k, \boldsymbol{e}_{i,j}, \boldsymbol{n}_i^k \middle| \boldsymbol{\theta}_k\right) \ \forall e_{i,j} \in \mathcal{B}_r$
8:         $\boldsymbol{h}_i^k \leftarrow Agg_k\left(\boldsymbol{h}_i^{k-1}, \{\boldsymbol{m}_{j \to i}^k\}_{j \in N_O(i)} \middle| \boldsymbol{\mu}_k\right) \ \forall v_i \in \mathcal{B}_r$
9:     **end for**
10:     $\hat{\boldsymbol{y}}_i \leftarrow Dec(\boldsymbol{h}_i^K | \boldsymbol{\omega}) \ \forall v_i \in \mathcal{B}_r$
11:     $L_r \leftarrow \sum_{v_i \in \mathcal{B}_r} l(\boldsymbol{y}_i, \hat{\boldsymbol{y}}_i)$
12:     Update parameters by gradients of L_r
13: **end for**

2.2 Graph Neural Networks

Existing graph learning tasks are often comprised of `encoders` and `decoders`. Encoders map high-dimensional graph information into low-dimensional embeddings. De-coders are application-driven. The essential difference be-tween GNNs relies on the encoders. Encoder computation can be performed by two established methods [34]: spectral and propagation. The spectral method generalizes convolution operations on a two-dimensional grid data to graph-structured data as defined in [21] [9], which uses sparse matrix multipli-cations to perform graph convolutions as described in [21]. The propagation method describes graph convolutions as a

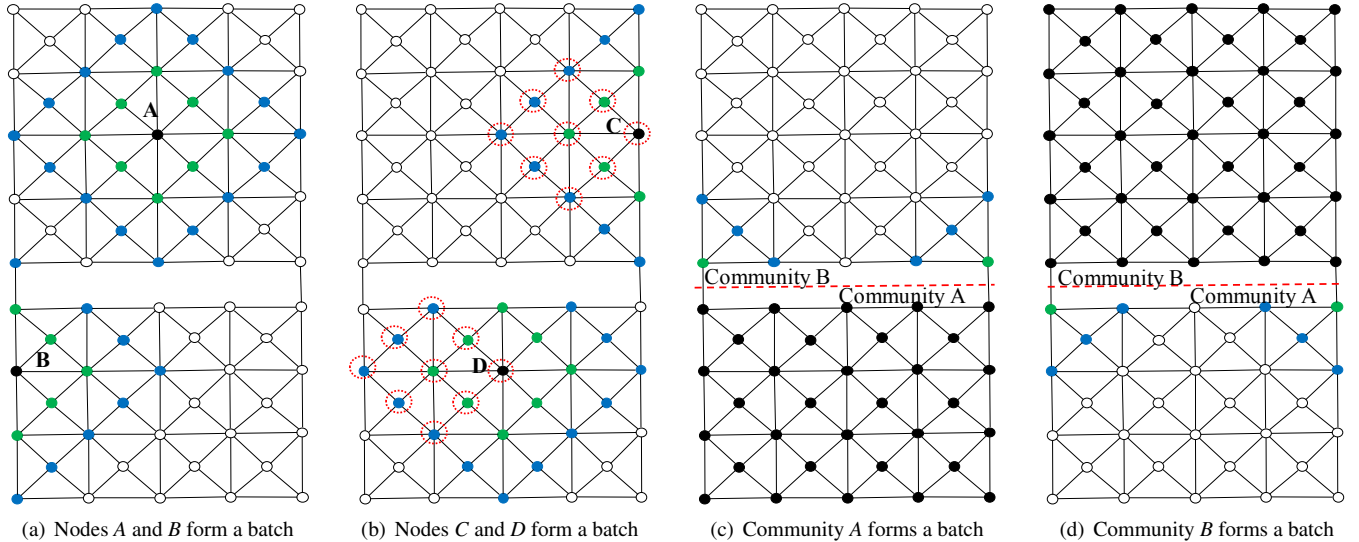|			
(a) Nodes *A* and *B* form a batch	(b) Nodes *C* and *D* form a batch	(c) Community *A* forms a batch	(d) Community *B* forms a batch

Figure 1: An example of a two-hop node classification: (a) and (b) are of mini-batch, (c) and (d) are of cluster-batch. The black solid points are the target nodes to generate mini-batches. The green and blue solid nodes are the one-hop and two-hop neighbors of their corresponding target nodes. The hollow nodes are ignored during the embedding computation. The nodes with circles are the shared neighbors bewteen mini-batches.

message propagation operation, which is equivalent to the spectral method (the proof refers to Appendix A.1).

In this paper, we present a framework of Message Propagation based Graph Neural Network (MPGNN) as a typical use case to elaborate the compute pattern of NN-TGAR and our new system GraphTheta. As shown in Algorithm 1, MPGNN can unify existing GNN algorithms under different training strategies. Recent work [30] [16] [12] focuses on propagating and aggregating messages, which aims to deliver a general framework for different message propagation methods. In fact, the core difference between existing propagation methods lie in the projection function (Line 6), the message propagation functions (Line 7) and the aggregation function (Line 8).

2.3   Cluster-batched Training

We study a new training strategy, namely cluster-batched gradient descent, to address the challenge of redundant neighbor embedding computation under the mini-batch strategy. This training strategy was first used by the Cluster-GCN [7] algorithm and shows superior performance to mini-batch in some applications. This method can maximize per-batch neighborhood sharing by taking the advantage of community detection (graph clustering) algorithms.

Cluster-batch first partitions a big graph into a set of smaller clusters. Then, it generates a batch of data either based on one cluster or a combination of multiple clusters. Similar to mini-batch, cluster-batch also performs localized graph convolutions. However, cluster-batch restricts the neighbors of a target node into only one cluster, which is equivalent to conducting a globalized convolution on a cluster of nodes. Typically, cluster-batch generates clusters by using a community

detection algorithm based on maximizing intra-community edges and minimizing inter-community connections [2]. Note that community detection can run either offline or at runtime, based on the requirements. Moreover, cluster sizes are often irregular, leading to varied batch sizes.

As shown in Algorithm 1, function $N_K(\cdots)$ is used to collect K-*hop* boundary neighbors and the corresponding edges. In case $P = 1, \gamma = 1$ runs MPGNN with a full-size training strategy. In case $P = N$, it runs with mini-batch, In case $N > P > 1$ and the graph is partitioned by a community detection method, it runs MPGNN with cluster-batch. The Cluster-GCN algorithm can be regarded as an implementation of MPGNN with cluster-batch.

Figure 1 illustrate the advantages of cluster-batch. An example of cluster-batched computation is shown in fig. 1(c)&1(d), where the graph is partitioned into two communities/clusters. The black nodes in Fig. 1(c) are in community *A* and the black nodes in Fig. 1(d) are the community *B*. The green or blue nodes in both graphs are the 1-*hop* or 2-*hop* boundaries of a community. Community *A* is selected as the first batch to train a 2-*hop* GNN model, while community *B* forms the second batch. In the embedding computation of the black nodes, their 1-*hop* or 2-*hop* boundary neighbors are also involved. The method generates embeddings of 32 and 41 target nodes, but only touched 40 and 49 nodes in *A* and *B*, resulting in an average computing cost of 1.22 nodes for each target node. In contrast, if mini-batch is used as shown in Fig. 1(a)&1(b), the average cost will be as heavy as 18.5 nodes.

Table 1 shows the comparisons among global-, mini- and cluster-batch. It is necessary to design a new GNN learning system that enables the exploration of different training strategies, which can solve the limitations of existing architectures.

3

Table 1: Comparison of three GNN training strategies

Strategies	Advantages	Disadvantages
Global-batch	• No redundant calculation • Stable training convergence	• The highest cost in one step
Mini-batch	• Friendly for parallel computing; • Easy to implement on modern training systems [1, 27].	• Redundant calculation among batches; • Exponential complexity with depth; • Power law graph challenge.
Cluster-batch	• Has advantages of mini-batch but with less redundant calculation.	• Limited support graphs without obvious community structures. • Instable learning speed and imbalance batch size.

