Analyzing the Performance of Graph Neural Networks with Pipe Parallelism

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ABSTRACT

Many interesting datasets ubiquitous in machine learning and deep learning can be described via graphs. As the scale and complexity of graph-structured datasets increase, such as in expansive social networks, protein folding, chemical interaction networks, and material phase transitions, improving the efficiency of the machine learning techniques applied to these is crucial. In this study, we focus on Graph Neural Networks (GNN), which have found great success in tasks such as node or edge classification and link prediction. However, standard GNN models have scaling limits due to necessary recursive calculations performed through dense graph relationships that lead to memory and runtime bottlenecks. While new approaches for processing larger networks are needed to advance graph techniques, and several have been proposed, we study how GNNs could be parallelized using existing tools and frameworks that are already known to be successful in the deep learning community. In particular, we investigate applying pipeline parallelism to GNN models with GPipe, introduced by Google in 2018.

1 INTRODUCTION

Traditional flat or sequential data delivery cannot fully satisfy many of today’s demanding deep learning models, especially as more data structures of interest can be better represented as high-dimensional graphs instead of low-dimensional grids. Graph learning has demonstrated successful applications in domains such as chemistry and drug design [10, 24], natural language processing [29], spatio-temporal forecasting [34], security [39], social networks [39], knowledge graphs [2], recommender systems [33], protein design discovery [28], and material phase transitions [4]. With its increased use, especially on large datasets, performance and scaling challenges with the Graph Neural Network (GNN) [38] are becoming prevalent when using existing machine learning frameworks and accelerators because of memory and data movement limitations [3].

A variety of new solutions to address these issues have been proposed and are highlighted in the next section. However, as a practical consideration, leveraging existing state-of-the-art tools and frameworks with demonstrated success at improving deep neural network performance is valuable to push these technologies forward.

Therefore, to better understand how training and inference can be more efficient for GNN models, we implement and analyze the performance of parallelized GNN models compared to their unparallelized counterparts when trained on a single CPU and GPU and multiple GPUs. As GNNs are executed sequentially, either layer-by-layer or stage-by-stage, the motivation for this study is to extend current techniques for improving performance by introducing pipeline parallelism into the GNN model architecture [37].

2 GRAPH NEURAL NETWORKS

The success of deep learning on traditional grid- or sequence-based inputs, such as images and sentences, cannot be overstated. Nevertheless, many datasets in the real-world cannot be expressed within a Euclidean coordinate system, and instead naturally take an arbitrary form of graphs or networks. Various studies exist on how to generalize neural networks for the application to arbitrary irregular graphs [5, 8, 10, 15, 19, 20], and we follow the exposition of Kipf and Welling [19] who first introduced the notion of a convolution architecture for a graph.

We consider the general scenario of node classification in a graph. The input is a graph $G = (V, E)$ where each node (or vertex) $i$ of the graph has a set of features $x_i$. Some pairs of nodes are connected, and the connections are called edges (or links). If $n$ is the number of nodes and there are $d$ features in each node, then the set of all features form a $n \times d$ matrix. Some nodes may have labels from a set of $C$ classes. The task is to classify each node into $C$ classes using the ingrained feature information through the edge connectivity between nodes across the graph.

A GNN approaches this problem by building a neural network layer atop a simultaneous message passing paradigm. Suppose there are $L+1$ layers, $H_0, \ldots, H_L$. Then, $H_0 = X$, the input set of features. For each layer $l$, the set of output features $H^{l+1}$ depends only on the previous layer $H^l$ and the input graph $G$. So, for some efficiently computable function $f$, $H^{l+1} = f(H^l, G)$ (1)

Approaches for the GNN model considers different choices of $f$. By setting the output of the last layer to be a single neuron, the model computes the logits for each node, which is then used to classify the nodes. Assuming $f$ is differentiable, this approach can be optimized by standard gradient descent algorithms.

In most instantiations of graph networks studied in the literature, the features $H^{l+1}$ (i) for node $i$ depend on the original feature $H^l(i)$ and the features of neighboring nodes $H^l(j)$, where $j$ being a neighbor of $i$ connected by edge $[i,j]$. In some settings, these edges can be of different types, such as being directed or undirected, as well as include features, in which case the edge properties also contribute to the calculation of $f$.

The message passing paradigm is designed by how the output features of a layer are simultaneously updated based on the input features of the layer, instead of through sequential updates. For many learning tasks on a graph, earlier approaches [6, 9] usually introduced problem-specific architectures or spectral graph theory.
to make predictions. However, these algorithms are limited as they require prior knowledge of the graph structure, and the GNN model provides a unified approach that allows for studying the properties of a graph itself.

