Toward Quantized Model Parallelism for Graph-Augmented MLPs Based on Gradient-Free ADMM Framework

Junxiang Wang, Hongyi Li, Zheng Chai, Yongchao Wang, Senior Member, IEEE, Yue Cheng, and Liang Zhao, Senior Member, IEEE

Abstract—While graph neural networks (GNNs) are popular in the deep learning community, they suffer from several challenges including over-smoothing, over-squashing, and gradient vanishing. Recently, a series of models have attempted to relieve these issues by first augmenting the node features and then imposing node-wise functions based on multilayer perceptron (MLP), which are widely referred to as graph-augmented MLP (GA-MLP) models. However, while GA-MLP models enjoy deeper architectures for better accuracy, their efficiency largely deteriorates. Moreover, popular acceleration techniques such as stochastic-version or data-parallelism cannot be effectively applied due to the dependency among samples (i.e., nodes) in graphs. To address these issues, in this article, instead of data parallelism, we propose a parallel graph deep learning Alternating Direction Method of Multipliers (pdADMM-G) framework to achieve model parallelism: parameters in each layer of GA-MLP models can be updated in parallel. The extended pdADMM-G-Q algorithm reduces communication costs by introducing the quantization technique. Theoretical convergence to a (quantized) stationary point of the pdADMM-G algorithm and the pdADMM-G-Q algorithm is provided with a sublinear convergence rate $\alpha(1/k)$, where $k$ is the number of iterations. Extensive experiments demonstrate the convergence of two proposed algorithms. Moreover, they lead to a more massive speedup and better performance than all state-of-the-art comparison methods on nine benchmark datasets. Last but not least, the proposed pdADMM-G-Q algorithm reduces communication overheads by up to 45% without loss of performance. Our code is available at https://github.com/xianggebenben/pdADMM-G.

Index Terms—Alternating direction method of multipliers (ADMM), convergence, graph neural networks (GNNs), model parallelism, quantization.

I. INTRODUCTION

Graph neural networks (GNNs) have accomplished the state-of-the-art performance in various graph applications such as node classification and link prediction. This is because they handle graph-structured data via aggregating neighbor information and extending operations and definitions of the deep learning approach [1]. However, their performance has significantly been restricted via their depths due to the over-smoothing problem (i.e., the representations of different nodes in a graph tend to be similar when stacking multiple layers) [2], the over-squashing problem (i.e., the information flow among distant nodes distorts along the long-distance interactions) [3], and the gradient vanishing problem (i.e., the signals of gradients decay with the depths of GNN models) [2]. These challenges still exist even though some models such as GraphSAGE [4] have been proposed to alleviate them.

On the other hand, the graph augmented multilayer perceptron (GA-MLP) models have recently received fast-increasing attention as an alternative to deal with the aforementioned drawbacks of conventional GNNs via the augmentation of graph features. GA-MLP models augment node representations of graphs and feed them into multilayer perceptron (MLP) models. Compared with GNNs, GA-MLP models are more resistant to the over-smoothing problem [2] and therefore demonstrate outstanding performance. For example, Wu et al. [5] showed that a two-layer GA-MLP approximates the performance of the GNN models on multiple datasets.

GA-MLP models are supposed to perform better with the increase of their depths. However, similar to GNNs, GA-MLP models still suffer from the gradient vanishing problem, which is caused by the mechanism of the classic backpropagation algorithm. This is because gradient signals diminish during the transmission among deep layers. Moreover, while the models go deeper, efficiency will become an issue, especially for medium- and large-size graphs. Compared to the data such as images and texts, where identically and independently distributed [independent identically distributed (i.i.d.)] samples are assumed, efficiency issues in graph data are much more
difficult to handle due to the dependency among data samples (i.e., nodes in graphs). Such dependency seriously troubles the effectiveness of using typical acceleration techniques such as sampling-based methods, and data-parallelism distributed learning in solving the efficiency issue. Therefore, parallelizing the computation along layers is a natural workaround, but the backpropagation prevents the gradients of different layers from being calculated in parallel. This is because the calculation of the gradient in one layer is dependent on its previous layers.

To handle these challenges, recently gradient-free optimization methods such as the Alternating Direction Method of Multipliers (ADMM) have been investigated to overcome the difficulties of the backpropagation algorithm. The spirit of ADMM is to decouple a neural network into layerwise subproblems such that each of them can be solved efficiently. ADMM does not require gradient calculation and therefore can avoid the gradient vanishing problem. Existing literature has shown its great potential. For example, Taylor et al. [6] and Wang et al. [7] proposed ADMM to train MLP models. Extensive experiments have demonstrated that the ADMM has outperformed most comparison methods such as gradient descent (GD).