3 Compute Pattern

3.1 NN-TGAR

To solve these problems in a data-parallel or hybrid-parallel system, we present a general computation pattern abstraction, namely NN-TGAR, which can perform the forwards and backwards of GNN algorithms on a big (sub-)graph distributively. This abstraction decomposes an encoding layer into a sequence of independent stages, i.e., NN-Transform, NN-Gather, Sum, NN-Apply, and Reduce. Our method allows distributing the computation over a cluster of machines. The NN-Transform (NN-T) stage is executed on each node to transform the results and generate messages. The NN-Gather (NN-G) stage is applied to each edge, where the inputs are edge values, source node, destination node, and the messages generated in the previous stage. After each iteration, this stage updates edge values and sends messages to the destination node (maybe on other workers). In the Sum stage, each node accumulates the received messages by means of a non-parameterized method like averaging, concatenation or a parameterized one such as LSTM. The resulting summation is updated to the node by NN-Apply (NN-A).

Different from the Gather-Sum-Apply-Scatter (GAS) proposed by PowerGraph [13], NN-T, NN-G and NN-A are implemented as neural networks. In forwards, the trainable parameters also join in the calculation of the three stages, but kept unchanged. In backwards, the gradients of these parameters are generated in NN-T, NN-G and NN-A stages, which is used in the final stage NN-Reduce for parameter updating. NN-TGAR can be executed either on the entire graph or subgraphs, subject to the training strategy used.

3.2 Forward

The forward of a GNN model can be described as $K + 2$ passes of NN-TGA, as each encoding layer can be described as one pass of NN-TGA. The decoder and loss functions can be separately described as a single NN-T operation. The decoder functions are application-driven. It can be described by a single NN-T operation in node classification, and a combination of NN-T and NN-G in link prediction. Without loss of generality, we use node classification as the default task in this paper.

The forward is comprised of K passes of NN-TGA from the first to K-th encoding layer, one NN-T operation for the decoder function, and one for the loss calculation. In the forward of each encoding layer, the projection function is executed on NN-T and the propagation function on NN-G. However, the aggregation function is implemented by a combination of Sum and NN-A, which corresponds to the accumulate part and the apply part defined as follows:

$$\boldsymbol{M}_i^k = Acc_k\big(\big\{\boldsymbol{m}_{j\to i}^k\big\}_{j\in N(v_i)}\big|\boldsymbol{\mu}_k^{(1)}\big), \tag{1a}$$

$$\boldsymbol{h}_i^k = Apy_k\big(\boldsymbol{h}_i^k, \boldsymbol{M}_{N_O(i)}^k\big|\boldsymbol{\mu}_k^{(2)}\big), \tag{1b}$$

where $\boldsymbol{\mu}_k = \big[\boldsymbol{\mu}_k^{(1)}, \boldsymbol{\mu}_k^{(2)}\big]$. If the accumulate part is not parameterized by mean-pooling, $\boldsymbol{\mu}_k^{(1)} = \boldsymbol{0}$ and $\boldsymbol{\mu}_k = \boldsymbol{\mu}_k^{(2)}$.

As shown in Fig. 2(a), the embedding of the $(k-1)$-th layer $\boldsymbol{h}_i^{k-1}$ is transformed to $\boldsymbol{n}_i^k$ using a neural network $Proj_k(*|\boldsymbol{W}_k)$ for all the three nodes in NN-T. The NN-G stage collects messages both from the neighboring nodes $\{v_2, v_3\}$ (and v_1) and from adjacent edges $\{e_{1,2}, e_{1,3}\}$ (and $e_{2,1}$) to the centric node v_1 (and v_2) through the propagation function $Prop_k(*|\theta_k)$. The output of this stage is automatically accumulated by $Acc_k(*)$, resulting in the summed message $\boldsymbol{M}_{N(1)}^k$ and $\boldsymbol{M}_{N(2)}^k$. The NN-A stage computes the new embeddings of nodes $\{v_1, v_2, v_3\}$, i.e. $\boldsymbol{h}_1^k, \boldsymbol{h}_2^k$ and $\boldsymbol{h}_3^k$, as the output of this encoding layer.

3.3 Auto-diff and Backward

Auto-differentiation is a prominent feature in deep learning and GraphTheta also implements auto-differentiation to simplify GNN programming by automating the backward gradient propagation during training. Like existing deep learning training systems, a primitive operation has two implementations: a forward version and a backward one. For instance, a data transformation function can implement its forward computation by a sequence of primitive operations. In this case, its backward computation can be automatically interpreted as a reverse sequence of the backward versions of these primitive operations. Assuming that $\boldsymbol{y} = f(\boldsymbol{x}, \boldsymbol{W})$ is a user-defined function composed of a sequence of built-in operations, GraphTheta can generate the two derivative functions automatically: $\partial\boldsymbol{y}/\partial\boldsymbol{x} = f_x'(\boldsymbol{W})$ and $\partial\boldsymbol{y}/\partial\boldsymbol{W} = f_W'(\boldsymbol{x})$.
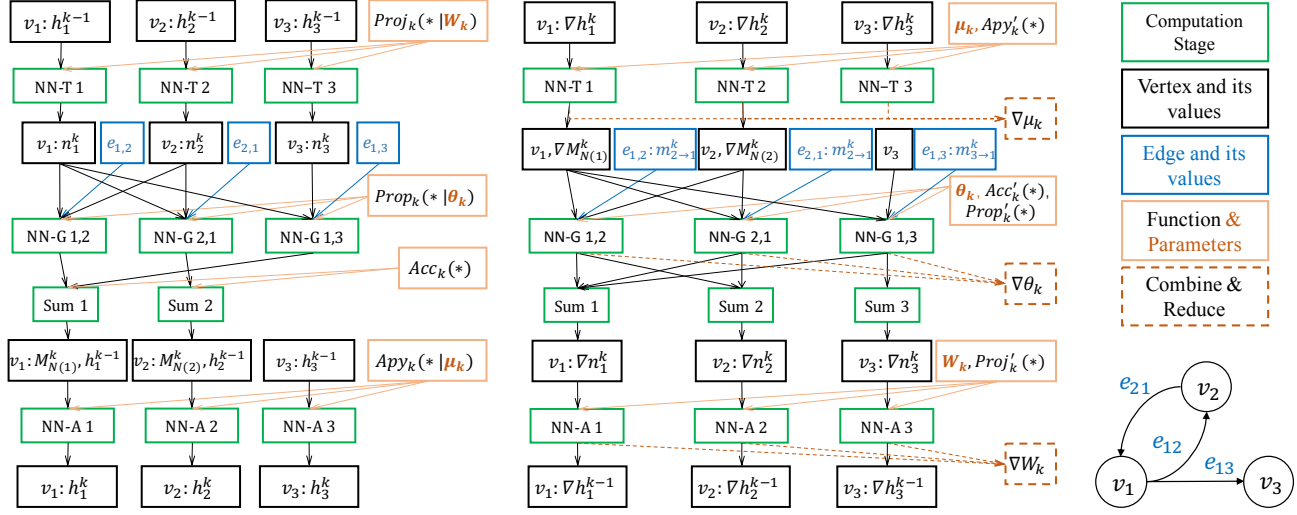
(a) Forward from h_i^{k-1} to h_i^k: NN-T uses the kth projection function, NN-G uses the kth propagation function and NN-A uses the kth aggregation function

(b) Backward from ∇h_i^k to ∇h_i^{k-1}: NN-T uses the derivation of Apy_k, NN-G uses the deriv. of $Acc_k\&Prop_k$, NN-A uses the deriv. of $Proj_k$, and NN-R processes gradients of parameters.

(c) The example graph used in (a\b), nodes may on different workers.

Figure 2: The computation pattern of NN-TGAR.

NN-TGAR will organize all these derivative functions to implement the backward progress of the whole GNN model. More details are listed in Appendix A.2 of a general proof of backward computation with message propagation, and in Appendix A.3 of the derivatives of MPGNN.

In the task of node classification, the backward of a GNN model can be described as $K+2$ passes of NN-TGAR, but in a reverse order. First, the differential of a loss function $\partial L/\partial \hat{\mathbf{y}}_i = l'(\mathbf{y}_i)$ is executed on each labeled node by a single NN-T stage. Then, the two stages NN-T and Reduce are used to the calculate the differential of the decoder function. In this phase, the gradients of the final embedding for each node are calculated as $\partial L/\partial \mathbf{h}_i^K = \partial L/\partial \hat{\mathbf{y}}_i \cdot Dec'(\boldsymbol{\omega})$ and updated to the corresponding node. Meanwhile, the gradients of the decoder parameters are calculated as $\partial L/\partial \boldsymbol{\omega} = \partial L/\partial \hat{\mathbf{y}}_i \cdot Dec'(\mathbf{h}_i^K)$ and sent to the optimizer. The K passes of NN-TGAR are executed backwards from the K-th to the first encoding layer.