The success of GNNs can clearly be seen in its application to the famous Zachary’s Karate Club problem [35]. Here, the graph describes a social network of 34 members of a karate club and documents links between members who interact outside the club. The task is to classify the members of the club as being part of a community centered around the karate instructor or the club president. Previous methods, such as DeepWalk [26], used complicated unsupervised learning procedures to compute this type of predictive task. On the other hand, [19] demonstrated that this could be done for “free” using a 3-layer Graph Convolutional Network (GCN), where the layer propagation rule is written as

$$H^{l+1}(i) = \sigma \left( \sum_{j \in \mathcal{N}(i)} \frac{1}{c_{ij}} W^l H^l(j) \right)$$  \hspace{1cm} (2)

Here, $\sigma$ is an appropriately chosen nonlinearity, $\mathcal{N}(i)$ are the neighbors of $i$, $c_{ij}$ are normalization coefficients computed from the graph structure, and $W^l$ is a simple, fully connected network. This approach of using the GCN model achieved state-of-the-art classification results for several graph datasets.

### 2.1 Graph Attention Network

The experiments presented in this paper are based on the Graph Attention Network (GAT), which is another novel GNN architecture that use attention layers on top of graph convolutions [30]. By leveraging this self-attention mechanism, GAT can achieve state-of-the-art accuracy results on several transductive and inductive graph benchmarks including the Cora, CiteSeer, and Pubmed datasets that we consider here.

We choose this model as our main experimentation model for the following reasons. GAT can be applied to graphs of different degrees by specifying arbitrary weights on the neighbors, making it a very useful model for a fairly wide variety of graph datasets. GAT is also applicable to inductive learning problems and has great generalization capabilities to unseen graph data. From our experiments, it does not perform as efficiently as even simpler graph convolutional networks. Therefore, it serves as a prime model to inform us on parallelization benchmarks.

We will first describe the main GAT layer. The GAT layer is described by supposing $n$ nodes exist in a graph, each with $f$ features given by $h_1, \ldots, h_n$. Then, the layer produces a set of $f'$ features, given by $h'_1, \ldots, h'_n$, as follows.

The initial step involves a linear transformation $W \in \mathbb{R}^{f \times f'}$ that is first applied to every node. This transforms each vector $h_i$ to $Wh_i$. Note that $W$ is a learnable parameter and is shared across the nodes. Then we compute an attention coefficient for each node, which is a single-layer feedforward network.

To do this, we first compute self-attention coefficients for each edge. For each edge $i, j$, an attention coefficient $a_{ij}$ is computed that indicates the importance of node $j$ on node $i$. Precisely at this stage, the graph structure is heavily utilized. This is known as masked attention. We first concatenate the embeddings on its nodes to obtain $Wh_i || Wh_j$, where $||$ denotes concatenation. Then, a weight vector $a$ linearly transforms this vector, and the LeakyRelu nonlinearity, with a default negative input slope of 0.2, is applied. Finally, a softmax layer normalizes the attention coefficients. Succinctly,

$$a_{ij} \propto \exp(\text{LeakyRelu}(a^T [Wh_i || Wh_j]))$$  \hspace{1cm} (3)

The output feature for each node is finally computed by taking a linear transformation of the embeddings, weighted by the attention coefficients and applying a nonlinearity, resulting in

$$h'_i = \sigma \left( \sum_{j \in \mathcal{N}(i)} a_{ij} Wh_j \right)$$  \hspace{1cm} (4)

Moreover, multi-head attention with 8 heads is used to stabilize the self-attention learning coefficients, where 8 such feature sets are simultaneously computed independently with their own set of learnable parameters.

The entire network has two main GAT layers where, in the first layer, the outputs of the eight attention nodes are concatenated and, in the second layer, which is also the prediction layer, the outputs of the eight layers are averaged.

The entire network begins with a dropout layer with a dropout probability of 0.6, followed by the first GAT layer, and then an Exponential Linear Unit (ELU) nonlinearity is applied with a default value of $\alpha = 1$. Then, another dropout layer with a dropout probability of 0.6 is applied, followed by the second GAT layer. Ultimately the logits are computed by a final softmax layer, which are then converted to prediction probabilities that are used for classification.

### 3 RELATED WORK

As described above, the core message-passing function of a GNN is the aggregation of features from the neighborhood of each node. Computing a gradient decent operation requires storing the entire graph as a single training batch. With increasing graph size or edge density, the time and memory complexity of this computation can grow exponentially and introduce an information bottleneck [1]. This effect limits the scalability of traditional GNNs, many of which, including GAT, do not address these concerns as their benchmark datasets were of a reasonable size for the available device capacities.

GraphSAGE [14] was the first attempt to address graph scalability by using a neighborhood sampling with mini-batch training to limit the number of nodes included in a batch. This approach can introduce redundant calculations as the same nodes may appear in multiple sampled batches and lead to “neighbor explosion” [36]. Similar sampling techniques responded to this challenge by batching sub-graphs instead of nodes, such as in [7]. However, graph clustering approaches are faced with the challenge of defining sub-graphs that sufficiently preserve the edge topology that guides the node feature updates during training, which is an issue directly observed in the analysis of the present study.