Differing from forward that runs the apply part at the last step, backward executes the differential of the apply part on nodes $\{v_1, v_2, v_3\}$ in the NN-T stage, as shown in Fig. 2(b). This stage calculates $\partial L/\partial \boldsymbol{\mu}^k$ that will be sent to the optimizer, $\{\partial L/\partial \mathbf{h}_i^{k-1} \cdot \partial Apy_k/\partial \mathbf{n}_i^k | i = 1,2,3\}$ that will be updated to the nodes as values, and $\{\partial L/\partial \mathbf{M}_i^k | i = 1,2\}$ that will be consumed by the next stage NN-G. Besides receiving messages from the previous stage, stage NN-G takes as input the values of the corresponding adjacent edges and centric nodes, and sends the result to neighbors and centric nodes, as well as the optimizer.

In NN-G, taking Gather$_{1,3}$ as an example, the differential of the accumulate function calculates $\partial L/\partial \mathbf{m}_{3\to1}^k$. Subsequently, the differential of the propagation function computes $\partial Prop_k/\partial \mathbf{n}_3^k$, $\partial Prop_k/\partial \mathbf{n}_1^k$, and $\partial Prop_k/\partial \boldsymbol{\theta}_k$, all of which are multiplied by $\partial L/\partial \mathbf{m}_{3\to1}^k$ and then sent to the source node v_3, destination node v_1, and the optimizer. The Sum stage receives gradient vectors computed in NN-G, as well as new node values computed in NN-T, and then element-wisely adds the gradients by node values for each of the three nodes, resulting in $\{\partial L/\partial \mathbf{n}_i^k | i = 1,2,3\}$. These three results will be passed to the next stage. The NN-A computes the gradients of the $(k-1)$-th layer embeddings $\partial L/\partial \mathbf{h}_i^{k-1}$ as $\partial L/\partial \mathbf{n}_i^k \cdot Proj_k'(\mathbf{W}_k)$, where the gradients of $\mathbf{W}_k$ are calculated similarly. The optimizer invokes Reduce to aggregate all the gradients of parameters (i.e., $\boldsymbol{\mu}_k$, $\boldsymbol{\theta}_k$, and $\mathbf{W}_k$), which are generated in stages NN-T, NN-G and NN-A and distributed over nodes/edges, and updates the parameters with this gradient estimation.

4 Implementation

Inspired by distributed graph processing systems, we present a new GNN training system which can simultaneously support all the three training strategies. Our new system enables deep GNN exploration without pruning graphs. Moreover, our system can balance memory footprint, time cost per epoch, and convergence speed. Fig. 3 shows the architecture of our system. It consists of five components: (*i*) a graph storage component with distributed partitioning and heterogeneous features and attributes management, (*ii*) a subgraph generation component with sampling methods, (*iii*) graph operators which manipulate nodes and edges, and (*iv*) learning core operations including neural network operators (including fully-connected layer, attention layer, batch normalization, concat, mean/attention pooling layers and etc.), typical loss functions

(including softmax cross-entropy loss w/o regularizations), and optimizers (including SGD and Adam [20]).

4.1 Distributed Graph Representation

Our graph programming abstraction follows the vertex-program paradigm and fits the computational pattern of GNNs which always centers around nodes. In our system, the underlying graphs are placed in a distributed environment, which requires efficient graph partitioning algorithms. A number of graph partitioning approaches have been proposed, such as vertex-cut, edge-cut, and hybrid-cut solutions. Popular graph partitioning algorithms are included in our system to support popular graph processing methods.

To efficiently run GNN-oriented vertex-programs, we propose a new graph partitioning method which evenly distributes nodes to partitions and cuts off cross-partition edges. Similar to PowerGraph, we use master and mirror nodes, where a master node is assigned to one partition and its mirrors are created in other partitions. For each edge, our method assigns it to the partition in which its source node is a master (target nodes also can be used as the indicator). This way, any edge contains at least one master node. The vertex-cut approach used by PowerGraph has the disadvantage of duplicating mirror nodes, resulting in memory overhead for the multi-layer GNN learning. To address this problem, our method allows mirror nodes to act as placeholders and only hold node states instead of the actual values. In this case, the replica factor is reduced to 1 from $(N_{master} + N_{mirror})/N_{master}$, where N_{master} and N_{mirror} are the number of master and mirror nodes. With the partitioning method, the implementation of each primitive in `GAS` abstraction is composed of several phases. Fig. 5 illustrates the computation of the `Gather` primitive.

In order to traverse graph efficiently, GraphTheta organizes outgoing edges in Compressed Sparse Row (CSR) and incoming edges in Compressed Sparse Column (CSC), and stores node and edge values separately. Our distributed graph traversal is completed in two concurrent operations: one traverses nodes with CSR and the other with CSC. For the operation with CSR, each master node sends its related values to all the mirrors and then gathers its outgoing edges with master neighbors, where the edges with mirror neighbors are directly skipped. For the operation with CSC, each mirror node gathers incoming edges with master neighbors. Mirror nodes receiving values from their corresponding masters will be passively gathered by their neighbors. Fig. 6 illustrates an example of our graph traversal. Assume that we would like to traverse all outgoing edges of the master node 3 in partition 0 held by worker 0. For the operation with CSR, worker 0 processes the outgoing edge of node 3 to the master node 0. As node 1 in worker 0 is a mirror, the edge from node 3 to node 1 is skipped. Meanwhile, worker 1 sends the value of its master node 1 to the mirror in worker 0. Concurrently, for the operation with CSC, worker 0 processes the incoming edge
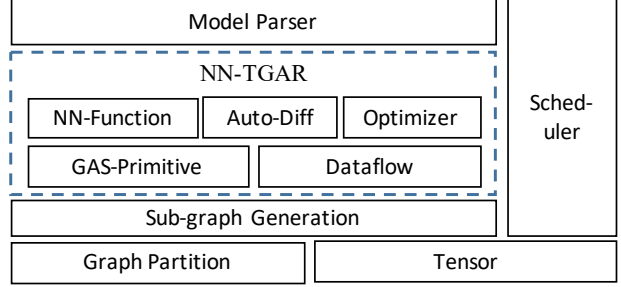

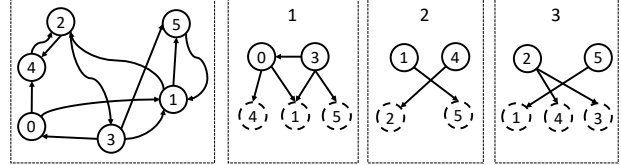Figure 3: The system architecture of GraphTheta.

Figure 4: An example of GraphTheta partitioning with nodes evenly assigned to three partitions. Mirrors are denoted by the dotted line.
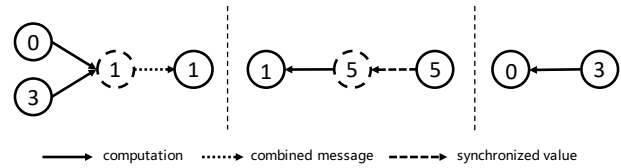

Figure 5: An example of computation and communication in the `Gather` primitive: compute, combine and synchronized.

of the mirror node 1 from node 3. Herein, the mirror node 1 receives its value sent from worker 1 and will be passively gathered by node 3 in worker 0. From the description, we can see that communication only occurs between master and mirror nodes.

The abstraction can address the local message bombing problem. On one hand, for a master-mirror pair, we only need one time of message propagation of node values and the results, which can reduces the traffic load from $O(M)$ to $O(N)$. On the other hand, we only synchronize node values involved in the computation per neural network layer, during the dataflow execution of a GNN model. Moreover, we remove the implicit synchronization phase after the original `Apply` primitive, instead of introducing implicit master-mirror synchronization to overlap computation and communication. Additionally, heuristic graph partitioning algorithms such as METIS [19], Louvain [2] are also supported to adapt cluster-batched training.