Another technique to enable GNN scalability is NeuGraph [22] that introduced parallel computation through a new graph-parallel abstraction of Scatter-ApplyEdge-Gather-ApplyVertex (SAGA-NN). This framework conveniently encapsulates almost all existing GNNs in the literature [37], and serves as a foundation for studying parallelized GNN performance optimization. The authors explored the design of a GNN processing framework on top of a dataflow based deep learning system, through which they optimized graph
computations, scheduling, and parallelism in a dataflow-based deep learning framework for graphs. Exploring computational efficiencies at the device level, $G^3$ [21] is a GNN training framework that implements graph-structured parallel operations that leverage the architectural features on GPUs. By directly utilizing graph-aware components of the GPU, they demonstrated significant speedups in training times over standard implementations in PyTorch and TensorFlow.

Finally, a recent approach that avoids graph sampling over nodes or sub-graphs is the Scalable Inception Graph Neural Network (SIGN) [13]. Here, graph convolutional filters of different sizes pre-compute intermediate node representations. This method enables its scaling to large graphs with classic mini-batching because it retains sufficient expressiveness from the node relationships for effective learning.

4 PIPELINE PARALLELISM

Google Brain introduced the scalable pipeline parallelism library GPipe [17] to enable the efficient distributed training of large, memory-consuming deep learning models on current accelerator architectures. According to their published results, GPipe increased training times of a 557 million-parameter model by 25 times using eight TPU devices and 3.5 times faster using four devices.

The basic scheme with GPipe is the distribution of a sequentially-designed deep neural network across multiple devices. To maximize these devices’ capability to calculate in parallel, it further splits the input mini-batch from the training samples into “micro-batches” to distribute across the devices. This technique, known as micro-batching, reduces the load for the available memory on the accelerators, resulting in effectively simultaneous training of the same batch across all devices.

Pipeline parallelism is like a stacked combination of model parallelism with small data parallelism. During the forward pass, when each partition finishes processing a micro-batch, it shifts the output to the next partition and immediately begins work on the next micro-batch. Following this approach, the partitions can overlap across GPUs. During the backward pass, the gradients for each micro-batch are calculated using the same model parameters from the forward pass, and are consistently accumulated at the end into the mini-batch to update the model parameters. Therefore, the number of partitions separating the data does not affect model quality.

In summary, GPipe splits neural network model layers across multiple accelerators and micro-batches the training batches to increase efficiency in the parallel computations. Hence, GPipe can be applied to any deep neural network comprised of sequential layers to perform distributed learning through synchronous stochastic gradient descent and pipeline parallelism. Of particular interest with this approach is the capability to easily scale the performance with additional accelerators without the need to re-tune hyperparameters.

Although originally designed for deep neural networks, the GPipe workflow is applicable to GNNs, with some necessary adaptations that we explore in this study. To the best of our knowledge, this is the first work to consider the idea of applying pipeline parallelism using existing libraries to potentially optimize the runtime of GNNs.

5 DATASETS

Cora, CiteSeer, and PubMed are well-established citation network datasets [27, 32] often used in benchmark training. Each dataset contains a bag-of-words representation of documents and citation links to represent relationships between published research. The feature vectors are the bag-of-words, and the graph is the network of citation links. If document $A$ cites $B$, then an undirected edge exists between the document nodes. The semi-supervised learning problem on these datasets is to classify each document into a class representing a topic or research theme.

The Cora dataset contains 2,708 machine learning research papers that form the nodes of a graph with 5,429 edges corresponding to citation relationships. Each publication is encoded by a TF-IDF vector that provides a feature vector of length 1,433 representing the input features. The classification task is to identify each paper into one of seven categories of Case-cased, Genetic Algorithms, Neural Networks, Probabilistic Methods, Reinforcement Learning, Rule Learning, and Theory.

The CiteSeer dataset contains 3,312 publications from the CiteSeer web database with a citation network consisting of 4,732 links. For a dictionary containing 3,703 unique words, each publication has a 0-1 word vector indicating if that word appears in the document. The graph node is to be classified into one of six classes of Agents, Artificial Intelligence, Database, Information Retrieval, Machine Language, and Human-computer Interaction.

The PubMed dataset consists of 19,717 scientific publications representing the nodes of a graph with 44,338 edges corresponding to the citation relationships. Each node includes 500 features, corresponding to the unique words from that individual document. For the training task, one of three classes is to be identified pertaining to diabetes classification of Diabetes Mellitus Experimental, Diabetes Mellitus Type 1, and Diabetes Mellitus Type 2.

We also briefly describe two larger datasets, the Reddit post dataset [14] and the Amazon data dump [23]. Although our experiments in this study do not cover these datasets due to memory limitations, it is useful to compare their sizes to the citation network datasets used for our analysis, which have served as a standard for GNNs and offer a strong benchmark for measuring the efficiency of parallelized GNNs.