4.2 Subgraph Training

To unify the processing of all the three types of training strategies, our new system uses subgraphs as the abstraction of graph structures and the GNN operations are applied. Both mini-batch and cluster-batch train a model on the subgraphs

generated from the initial batches of target nodes, whereas global-batch does on the entire graph. The size of a subgraph can vary from one node to the entire graph based on three factors, i.e., number of GNN layers, graph topology and community detection algorithms. The number of GNN layers determines the neighbor exploration depth and has an exponential growth of subgraph sizes. For graph topology, node degree determines the exponential factor of subgraph growth.

Fig. 7 shows a mini-batch training example, where a GNN model containing two graph convolution layers is interleaved by two fully-connected layers. The right part shows a subgraph constructed from a batch of initial target nodes $\{1, 2, 3\}$, which has one-hop neighbors $\{4, 5, 6\}$ and two-hop neighbors $\{7, 8\}$. The left part shows the forward and backward computation of this subgraph, with arrows indicating the propagation direction. For subgraph computation, a straightforward method is to load the subgraph structure and the related data into memory and perform matrix operations on the subgraph located at the same machine. As the memory overhead of a subgraph may exceed the memory limit, this method has inherent limitation in generalization. Instead, GraphTheta completes the training procedure with distributed computing by only spanning the structure of the distributed subgraph. To construct a subgraph, our system introduces a breadth-first-search traverse operation. For each target node, this operation initializes a minimal number of layers per node, which are involved in the computation, in order to reduce unnecessary propagation of graph computing. Furthermore, to avoid the cost of subgraph structure construction and preserve graph access efficiency, we build a vertex-ID mapping between the subgraph and the local graph within each process/worker to reuse CSR/CSC indexing. In addition, our system has implemented a few sampling methods, including random neighbor sampling [16], which can be applied to subgraph construction.

4.3 Parallel Execution Model

Training subgraphs sequentially cannot fully unleash the power of a distributed system. GraphTheta is designed to concurrently train multiple subgraphs with multi-versioned parameter in a distributed environment, and support concurrent lookups and updates. That lead to two distinguished features from the existing GNN training systems: (*i*) parallel subgraph tensor storage built upon distributed graphs, and (*ii*) `GraphView` abstraction and multi-versioned parameter management to enable parallelized batched training.

Parallel tensors storage For subgraph training, we investigate two key techniques to enable low-latency access to distributed subgraphs and lower total memory overhead. The first technique is reusing the CSR/CSC indexing. It is inefficient in high-concurrency environment to construct and release the indexing data for each subgraph on the fly. Instead, the global indexing of the whole graph is reused, and a private
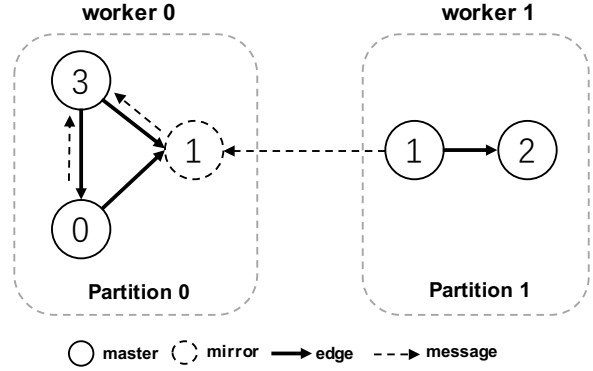

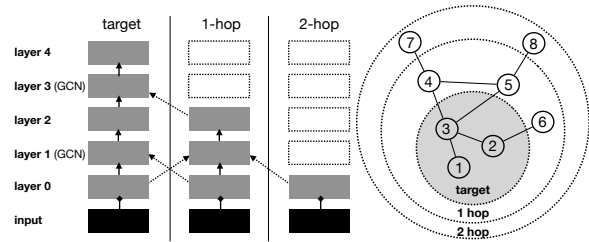Figure 6: An example of distributed graph traversal

Figure 7: The tensor stacks of a target node and its 2-hop neighbors in the training process with a 2-hop GNN model.
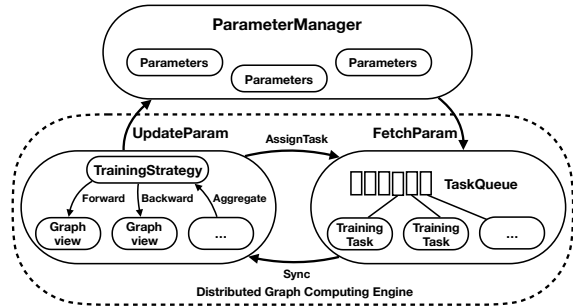

Figure 8: The parallel batched training paradigm.

cache-friendly vertex-ID mapping is adopted to efficiently access a graph topology, as described in section 4.2.

The second technique is task-oriented tensor storage. In GNNs, the same node can be incorporated in different subgraphs constructed from different batches of target nodes, especially high degrees nodes. To make tasks context-independent and hide underlying implementation details, the memory layout of nodes is task-specific (a task can be an individual forward, backward, or aggregation phase) and sliced into frames. A frame of a given node is a stack of consecutive resident memory, storing raw data and tensors. To alleviate peak memory pressure, the memory can be allocated and released dynamically per frame on the fly. More specifically, in the forward/backward phase, output tensors for each layer is calculated and released immediately after use. As the allocation and de-allocation of tensors has a context-aware memory

usage pattern, we design a tensor caching between frames and standard memory manipulation libraries to avoid frequently trapping into operating system kernel spaces.

`GraphView` and multi-versioned parameters To train multiple subgraphs concurrently, we design the abstraction `GraphView`, which maintains all key features of the underlying parallel graph storage including reused indexing, embedding lookup, and the distributed graph representation. Implemented as a light-weight logic view of the global graph, the `GraphView` exposes a set of interfaces necessary to all training strategies, and allows to conveniently communicate with storages. Besides the global-, mini- and cluster-batch, other training strategies can also be implemented base `GraphView`. And training tasks with `GraphViews` are scheduled in parallel. That enables to concurrently assign the separated forward, backward and aggregation phases to a training worker. Due to varied workloads of subgraphs, a work-stealing scheduling strategy is adopted to improve load balance and efficiency.

Fig. 8 depicts the parallel batched training paradigm with graph view and multi-version parameter management. `ParameterManager` manages multiple versions of trainable parameters. In a training step, workers can fetch parameters of a specific version from `ParameterManager`, and use these parameters within the step. For each worker, it computes on a local slice of the target subgraph being trained, and uses a task queue (i.e., `TaskQueue`) to manage all the tasks assigned to itself and then execute them concurrently. In the end of a training step, parameter gradients are aggregated, and sent to `ParameterManager` for version update. `UpdateParam` performs the actual parameter update operations either in a synchronous or an asynchronous mode.

5   Experiments and Results

5.1   Datasets

We evaluate the performance of our system by training node classification models using 6 datasets. As shown in Table 2, the sizes vary from small-, modest-, to large-scale. The popular GCN [21] algorithm and our EAGNN algorithm are used for comparison. From Table 2, Cora, Citeseer and Pubmed [29] are three citation networks with nodes representing documents and edges indicating citation relationship between documents. In the three datasets, the attribute of a node is a bag-of-words vector, which is sparse and high-dimensional, while the label of the node is the category of the corresponding document. Reddit is a post-to-post graph in which one post forms one node and two posts are linked if they are both commented by the same user. In Reddit, a node label presents the community a post belongs to [16]. Amazon is a co-purchasing graph, where nodes are products and two nodes are connected if purchased together. In Amazon, node labels represent the categories of products [7]. These five

datasets are publicly available and have only node attributes, without edge attributes or types.

In Alipay dataset, nodes are users, attributes are user profiles and class labels are the financial risk levels of users. Edges are bulit from a series of relations among users such as chatting, online financial cooperation, payment, and trade. This dataset contains 1.4 billion nodes and 4.1 billion attributed edges. In our experiments, we equally split the data set into two parts, one for training and the other for testing. To our knowledge, Alipay dataset is the largest edge-attributed graph ever used to test deep GNN models in the literature.

In addition, even though there are only node classification tasks in our testing, our system can actually support other types of tasks with moderate changes, such as revising the decoders to accommodate specific task and keeping graph embedding encoder part unchanged.