Reddit is a discussion website that aggregates social news and features a web content rating system. Posts are classified into many categories known as subreddits. The dataset contains 232,965 posts from 50 different large subreddits that serve as the nodes of a graph. Two posts are connected by an edge if the same user comments on both posts, resulting in nearly 150 million edges. The features are 300-dimensional word vector embeddings from each post, and the labels are the subreddits that contain the post.

The Amazon dataset [23] contains approximately 180 million relationships or edges among nearly 6 million objects or nodes, taken from the Amazon e-commerce storefront. These relationships are represented as recommendations provided by Amazon when visiting the web page for a specific product. Each edge is further
classified into multiple categories based on additional relationships between the products. The labels are the type of objects chosen from 11 categories. So, this dataset serves as an interesting real-world application for a related edge classification task for GNNs.

6 IMPLEMENTATION

Experiments included training a GAT-based multi-layer sequential neural network on the task of node classification with the citation datasets described above. The PubMed set was solely used to compare performance with pipeline parallelism and graph data batching. The forward propagation model structure remained consistent across all experiments designed with a drop-out layer ($p = 0.6$) followed by a GAT layer with eight heads (attention drop-out $= 0.6$), a leaky ReLU activation function, a second drop-out layer ($p = 0.6$), a second GAT layer (eight heads, attention drop-out $= 0.6$) where the outputs are averaged, and, finally, a log softmax function.

The neural network model was implemented in PyTorch with the graph frameworks, PyTorch Geometric (PyG) [12] and Deep Graph Library (DGL) [31]. Each framework was compared for performance on each device architecture. Pipeline and data parallelism through $GPipe$ was only implemented through DGL. Trials included performance measures for a single CPU, single GPU, and pipe parallel distribution across four GPUs with and without micro-batching of the graph data.

The following were used for the single device benchmarks,

- Intel(R) Xeon(R) CPU @ 2.20GHz
- NVIDIA Tesla T4 GPU

and four NVIDIA Tesla V100-SXM2 GPUs (the DGX user system available at Argonne National Laboratory) were used for the distributed pipeline parallel experiments.

$GPipe$ was incorporated into the GNN models for each framework with the $torchpipe$ [18] library, which is an implementation of the $GPipe$ framework in PyTorch. The defined model is wrapped in a method that takes as parameters a defined distribution of the model layers across the available GPUs as the number of micro-batches (called “chunks”) to be applied. A value of one corresponds to the data parallelism feature being disabled.

```python
import torch.nn as nn

# Define a sequential model
model = nn.Sequential(
    nn.Dropout(0.6),
    GAT(g, numfeats, 8),
    nn.ELU(),
    nn.Dropout(0.6),
    GAT(g, 8 * 8, nclasses, take_mean=True),
    nn.LogSoftmax(1))

# Wrap the model for pipeline parallelism management
model = $GPipe$(model, balance=[1, 2, 1, 2], chunks=4)
```

Listing 1: Illustrative $GPipe$ implementation with $torchpipe$.

In Listing 1, $g$ contains the complete graph, $numfeats$ represents the number of features per node, and $nclasses$ is the number of classes in the classification task. The customizable balance array specifies how many layers from the sequence to distribute to each GPU. From this, $GPipe$ automatically manages the necessary movements of the model and data across devices. An automated distribution algorithm is also available to optimize this layer assignment. However, for the uniform analysis presented in this paper, we manually set the layer distribution across four devices to ensure consistency for all experiments.

With chunks $> 1$, the complete dataset or batches from the training is split into micro-batches by $GPipe$ to increase device parallelism. After a partition completes its processing of a micro-batch, it passes the output to the next partition and begins on the next incoming micro-batch in the pipeline. Through this approach, the multiple devices effectively process the same mini-batch (or entire dataset) simultaneously during a training epoch.

A key challenge with this implementation for a GNN is that a sequential module is required for the network layers. With this format comes a cascade of additional restrictions, beginning with the condition that only a single input of features may be passed through the layers. However, the graph convolution layer expects as input the graph data object and its corresponding features.

For our experiments that did not incorporate model parallelism across multiple GPUs, this did not pose an issue because we could simply include the full graph data object, $g$, into the GNN model definition and pass the single tensor of features. However, when model parallelism is activated, $GPipe$ applies micro-batching to this feature tensor, and the corresponding subset of graph nodes must instead be presented to the graph convolution layer, instead of the full graph data object.

As a workaround for enabling micro-batching, we exploited the option that the sequential module can pass a single tuple comprised of multiple tensors. Then, we can pass the node indices of the graph as the first tensor along with the corresponding features in a second tensor. $GPipe$ applies its micro-batching to each tensor in the tuple, so a subset of graph nodes with the corresponding features are passed along the sequence of layers, as needed.

When the graph convolution layer receives the passed tuple, our adapted code extracts the node tensor comprised of the sub-graph as determined by the micro-batch from $GPipe$. Both DGL and PyG graph frameworks include a method to re-build a graph structure from a subset of graph nodes. This process requires the full graph data object, $g$, for the re-build, and the output is a sub-graph structure expected by the graph convolution layer.

The second tensor of the passed tuple that includes the features is subsequently extracted in the graph convolution layer and used in the forward calculation. Upon completion, the two-tensor tuple is reformatted with the original nodes of the sub-graph and the updated features to be passed along through the remaining layers of the sequence.

7 RESULTS

All experimental training runs were performed for 300 epochs on the same GNN model structure. This model was not optimized for best training performance but remained consistent for all scenarios so that direct comparisons focusing on the graph frameworks, hardware, and parallelism approach could be observed independent of the model structure.
### 7.1 Benchmarks

As a first comparison benchmark, we trained the GNN model on single devices with the citation datasets of Cora, CiteSeer, and PubMed. The training time and test accuracy results are summarized in Table 1. As expected, training times, as measured by the average time per training epoch, on the GPU are faster for both graph frameworks across all datasets. Interestingly, DGL trained on average 35% faster than PyG on a CPU, while PyG trained on average 29% faster than DGL on a GPU. This outcome suggests, at least for our applied GNN model training on a single device, PyG may be better optimized for a GPU and DGL for a CPU. Training accuracy remained within a range of 15.5%, with PyG averaging 2.4% better than DGL over all datasets.

Next, we compare the average training time per epoch on three compute architectures, including the single CPU and GPU, as previously measured, with the DGX system comprised of four GPUs leveraging GPipe pipeline parallelism without micro-batching. In each case presented in Figure 1, the complete graph data object was included in the graph convolution layer during each training epoch.

The comprehensive benchmark report in Table 2 implements the GAT model on the PubMed dataset across combinations of frameworks and compute clusters for an expanded analysis and comparison of the runtimes and accuracy. Here, we also include the duration of the first epoch in the reported training times to provide a complete comparison of the graph frameworks and hardware. The duration of the first “setup” epoch varied slightly across graph frameworks and architectures, while the remaining training epochs ran on the order of 80–100 times faster on the single GPU compared to the single CPU.

![Figure 1: Benchmark training times for DGL and PyG on the PubMed dataset comparing the single devices to multiple devices with pipeline parallelism. Here, data parallelism is disabled.](image-url)

Surprisingly, no significant performance improvement in training time is observed in the four GPU system using GPipe with a “chunk size” = 1 (i.e., no micro-batching) compared to a single GPU. The PubMed dataset used in these experiments is considered small compared to those that are intended to benefit from pipeline parallelism.
parallelism. Therefore, the added cost of shifting data across the four GPUs may overtake the minimal speedup provided by GPipe. This may also suggest that the additional feature of data parallelism (via the data “chunks”) provided by GPipe is crucial to realizing meaningful performance improvements.

We also measured the training accuracy resulting from both graph learning frameworks applied with GPipe across four GPUs, but without micro-batching, exactly as in the timing measurements. As plotted in Figure 2, each framework converged similarly in accuracy over 300 training epochs in this configuration.

7.2 Increased training time

To investigate the impact of data parallelism within GPipe, we activated micro-batching and ran the training with the DGL graph framework to compare total training times between a single GPU and multiple distributed GPUs. As seen in Figure 3, the training times dramatically increase with micro-batching enabled at two, three, and four batches, as generated by GPipe.

As described above, our approach adapts the forward training to pass the graph information along with the features through a tuple of tensors into the sequential model. The GPipe micro-batching splits each tensor within the tuple so that only a subset of nodes is passed through, along with its corresponding set of features, as expected. The first convolution layer receives this subset of nodes indices but still must have a complete graph structure as its input with the feature tensor. So, a re-build of a graph is first performed with a DGL framework-delivered method. This sub-graph creation from the provided subset of nodes requires the full graph data object as a reference. However, DGL necessitates that the full graph, g, must remain on the CPU.

Therefore, to generate the sub-graph within the convolution layer, a copy of the subset node tensor must first be moved from the GPU onto the CPU, then the sub-graph is built and moved back onto the GPU. This data flow across devices was performed twice because our model includes two convolution layers. So, significant overhead was added to the total time just to enable the basic training calculations. As the chunk size increased, more micro-batches were generated, resulting in even more sub-graph build steps. Fortunately, the feature tensor extracted from the passed tuple could remain on the GPU. However, the updated values were still re-packaged into a tuple with the original sub-graph nodes to be returned into the forward pass of the model sequence.

7.3 Degraded accuracy

As discussed above, the training time significantly increases due to the necessity to re-build the micro-batched sub-graphs within each sequential GNN layer. We also observed the training accuracy suffered severely with an increasing number of micro-batches.