5.2   Evaluation on Public Datasets

On the public datasets, we train a two-layer GCN model [21] using our system and compare the performance with the state-of-the-art counterparts, including a TensorFlow-based implementation (TF-GCN) from [21], a DGL-based one (DGL) [31], and two neighbor-sampling-based ones: Fast-GCN [4] and VR-GCN [3]. Cluster-GCN [7] is not compared because the performance of a two-layer GCN on these datasets are not available in the original paper. Different datasets are configured to have varied hidden layer sizes. Specifically, hidden layer sizes are 16, 128 and 200 for the three citation networks (i.e., Cora, Citeseer and PubMed), Reddit and Amazon. Except for Amazon, all the others have their own sub-sets for validation. Moreover, the latter enables dropout for each layer, whereas the former does not. In terms of global-batch, we train the model up to 1,000 epochs and select the trained model with the highest validation accuracy to test generalization performance for the latter. With respect to mini-batch, early stop is exerted once stable convergence has reached for each dataset. In all tests, cross-entropy loss function is used to measure convergence and prediction results are produced by feeding node embeddings to a softmax layer. Due to the small sizes of the three networks, we run one worker of 2 GB memory to train each of them. In terms of the average time per epoch/step, our method obtains on the Cora, Citeseer and PubMed datasets 0.46 (0.75) seconds, 0.97 (0.47) seconds, and 0.85 (0.33) seconds respectively with respect to the global-batch (mini-batch) training.

Comparison to other systems with non-sampling-based methods First, we compare our system with TF-GCN and DGL to demonstrate that our system can achieve highly competitive or superior generalization performance on the same datasets and models, even without using sampling. Table 3 shows the performance comparison between GraphTheta, TF-GCN and DGL on the three small-scale citation networks, i.e.,

Table 2: Datasets

Name	#Nodes	#Node attr.	#Edges	#Edge attr.	Max cluster size	Cluster number
Cora	2,708	1433	5,429	0	-	-
Citeseer	3,327	3703	4,732	0	-	-
Pubmed	19,717	500	44,338	0	-	-
Reddit	232,965	602	11,606,919	0	30,269	4300
Amazon	2,449,029	100	61,859,140	0	36,072	8500
Alipay Dataset	1.40 Billion	575	4.14 Billion	57	24 Million	4.9Million

Table 3: The comparison to other systems with non-sampling 2-hop GCN

Dataset	Accuracy in Test Set (%)			
	GCN with GB*	GCN with MB*	GCN On DGL	GCN On TF
Cora	**82.70**	82.40	81.31	81.50
Citeseer	**71.90**	**71.90**	70.98	70.30
Pubmed	**80.00**	79.50	79.00	79.00

*Training and inference on GraphTheta.

Table 4: The comparison to other systems with 2-hop GCN and sampling-based training.

Dataset	Accuracy in Test Set (%)				
	Global-batch*	Mini-batch*	Cluster-batch*	Fast GCN	VR-GCN
Reddit	**96.44**	95.84	95.60	93.70	96.30
Amazon	**89.77**	87.99	88.34	–	89.03

*Training and inference on GraphTheta.

Table 5: Comparison results on Alipay dataset

Strategies	Performance in Test Set (%)		Time (h)
	F1 Score	AUC	
Global-batch	12.18	87.64	30
Mini-batch	13.33	88.12	36
Cluster-batch	**13.51**	**88.36**	**26**

Cora, Citeseer and PubMed. For DGL, we resue the results presented in [31], instead of evaluating it. This is because [31] did not expose its hyper-parameters and pose challenges for result reproduction. Both GraphTheta and TF-GCN use the same set of hyper-parameter values, including learning rate, dropout keep probability, regularization coefficient, and batch size, as proposed in [21]. And train the model 300 steps for mini-batch. From the table, global-batch yields the best accuracy for each dataset, with an exception that its performance is neck-by-neck with that of mini-batch on Citeseer. Mini-batch also outperforms both DGL and TF-GCN for each case.

Comparison to other systems with sampling-based methods Second, we compare our implementations (without sampling) with FastGCN and VR-GCN on the two modest-scale datasets: Reddit and Amazon. FastGCN employs importance neighbor sampling, while VR-GCN adopts variance reduction. And both of them train models in a mini-batched manner. Table 4 gives the test accuracy of each experiment. For FastGCN and VR-GCN, we directly use the results from their corresponding publications. Note that the performance of FastGCN on Amazon is unavailable, and the algorithm will not participate in performance evaluation with respect to Amazon.

For global-batch, we set 500 epochs for Reddit at maximum, and activate early stop as long as validation accuracy reaches stable. Meanwhile, a maximum number of 750 epochs is used for Amazon. For mini-batch, each training step randomly chooses 1% labeled nodes to form the initial batch for Reddit, and 0.1% for Amazon. This results in a batch size of 1,500 for the former and 1,710 for the latter. We train Reddit for 600 steps and Amazon for 2,750 steps with respect to mini-batch. Note that as Reddit (and Amazon) is a dense co-comment (and co-purchasing) network, the two-hop neighbors of only 1% (and 0.1%) labeled nodes almost touch 80% (and 65%) of all nodes. For cluster-batch, each training step randomly chooses 1% clusters to form the initial batch for Reddit and Amazon, where clusters are created beforehand. Moreover, cluster-batch applies the same early stop strategy as mini-batch. We train the two networks of Reddit and Amazon on a Linux CPU Docker cluster and launch 600 and 200 workers, each of which has a memory size of 2 GB. For Reddit, our method obtains an average time per epoch/step of 78.0 seconds, 80.2 seconds and 60.4 seconds in terms of global-batch, mini-batch and cluster-batch. For Amazon, the results are 45.1 seconds, 55.8 seconds and 35.3 seconds respectively.

On both datasets, global-batch yields the best accuracy, while mini-batch performs the worst with cluster-batch in between. Moreover, FastGCN is inferior to VR-GCN. It is worth mentioning that the relatively lower performance of cluster-batch may be caused by the fact that both networks are dense and do not have good cluster partitioning. Based on these observations, it is reasonable to draw the conclusion that sampling-based training methods are not always better than non-sampling-based ones.

5.3 Evaluation on Alipay dataset

In this test, we use our in-house developed variant of the graph attention network (GAT) [30], namely GAT with edge
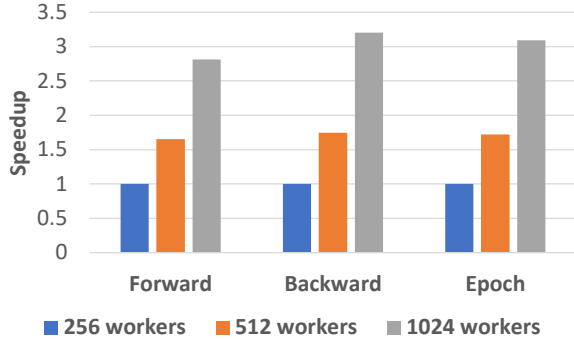
Figure 9: Scaling results of GraphTheta on Alipay dataset

features (GAT-E), which adapts GAT to utilize edge features. This model is trained with Alipay dataset using the following three training strategies: global-batch, mini-batch and cluster-batch. Alipay dataset is a very sparse graph with a density of about 3. GAT-E is based on the assumption that given a node, different neighbor relationship has different influence on the node. Differing from the original GAT described in [30], the inputs of the attention function further involve the edge feature, besides the features of both the source and the destination nodes.

Table 5 shows the performance of three training strategies. We run 400 epochs for global-batch, and 3,000 steps for all the others. Cluster-batch performs the best, with mini-batch better than global-batch, in terms of both F1 score and accuracy. In terms of the convergence speed in the same distributed environment, we can observe that cluster-batch converges the fastest. The second fastest method is global-batch, and the third one is mini-batch. Specifically, the overall training time of 1,024 workers is 30 hours for global-batch, 36 hours for mini-batch, and 26 hours for cluster-batch, and the peak memory footprint per worker is 12 GB, 5 GB and 6 GB respectively.

5.4 Scaling Results

We evaluate the capability of scaling to big graphs of Graph-Theta with respect to the number of workers, in a distributed environment, using Alipay dataset. In this testing, each worker is equipped with one computing thread and runs in a Linux CPU Docker. We employ global-batch, and conduct 10 rounds of tests. Then, we report the average runtime of speedup. Due to the large memory footprint of Alipay dataset, we start from 256 workers and use the average training time as the baseline.

Fig. 9 shows the speedup results with respect to the number of workers. From the results, we can see that the forward, backward and full training steps are consistent in terms of the scaling size. They all scale linearly with the number of workers. By increasing the number of workers from 256 to 512, the forward runs $1.66\times$ faster, the backward runs $1.75\times$ faster, and the full training steps run $1.72\times$ faster. Furthermore, we

increase the number of works from 512 to 1,024, the speeds increase by 2.81, 3.21 and 3.09 times respectively. Considering parallel efficiency, the forward achieves 83% (and 70%), backward of 87% (and 80%), and full training steps of 86% (and 77%) in terms of efficiency by using 512 workers (and 1,024 workers). Neither mini-batch nor cluster-batch is as good as global-batch with respect to parallel scalability, which means mini-batch and cluster-batch cannot fully unleash the computation power of the distributed system, out of the relatively small amount of computation in subgraphs.

6 Related Work

Existing GL systems/frameworks for GNNs are either shared-memory or distributed-memory. They are designed for mini-batch and global-batch trainings. Specifically, DGL is a shared-memory GL system, which implements a graph message passing method [11]. To overcome the memory constraint when processing big graphs, DGL recently introduces a graph storage server to store the graph. However, this method does not always work because clients have to pull subgraphs from the server remotely. Pixie and PinSage are shared-memory frameworks based on the mini-batch training. Pixie targets real-time training and inference, while PinSage is designed for off-line applications. NeuGraph takes advantage of GPUs sharing the same host to perform the global-batch training by splitting a graph into partitions and implementing global convolutions partition-by-partition. GPNN is a distributed global-batch node classification method. GPNN first partitions the graphs and then conducts transductive learning using greedy training that interleaves intra-partition training with inter-partition training. AliGraph and AGL are two distributed methods for the mini-batch training. Similar to DGL, AliGraph uses a graph storage server (distributed) as the solution for big graphs. In contrast, AGL used a naïve storage method instead, which extracts subgraphs offline ahead of time and stores them in disk for possible future use. Note that both AliGraph and AGL perform the forward and backward computation over a mini-batch by only one process/worker, i.e., conducting data-parallel execution.

Our system intrinsically differs from existing methods by implementing hybrid-parallel execution, which computes each mini-batch by a group of processes/workers, and supporting multiple training strategies. It is worth mentioning that though general-purpose graph processing systems [26] [14] [13] [36] [5] are incapable of directly supporting graph learning, the graph processing techniques can be taken as the infrastructure of graph learning systems.

7 Conclusion

In this paper, we presented GraphTheta, a distributed GNN learning system supporting multiple training strategies, in-

cluding global-batch, mini-batch and cluster-batch. Extensive experimental results show that our system scales almost linearly to 1,024 workers in a distributed Linux CPU Docker environment. Considering the affordable access to a cluster of CPU machines in public clouds such as Alibaba Aliyun, Amazon Web Services, Google Cloud and Microsoft Azure, our system shows promising potential to achieve low-cost graph learning on big graphs. Moreover, our system demonstrates better generalization results than the state-of-the-art on a diverse set of networks. Especially, experimental results on Alipay dataset of 1.4 billion nodes and 4.1 billion edges show that the new cluster-batch training strategy is capable of obtaining the best generalization results and the fastest convergence speed on big graphs. Specifically, GraphTheta makes our in-house developed GNN to reach convergence in 26 hours using cluster-batch, by launching 1,024 workers on Alipay dataset.

Acknowledgments

References

[1] Martín Abadi, Paul Barham, Jianmin Chen, Zhifeng Chen, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Geoffrey Irving, Michael Isard, et al. Tensorflow: A system for large-scale machine learning. In *12th {USENIX} Symposium on Operating Systems Design and Implementation ({OSDI} 16)*, pages 265–283, 2016.

[2] Vincent D. Blondel, Jean-Loup Guillaume, Renaud Lambiotte, and Etienne Lefebvre. Fast unfolding of communities in large networks. *Journal of Statistical Mechanics: Theory and Experiment*, P10008:1–12, Oct 2008.

[3] Jianfei Chen, Jun Zhu, and Le Song. Stochastic training of graph convolutional networks with variance reduction. In Jennifer Dy and Andreas Krause, editors, *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pages 942–950, Stockholmsmässan, Stockholm Sweden, 10–15 Jul 2018. PMLR.

[4] Jie Chen, Tengfei Ma, and Cao Xiao. Fastgcn: fast learning with graph convolutional networks via importance sampling. *arXiv preprint arXiv:1801.10247*, 2018.

[5] Rong Chen, Jiaxin Shi, Yanzhe Chen, Binyu Zang, Haibing Guan, and Haibo Chen. Powerlyra: Differentiated graph computation and partitioning on skewed graphs. *ACM Transactions on Parallel Computing (TOPC)*, 5(3):1–39, 2019.

[6] Tianqi Chen, Mu Li, Yutian Li, Min Lin, Naiyan Wang, Minjie Wang, Tianjun Xiao, Bing Xu, Chiyuan Zhang, and Zheng Zhang. Mxnet: A flexible and efficient machine learning library for heterogeneous distributed systems. *arXiv preprint arXiv:1512.01274*, 2015.

[7] Wei-Lin Chiang, Xuanqing Liu, Si Si, Yang Li, Samy Bengio, and Cho-Jui Hsieh. Cluster-gcn: An efficient algorithm for training deep and large graph convolutional networks. In *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, page 257–266, New York, NY, USA, 2019. Association for Computing Machinery.

[8] Hanjun Dai, Bo Dai, and Le Song. Discriminative embeddings of latent variable models for structured data. In *International conference on machine learning*, pages 2702–2711, 2016.

[9] Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on graphs with fast localized spectral filtering. In D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, editors, *Advances in Neural Information Processing Systems 29*, pages 3844–3852. Curran Associates, Inc., 2016.

[10] Chantat Eksombatchai, Pranav Jindal, Jerry Zitao Liu, Yuchen Liu, Rahul Sharma, Charles Sugnet, Mark Ulrich, and Jure Leskovec. Pixie: A system for recommending 3+ billion items to 200+ million users in real-time. In *Proceedings of the 2018 world wide web conference*, pages 1775–1784, 2018.

[11] Justin Gilmer, Samuel S Schoenholz, Patrick F Riley, Oriol Vinyals, and George E Dahl. Neural message passing for quantum chemistry. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 1263–1272. JMLR. org, 2017.

[12] Justin Gilmer, Samuel S. Schoenholz, Patrick F. Riley, Oriol Vinyals, and George E. Dahl. Neural message passing for quantum chemistry. In *Proceedings of the 34th International Conference on Machine Learning - Volume 70*, ICML'17, page 1263–1272. JMLR.org, 2017.

[13] Joseph E Gonzalez, Yucheng Low, Haijie Gu, Danny Bickson, and Carlos Guestrin. Powergraph: Distributed graph-parallel computation on natural graphs. In *Presented as part of the 10th {USENIX} Symposium on Operating Systems Design and Implementation ({OSDI} 12)*, pages 17–30, 2012.

[14] Joseph E Gonzalez, Reynold S Xin, Ankur Dave, Daniel Crankshaw, Michael J Franklin, and Ion Stoica. Graphx: Graph processing in a distributed dataflow framework. In *11th {USENIX} Symposium on Operating Systems Design and Implementation ({OSDI} 14)*, pages 599–613, 2014.

[15] Marco Gori, Gabriele Monfardini, and Franco Scarselli. A new model for learning in graph domains. In *Proceedings. 2005 IEEE International Joint Conference on Neural Networks, 2005.*, volume 2, pages 729–734. IEEE, 2005.

[16] Will Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs. In *Advances in neural information processing systems*, pages 1024–1034, 2017.

[17] David K. Hammond, Pierre Vandergheynst, and Rémi Gribonval. Wavelets on graphs via spectral graph theory. *Applied and Computational Harmonic Analysis*, 30(2):129 – 150, 2011.

[18] Wenbing Huang, Tong Zhang, Yu Rong, and Junzhou Huang. Adaptive sampling towards fast graph representation learning. In *Advances in neural information processing systems*, pages 4558–4567, 2018.

[19] George Karypis and Vipin Kumar. A fast and high quality multilevel scheme for partitioning irregular graphs. *SIAM J. Scientific Computing*, 20(1):359–392, 1998.

[20] Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *International Conference on Learning Representations*, 2015.

[21] Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. *arXiv preprint arXiv:1609.02907*, 2016.

[22] Kai Lei, Meng Qin, Bo Bai, Gong Zhang, and Min Yang. Gcn-gan: A non-linear temporal link prediction model for weighted dynamic networks. In *IEEE INFOCOM 2019-IEEE Conference on Computer Communications*, pages 388–396. IEEE, 2019.