Although GPipe micro-batching can be disabled, as we configured for our benchmark tests (see Figure 1 and Figure 2), the expected benefit of pipeline parallelism requires this micro-batching. To observe the effects of micro-batching in our adapted implementation, we next ran the same DGL framework-based model with GPipe across four GPUs, sequentially distributed as before.

The challenge involved here is that the intended design of the GPipe micro-batching through the torchgpipe library implementation is to separate the features tensor passed into the model into uniform batches. As our adaptation passes a tuple containing both a node tensor and feature tensor, we observed this micro-batching to be applied to each tensor by sequentially selecting the tensor indices into a number of batches equal to the set chunk size parameter.
While this sequential separation preserved the nodes of the resulting sub-graph with their corresponding features, the edge relationships between the nodes were lost. Edges are re-established during the sub-graph build in the convolution layers, as detailed above. However, as the original graph structure is not expected to store its edges sequentially, separating the graph in this way likely eliminates many relationships that are crucial to be aggregated during the graph convolution layer calculations.

Due to this potential for significant information loss during the GPipe micro-batching, with an increasing number of batches generated, the resulting training accuracy dropped, as seen in Figure 4 with comparisons to the previous training accuracy results run without batching.

![Graph model training accuracy: DGL on GPUs](image)

**Figure 4: Accuracy drop-off with GPipe and graph micro-batching.**

On the other hand, both DGL and PyG provide more sophisticated approaches to generate mini-batches from the complete graph structures. For example, available in DGL as of v0.5.3, stochastic mini-batch training can be applied when not all the features from all nodes must be stored on a single GPU. This approach takes a sample of the neighborhood about a node from its previous layer and iterates until the sample search reaches the input. From this process, a dependency graph is built backward from the output to the input, maintaining the relationship structure throughout the training for a single node.

The initial intention of our implementation was to leverage these stochastic mini-batch “blocks,” as they are referred to in DGL, as the batches for GPipe. However, GPipe sequentially split these blocks into smaller batches, as they did on the sub-set of nodes tensor, so the relationships from the predetermined dependency graph is still lost.

In addition, DGL also offers a distributed training mechanism that uses its stochastic mini-batch blocks to parallelize the computation and partition graph data during training. However, at the time of this study, the distributed training in DGL only supports homogeneous graph structures with one node type and one edge type. So, we could not compare this technique with our benchmark datasets.

### 8 CONCLUSION AND FUTURE WORK

In this work, we analyzed the performance of GNNs using pipeline parallelism via GPipe. Our results suggest that although GPipe has demonstrated great success in optimizing deep neural networks, its ability to deliver efficiency for a graph neural network remains limited with our current adapted implementation.

The stochastic graph batching algorithms available in DGL and PyG take into account the graph structure while batching to ensure minimal structure loss across partition clusters. However, this is not immediately enforceable in GPipe because its micro-batching further splits these batches. So, an immediate scope for future work is to determine how to customize the GPipe data parallelism to utilize intelligent graph batching instead of a sequential separation by index. Such an improvement is expected to increase accuracy to match the benchmark levels while benefitting from the parallelism in runtime efficiency. In addition, the SIGN technique described in Section 3 may be the best batching approach to consider for parallelizing GNNs with our implementation because it avoids the experienced pitfalls of node and graph sampling and instead provides precomputed node representations that may be straightforwardly mini-batched by GPipe.

Additional experimentation incorporating other GNN models, such as GraphConv [25], GatedGraphConv [20], and SplineCNN [11] with the graph frameworks studied here will offer more insights into the accuracy performance of these predictions across various computing architectures.

Of particular importance to this study, pipeline parallelism is intended to benefit neural network training on very large datasets, much greater in size than the PubMed set used here. For the scope of this work, PubMed was useful for establishing the adapted implementation without being initially overburdened with managing memory. Also, PubMed, along with the other citation networks included for benchmarking, were pre-packaged by both graph frameworks, which greatly minimize data preparation and configuration into our model. We anticipate that runtime performance will increase for training on extremely large graphs after memory bottlenecks or computational complexity overtake the capability offered by a single GPU.

Therefore, as another next step, extending these experiments with the current implementation to massive datasets, such as the Reddit post dataset [14] and the Amazon data dump [23], will better illustrate the impact of GPipe parallelism on GNNs, and provide a more clear understanding for potential enhancements. Released in 2020, the Open Graph Benchmark (OGB) [16] is a collection of large graph benchmark datasets with data loaders available for DGL and PyG, which will allow for a straightforward and streamlined extension of our model to larger graphs. For the node classification task performed in this study, OGB offers graphs ranging from approximately 170,000 nodes and 1,170,000 edges up to very large networks with 111 million nodes and over 1.6 billion edges. These datasets represent the necessary scale to properly understand how to best adjust our current implementation and determine if there
remains a possibility to improve training performance with existing tools and frameworks.