[23] Renjie Liao, Marc Brockschmidt, Daniel Tarlow, Alexander L Gaunt, Raquel Urtasun, and Richard Zemel. Graph partition neural networks for semi-supervised classification. In *Workshop of International Conference on Learning Representations*, 2018.

[24] Ziqi Liu, Chaochao Chen, Longfei Li, Jun Zhou, Xiaolong Li, Le Song, and Yuan Qi. Geniepath: Graph neural networks with adaptive receptive paths. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pages 4424–4431, 2019.

[25] Lingxiao Ma, Zhi Yang, Youshan Miao, Jilong Xue, Ming Wu, Lidong Zhou, and Yafei Dai. Neugraph: parallel deep neural network computation on large graphs. In *2019 {USENIX} Annual Technical Conference ({USENIX}{ATC} 19)*, pages 443–458, 2019.

[26] Grzegorz Malewicz, Matthew H Austern, Aart JC Bik, James C Dehnert, Ilan Horn, Naty Leiser, and Grzegorz Czajkowski. Pregel: a system for large-scale graph processing. In *Proceedings of the 2010 ACM SIGMOD International Conference on Management of data*, pages 135–146, 2010.

[27] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, et al. Pytorch: An imperative style, high-performance deep learning library. In *Advances in Neural Information Processing Systems*, pages 8024–8035, 2019.

[28] Franco Scarselli, Marco Gori, Ah Chung Tsoi, Markus Hagenbuchner, and Gabriele Monfardini. The graph neural network model. *IEEE Transactions on Neural Networks*, 20(1):61–80, 2008.

[29] Prithviraj Sen, Galileo Namata, Mustafa Bilgic, Lise Getoor, Brian Gallagher, and Tina Eliassi-Rad. Collective classification in network data. *AI Magazine*, 29(3):93–106, 2008.

[30] Petar Velickovic, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. Graph attention networks. *ArXiv*, abs/1710.10903, 2017.

[31] Minjie Wang, Lingfan Yu, Da Zheng, Quan Gan, Yu Gai, Zihao Ye, Mufei Li, Jinjing Zhou, Qi Huang, Chao Ma, et al. Deep graph library: Towards efficient and scalable deep learning on graphs. In *Seventh International Conference on Learning Representations*, 2019.

[32] Rex Ying, Ruining He, Kaifeng Chen, Pong Eksombatchai, William L Hamilton, and Jure Leskovec. Graph convolutional neural networks for web-scale recommender systems. In *Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pages 974–983, 2018.

[33] Dalong Zhang, Xin Huang, Ziqi Liu, Zhiyang Hu, Xianzheng Song, Zhibang Ge, Zhiqiang Zhang, Lin Wang, Jun Zhou, and Yuan Qi. Agl: a scalable system for industrial-purpose graph machine learning. *Proceedings of the VLDB Endowment*, 13(12), 2020.

[34] Ziwei Zhang, Peng Cui, and Wenwu Zhu. Deep learning on graphs: A survey. *IEEE Transactions on Knowledge and Data Engineering*, 2020.

[35] Rong Zhu, Kun Zhao, Hongxia Yang, Wei Lin, Chang Zhou, Baole Ai, Yong Li, and Jingren Zhou. Aligraph: a comprehensive graph neural network platform. *Proceedings of the VLDB Endowment*, 12(12):2094–2105, 2019.

[36] Xiaowei Zhu, Wenguang Chen, Weimin Zheng, and Xiaosong Ma. Gemini: A computation-centric distributed graph processing system. In *12th {USENIX} Symposium on Operating Systems Design and Implementation ({OSDI} 16)*, pages 301–316, 2016.

A   Theoretical Analysis

A.1   Equivalence Relation

Indeed, the propagation on graphs and sparse matrix multiplication are equivalent in the foward. The general convolutional operation on graph $\mathcal{G}$ can be defined [21] [9] as,

$$\boldsymbol{x} *_{\mathcal{G}} \mathcal{K} = \boldsymbol{U}((\boldsymbol{U}^T \boldsymbol{x}) \odot (\boldsymbol{U}^T \mathcal{K})), \qquad (2)$$

where $U = [u_0, u_1, ..., u_{N-1}] \in \mathbb{R}^{N \times N}$ is the complete set of orthonormal eigenvectors of normalized graph Laplacian $\boldsymbol{L}$, $\odot$ is the element-wise Hadamard product, $\boldsymbol{x} \in \mathbb{R}^{N \times 1}$ is the 1-dimension signal on graph $\mathcal{G}$ and $\mathcal{K}$ is the convolutional kernel on the graph. The graph Laplacian defined as $\boldsymbol{L} = \boldsymbol{I}_N - \boldsymbol{D}^{(-1/2)} \boldsymbol{A} \boldsymbol{D}^{(-1/2)})$, where $\boldsymbol{D} = diag\{d_1, d_2, ..., d_N\}$ and $d_i = \sum_{j=0}^{N} A(i,j)$. Equation (2) can be approximated by a truncated expansion with K-order Chebyshev polynomials as follows (more details are given in [17] [21]).

$$\begin{aligned} \boldsymbol{x} *_{\mathcal{G}} \mathcal{K} &\approx \sum_{k=0}^{K} \theta_k T_k(\hat{\boldsymbol{L}}) \boldsymbol{x} \\ &= \theta_0 T_0(\hat{\boldsymbol{L}}) \boldsymbol{x} + \theta_1 T_1(\hat{\boldsymbol{L}}) \boldsymbol{x} + \cdots + \theta_K T_K(\hat{\boldsymbol{L}}) \boldsymbol{x}, \end{aligned} \qquad (3)$$

where the Chebyshev polynomials are recursively defined by,

$$T_k(\hat{\boldsymbol{L}}) = 2\hat{\boldsymbol{L}} T_{k-1}(\hat{\boldsymbol{L}}) - T_{k-2}(\hat{\boldsymbol{L}}) \qquad (4a)$$

$$with \quad T_0(\hat{\boldsymbol{L}}) = \boldsymbol{I}_N, \ T_1(\hat{\boldsymbol{L}}) = \hat{\boldsymbol{L}}, \qquad (4b)$$

where $\hat{\boldsymbol{L}} = 2\boldsymbol{L}/\lambda_M - \boldsymbol{I}_N$, λ_M is the the largest eigenvalue of $\boldsymbol{L}$, and $\theta_0, \theta_1, \cdots, \theta_K$ are the Chebyshev coefficients, which parameterize the convolutional kernel $\mathcal{K}$. Substituting (4a) into (3), and considering λ_M as a learnable parameters, the truncated expansion can be rewritten as,

$$\sum_{k=0}^{K} \eta_k \boldsymbol{L}^k \boldsymbol{x} = \eta_0 \boldsymbol{I}_N \boldsymbol{x} + \eta_1 \boldsymbol{L} \boldsymbol{x} + \cdots + \eta_K \boldsymbol{L}^K \boldsymbol{x}, \qquad (5)$$

where $\eta_0, \eta_1, \cdots, \eta_K$ are learnable parameters. This polynomials can also be written in a recursive form of

$$\sum_{k=0}^{K} \eta_k \boldsymbol{L}^k \boldsymbol{x} = \sum_{k=0}^{K} \eta'_k T'_k(\boldsymbol{x}) \qquad (6a)$$

$$with \quad T'_k(\boldsymbol{x}) = \boldsymbol{L} \eta'_{k-1} T'_{k-1}(\boldsymbol{x}), \ T'_0(x) = x \qquad (6b)$$

$$and \quad \eta'_k = \eta_k / \eta_{k-1}, \ \eta'_0 = \eta_0. \qquad (6c)$$

and $\eta'_0, \eta'_1, \cdots, \eta'_K$ are also considered as a series of learnable parameters. We generalize it to high-dimensional signal $\boldsymbol{X} \in \mathbb{R}^{N \times d_I}$ as follows: each item in (6a) can be written as $\boldsymbol{H}_k = T'_k(\boldsymbol{X}) \boldsymbol{W}_k$. Recalling (6b), the convolutional operation on graph with high-dimensional signal can be simplified as K-order polynomials and defined as,

$$\boldsymbol{x} *_{\mathcal{G}} \mathcal{K} \approx \sum_{k=0}^{K} \boldsymbol{H}_k, \ with \ \boldsymbol{H}_k = \boldsymbol{L} \boldsymbol{H}_{k-1} \boldsymbol{W}_k, \boldsymbol{H}_0 = \boldsymbol{X} \boldsymbol{W}_0, \quad (7)$$

where $\boldsymbol{H}_k \in \mathbb{R}^{N \times d}$, and $\boldsymbol{W}_k \in \mathbb{R}^{d \times d}$, which are also learnable and parameterize the convolutional kernel. Based on the matrix multiplication rule, the i-th line $\boldsymbol{h}_i^k$ in $\boldsymbol{H}_k$ can be written as,

$$\boldsymbol{h}_i^k = \sum_{j=1}^{N} \boldsymbol{L}(i,j)(\boldsymbol{h}_j^{k-1} \boldsymbol{W}_k). \qquad (8)$$