Finally, this study suggests interesting new research directions appropriate for short- and long-term considerations. First, can we design and innovate better algorithms to build within the GPipe paradigm for more efficient parallelization of GNNs? Second, expanding on the value of practicality by leveraging existing toolsets, do opportunities exist with other well-established techniques from the vast archives of deep learning research that can be transferred or adapted to GNNs and other new deep learning fields? On an even broader scale and vision, we can imagine how these graph data structures used today suggest a similarity, or at least the possibility for similarity, to real-world biological brain networks. Establishing advanced understandings on how to adapt current compute frameworks and distributed architectures to efficiently process extremely large, complex, and arbitrarily dense graphs could guide future approaches in neurotechnology. For example, by understanding how computational graphs of such a scale function based on the underlying structure, we might discover more about how to accurately simulate emergent neural behavior, such as the appearance of consciousness, or even directly augment functional capabilities through software integration with living mammalian brains.

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REFERENCES

[1] U. Alon and E. Yahav. 2020. On the Bottleneck of Graph Neural Networks and its Practical Implications. arXiv preprint arXiv:2006.05205 (2020).
[2] Siddharat Arora. 2020. A Survey on Graph Neural Networks for Knowledge Graph Completion. arXiv:2007.12974 [cs.CL]
[3] Adam Auten, Matthew Tomei, and Rakesh Kumar. 2020. Hardware Acceleration of Graph Neural Networks. In 2020 57th ACM/IEEE Design Automation Conference (DAC). IEEE, 1–6.
[4] V. Iuaptop, T. Keek, A. Grabska-Barwińska, C. Donner, E.D. Cubuk, S.S. Schoenholz, A. Obika, A.W.R. Nelson, T. Back, D. Hassabis, and P. Kohli. 2020. Unveiling the predictive power of static structure in glassy systems. Nature Physics 16, 4 (2020), 448–454.
[5] Joan Bruna, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. 2013. Spectral networks and locally connected networks on graphs. arXiv preprint arXiv:1312.6203 (2013).
[6] D. Cheriton and R.E. Tarjan. 1976. Finding Minimum Spanning Trees. SIAM J. Comput. 5, 4 (1976), 724–742.
[7] W.-L. Chiang, X. Liu, S. Yi, L. Bengio, and C.-J. Hsieh. 2019. 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 and Data Mining. 257–266.
[8] Michael Defferrard, Xavier Bresson, and Pierre Vandergheynst. 2016. Convolutional neural networks on graphs with fast localized spectral filtering. In Advances in neural information processing systems. 3844–3852.
[9] E.W. Dijkstra. 1959. A note on two problems in connexion with graphs. Numer. Math. 1, 1 (1959), 269–271.
[10] David K Duvenaud, Dougal Maclaurin, Jorge Iparraguirre, Rafael Bombarell, Armand-guillaume Pascanu, Timothy Hirzel, Alain Aspuru-Guzik, and Ryan P Adams. 2015. Convolutional networks on graphs for learning molecular fingerprints. In Advances in neural information processing systems. 2224–2232.
[11] Matthias Fey, Jan Eric Lenssen, Frank Weichert, and Heinrich Müller. 2018. Splinecnn: Fast geometric deep learning with continuous b-spline kernels. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition. 869–877.
[12] Matthias Fey and Jan Eric Lenssen. 2019. Fast graph representation learning with PyTorch Geometric. arXiv preprint arXiv:1903.02428 (2019).
[13] F Frasca, E. Rossi, D. Eynard, B. Chamberlain, M. Bronstein, and F. Monti. 2020. SIGN: Scalable Inception Graph Neural Network. arXiv preprint arXiv:2004.11188 (2020).
[14] Will Hamilton, Zhitao Ying, and Jure Leskovec. 2017. Inductive representation learning on large graphs. In Advances in neural information processing systems. 1024–1034.
[15] Matthias Hemaff, Jo-An Brunza, and Yann LeCun. 2015. Deep convolutional networks on graph-structured data. arXiv preprint arXiv:1506.05653 (2015).
[16] W. Hu, M. Fey, M. Zitnik, Y. Dong, H. Ren, B. Liu, M. Catasta, and J. Leskovec. 2020. Open Graph Benchmark: Datasets for Machine Learning on Graphs. arXiv preprint arXiv:2005.06667 (2020).