Thus, we can translate convolutional operation into K rounds of propagation and aggregation on graphs. Specifically, at round k, the projection function is $\boldsymbol{n}_i^k = \boldsymbol{h}_i^{k-1} \boldsymbol{W}_k$, the propagation function is $\boldsymbol{m}_{j \to i}^k = \boldsymbol{L}(i,j) \boldsymbol{n}_i^k$, the aggregation function is $\boldsymbol{h}_i^k = \sum_{j \in N(i)} \boldsymbol{m}_{j \to i}^k$. In other words, $\boldsymbol{h}_i^{k-1}$ (or $\boldsymbol{h}_i^k$) is the j-th line (or i-th line) of $\boldsymbol{H}_k$ (or $\boldsymbol{H}_{k-1}$) and also the output embedding of v_i (or the input embedding of v_j). Each node propagates its message $\boldsymbol{n}_i^k$ to its neighbors, and also aggregates the received messages sent from neighbors by summing up the values weighted by the corresponding Laplacian weights.

A.2   Backwards of GNN

A general GNN model can be abstracted into K combinations of individual stage and conjunction stage. Each node on the graph can be treated as a data node and transformed separately in a separated stage, which can be written as,

$$\boldsymbol{n}_i^k = f_k(\boldsymbol{h}_i^{k-1} | \boldsymbol{W}_k). \qquad (9)$$

But the conjunction stage is related to the node itself and its neighbors, without loss of generality, it can be written as,

$$\boldsymbol{h}_i^k = g_k(A(i,1)\boldsymbol{n}_1^k, A(i,2)\boldsymbol{n}_2^k, \cdots, A(i,N)\boldsymbol{n}_N^k | \boldsymbol{\mu}_k), \qquad (10)$$

where $A(i,j)$ is the element of adjcency matrix and is equal to the weight of $e_{i,j}$ (refer to the first paragraph in 2). The forward formula (10) can be implemented by message passing, as n_j^k is propagated from v_j along the edges like $e_{i,j}$ to its neighbor v_i. The final summarized loss is related to the final embedding of all the nodes, so can be written as,

$$L = l(\boldsymbol{h}_0^K, \boldsymbol{h}_1^K, \cdots, \boldsymbol{h}_N^K). \qquad (11)$$

According to the multi-variable chain rule, the derivative of previous embeddings of a certain node is,

$$\frac{\partial L}{\partial \boldsymbol{n}_i^k} = \frac{\partial L}{\partial \boldsymbol{h}_1^k} a_{1,i} \frac{\partial \boldsymbol{h}_1^k}{\partial \boldsymbol{n}_i^k} + \frac{\partial L}{\partial \boldsymbol{h}_2^k} a_{2,i} \frac{\partial \boldsymbol{h}_2^k}{\partial \boldsymbol{n}_i^k} + \cdots + \frac{\partial L}{\partial \boldsymbol{h}_N^k} a_{N,i} \frac{\partial \boldsymbol{h}_N^k}{\partial \boldsymbol{n}_i^k}. \qquad (12)$$

Thus, (12) can be rewritten as,

$$\frac{\partial L}{\partial \boldsymbol{n}_i^k} = \sum_{j \in N_{in}(i)} a_{j,i} \frac{\partial L}{\partial \boldsymbol{h}_j^k} \frac{\partial \boldsymbol{h}_j^k}{\partial \boldsymbol{n}_i^k} \qquad (13)$$

So the backwards of a conjunction stage also can be calculated by a message passing, where each node (i) broadcasts the current gradient $\partial L / \partial \boldsymbol{h}_j^k$ to its neighbors along edges $e_{j,i}$;

(ii) calculates the differential $\partial \boldsymbol{h}_j^k / \partial \boldsymbol{n}_i^k$ on each edge $e_{j,i}$, multiplies the received gradient and edge weight $a_{j,i}$, and sends the results (vectors) to the destination node v_i; (iii) sums up the received derivative vectors, and obtains the gradient $\partial L / \partial \boldsymbol{n}_i^k$. Meanwhile, the forward and backward of each stage is similar to the normal neural network. The above derivation can expand to the edge-attributed graph.

A.3 Derivation in MPGNN

The previous section gives the derivatives for a general GNN model, and this part describes the derivation for the MPGNN framework. As in Algorithm 1, a MPGNN framework contains K passes' procedure of "projection-propagation-aggregation", where the projection function (Line 6) can be considered as the implementation of an individual stage, while the propagation function (Line 7) and aggregation function for the conjunction stage. Aggregation function adopts the combination of (1a) and (1b). If the gradients of the k-th layer node embeddings $\partial L / \partial \boldsymbol{h}_i^k$ are given, the gradients of $(k-1)$-th layer node embeddings and the corresponding parameters are computed as,

$$\frac{\partial L}{\partial \boldsymbol{\mu}_k^{(2)}} = \sum_{i=1}^{N} \frac{\partial L}{\partial \boldsymbol{h}_i^k} \frac{\partial \boldsymbol{h}_i^k}{\partial \boldsymbol{\mu}_k^{(2)}}, \tag{14}$$

$$\frac{\partial L}{\partial \boldsymbol{\mu}_k^{(1)}} = \sum_{i=1}^{N} \frac{\partial L}{\partial \boldsymbol{h}_i^k} \frac{\partial \boldsymbol{h}_i^k}{\partial \boldsymbol{M}_i^k} \frac{\partial \boldsymbol{M}_i^k}{\partial \boldsymbol{\mu}_k^{(1)}}, \tag{15}$$

$$\frac{\partial L}{\partial \boldsymbol{m}_{j \to i}^k} = \frac{\partial L}{\partial \boldsymbol{h}_i^k} \frac{\partial \boldsymbol{h}_i^k}{\partial \boldsymbol{M}_i^k} \frac{\partial \boldsymbol{M}_i^k}{\partial \boldsymbol{m}_{j \to i}^k}, \tag{16}$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_k} = \sum_{i=1}^{N} \sum_{j \in N_O(i)} \frac{\partial L}{\partial \boldsymbol{m}_{j \to i}^k} \frac{\partial \boldsymbol{m}_{j \to i}^k}{\partial \boldsymbol{\theta}_k}, \tag{17}$$

$$\begin{aligned} \frac{\partial L}{\partial \boldsymbol{n}_i^k} = & \sum_{j \in N_O(i)} \frac{\partial L}{\partial \boldsymbol{m}_{j \to i}^k} \frac{\partial \boldsymbol{m}_{j \to i}^k}{\partial \boldsymbol{n}_i^k} + \\ & \sum_{j \in N_I(i)} \frac{\partial L}{\partial \boldsymbol{m}_{i \to j}^k} \frac{\partial \boldsymbol{m}_{i \to j}^k}{\partial \boldsymbol{n}_i^k} + \frac{\partial L}{\partial \boldsymbol{h}_i^k} \frac{\partial Apy_k}{\partial \boldsymbol{n}_i^k}, \end{aligned} \tag{18}$$

$$\frac{\partial L}{\partial \boldsymbol{W}_k} = \sum_{i=1}^{N} \frac{\partial L}{\partial \boldsymbol{n}_i^k} \frac{\partial \boldsymbol{n}_i^k}{\partial \boldsymbol{W}_k}, \tag{19}$$

$$\frac{\partial L}{\partial \boldsymbol{h}_i^{k-1}} = \frac{\partial L}{\partial \boldsymbol{n}_i^k} \frac{\partial \boldsymbol{n}_i^k}{\partial \boldsymbol{h}_i^{k-1}}. \tag{20}$$