[17] Yangning Huang, Youdong Cheng, Ankur Bapna, Orhan Firat, Dehao Chen, Mia Chen, HyoukJoong Lee, Jiaqun Ngiam, Quoc V Le, Yonghui Wu, et al. 2019. Gpipe: Efficient training of giant neural networks using pipeline parallelism. In Advances in neural information processing systems. 103–112.
[18] Chiheon Kim, Heungseung Lee, Myungyong Jeong, Wooyunh Bae, Boogeon Yoon, Ilido Kim, Sunghin Lim, and Sungwoong Kim. 2020. torchgpipe: On-the-fly Pipeline Parallelism for Training Giant Models. (2020). arXiv:2004.09910
[19] Thomas Kipf and Max Welling. 2016. Semi-supervised classification with graph convolutional networks. arXiv preprint arXiv:1609.02907 (2016).
[20] Yuja Li, Daniel Tarlow, Marc Brockschmidt, and Richard Zemel. 2015. Gated sequence graph neural networks. arXiv preprint arXiv:1511.05493 (2015).
[21] Housong Liu, Shengliang Lu, Xinyu Chen, and Bengsheng He. 2020. G3: when graph neural networks meet parallel graph processing systems on GPUs. Proceedings of the VLDB Endowment 13, 12 (2020), 2813–2816.
[22] Lingxiang Ma, Zhi Yang, Youshan Miao, Jilong Xue, Ming Wu, Lidong Zhou, and Yairait Dai. 2019. Neugraph: parallel deep neural network computation on large graphs. In 2019 [USENIX] Annual Technical Conference (USENIX ATC) (2019), 443–458.
[23] Julian McCleary, Christopher Targett, Qinfeng Shu, and Anton Van Den Hengel. 2015. Image-based recommendations on styles and substitutes. In Proceedings of the 38th international ACM SIGIR conference on research and development in information retrieval. 43–52.
[24] Rocio Mercado, Tobias Rastemo, Edward Lindelof, Gunter Klabmainer, Ola Englund, Hongming Chen, and Edspon Jannik Bjerrum. 2020. Graph Networks for Molecular Design. (8 2020). https://doi.org/10.26434/chemrxiv.1284317.v1
[25] Christopher Morris, Martin Ritzert, Matthias Fey, William L Hamilton, Jan Eric Lenssen, Gaurav Rattan, and Martin Grohe. 2019. Wessfeler and lenan go neural: Higher-order graph neural networks. In Proceedings of the AAAI Conference on Artificial Intelligence, Vol. 33. 4602–4609.
[26] Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. 2014. Deepwalk: Online Learning of social representations. In Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining. 701–710.
[27] Prithviraj Sen, Galileo Namata, Mustafa Bilgic, Lise Getoor, Brian Gallagher, and Tina Eliassi-Rad. 2008. Collective classification in network data. AI magazine, 29, 3 (2008), 93–93.
[28] A. Strøkasch, D. Beccera, C. Corbi-Verge, A. Perez-Riba, and P. F. Kim. 2020. Fast and Flexible Protein Design Using Deep Graph Neural Network. Cell Systems 11, 4 (2020), 402–411.e4.
[29] Shikhar Vashisth. 2019. NeurGraph: Embedding Methods for Natural Language Processing. CoRR abs/1911.03042 (2019). arXiv:1911.03042 http://arxiv.org/abs/1911.03042
[30] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. 2017. Graph attention networks. arXiv preprint arXiv:1710.10903 (2017).
[31] Minjie Wang, Da Zheng, Zihao Ye, Quan Gan, Mufei Li, Xiang Song, Jingjing Zhou, Chao Ma, Lingfan Yu, Gaif Tian, Xiaojun Xiao, Tong He, George Karypis, Jinyang Li, and Zheng Zhang. 2019. Deep Graph Library: A Graph-Centric, Highly-Performant Package for Graph Neural Networks. arXiv preprint arXiv:1909.01315 (2019).
[32] Zhilin Yang, William Cohen, and Ruslan Salakhudinov. 2016. Revisiting semi-supervised learning with graph embeddings. In International conference on machine learning. PMLR, 40–48.
[33] Rex Ying, Ruining He, Kaifeng Chen, Pong Eksombatchai, William L. Hamilton, and Jure Leskovec. 2018. Graph Convolutional Neural Networks for Web-Scale Recommender Systems. CoRR abs/1806.01973 (2018). arXiv:1806.01973 http://arxiv.org/abs/1806.01973
[34] Bing Yu, Haoteng Yin, and Zhanxing Zhu. 2017. Spatio-temporal Graph Convolutional Neural Network: A Deep Learning Framework for Traffic Forecasting. CoRR abs/1709.04875 (2017). arXiv:1709.04875 http://arxiv.org/abs/1709.04875
[35] Wayne W Zachary. 1977. An information flow model for conflict and fission in small groups. Journal of anthropological research 33, 4 (1977), 452–473.
[38] Jie Zhou, Ganqu Cui, Zhengyan Zhang, Cheng Yang, Zhiyuan Liu, Lifeng Wang, Changcheng Li, and Maosong Sun. 2018. Graph neural networks: A review of methods and applications. arXiv preprint arXiv:1812.08434 (2018).

[39] Jiawei Zhou, Zhiying Xu, Alexander M Rush, and Minlan Yu. 2020. Automating Botnet Detection with Graph Neural Networks. arXiv preprint arXiv:2003.06344 (2020).