In this article, we propose a novel parallel graph deep learning ADMM (pdADMM-G) optimization framework to train large-scale GA-MLP models, and the extended pdADMM-G-Q algorithm reduces the communication cost of the pdADMM-G algorithm by the quantization techniques. Our contributions to this article include the following.

1) We propose a novel reformulation of GA-MLP models, which splits a neural network into independent layer partitions and allow for ADMM to achieve model parallelism.

2) We propose a novel pdADMM-G framework to train a GA-MLP model. All subproblems generated by the ADMM algorithm are discussed. The extended pdADMM-G-Q algorithm reduces communication costs by introducing the quantization technique.

3) We provide the theoretical convergence guarantee of the proposed pdADMM-G algorithm and the pdADMM-G-Q algorithm. Specifically, they converge to a (quantized) stationary point of GA-MLP models when the hyperparameters are sufficiently large, and their sublinear convergence rates are $\mathcal{O}(1/k)$.

4) We conduct extensive experiments on nine benchmark datasets to show the convergence, the massive speedup of the proposed pdADMM-G algorithm and the pdADMM-G-Q algorithm, as well as their outstanding performance when compared with all the state-of-the-art optimizers. Moreover, the proposed pdADMM-G-Q algorithm reduces communication overheads by up to 45%.

The organization of this article is shown as follows: In Section II, we summarize recent related research work to this article. In Section III, we propose the pdADMM-G algorithm and the pdADMM-G-Q algorithm to train deep GA-MLP models. Section IV details the convergence properties of the proposed pdADMM-G algorithm and the pdADMM-G-Q algorithm. Extensive experiments on nine benchmark datasets to demonstrate the convergence, speedup, communication savings, and outstanding performance of the pdADMM-G algorithm and the pdADMM-G-Q algorithm are shown in Section V, and Section VI concludes this work.

II. RELATED WORK

This section summarizes existing literature related to this research.

A. Distributed Deep Learning

With the increase of public datasets and layers of neural networks, it is imperative to establish distributed deep learning systems for large-scale applications. Many systems have been established to satisfy such needs. Famous systems include Terngrad [8], Horovod [9], SINGA [10] Mxnet [11], TicTac [12], and Poseidon [13]. They applied some parallelism techniques to reduce computational time, and therefore improved the speedup. Existing parallelism techniques can be classified into two categories: data parallelism and model parallelism. Data parallelism focuses on distributing data across different processors and then aggregating results from them into a server. Scaling GD is one of the most common ways to reach data parallelism [14]. For example, the distributed architecture, Poseidon, is achieved by scaling GD through overlapping communication and computation over networks. The recently proposed ADMM [6], [7] is another way to achieve data parallelism. However, data parallelism suffers from the bottleneck of a neural network: for GD, the gradient should be transmitted through all processors; for ADMM, the parameters in one layer are subject to those in its previous layer. As a result, this leads to heavy communication costs and time delays. Model parallelism, however, can solve this challenge because model parallelism splits a neural network into many independent partitions. In this way, each partition can be optimized independently and reduce layer dependency. For instance, Parpas and Muir [15] proposed a parallel-in-time method from the perspective of dynamic systems; Huo et al. [16] introduced a feature replay algorithm to achieve model parallelism. Zhuang et al. [17] broke layer dependency by introducing the delayed gradient.

B. Deep Learning on Graphs

Graphs are ubiquitous structures and are popular in real-world applications. There is a surge of interest to apply deep learning techniques to graphs. For a comprehensive summary please refer to [18]. It classified existing GNN models into four categories: recurrent GNNs (RecGNNs), convolutional GNNs (ConvGNNs), graph autoencoders (GAEs), and spatial–temporal GNNs (STGNNs). RecGNNs learn node representation with recurrent neural networks via the message passing mechanisms [19], [20], [21]; ConvGNNs generalize the operations of convolution to graph data and stack multiple convolution layers to extract high-level node features [22], [23], [24]; GAEs encode node information into a latent space and reconstruct graphs from the encoded node representation [25], [26], [27]; the idea of STGNNs is to capture spatial dependency and temporal dependency simultaneously [28], [29], [30].
III. PDADMM-G ALGORITHM

We propose the pdADMM-G algorithm to solve GA-MLP models in this section. Specifically, Section III-A formulates the GA-MLP model training problem, and Section III-B proposes the pdADMM-G algorithm. Section III-C extends the proposed pdADMM-G algorithm to the pdADMM-G-Q algorithm for quantization. Important notations are given in Table I.

A. Problem Formulation

Consider a graph $G = (V, E)$, where $V$ and $E$ are sets of nodes and edges, respectively; $|V|$ is the number of nodes, and $\Psi = \{\psi_1(A), \ldots, \psi_K(A)\}$ be a set of (usually multihop) operators $\psi_i(A): \mathbb{R}^{|V|} \rightarrow \mathbb{R}^{|V|}(i = 1, \ldots, K)$ that are functions of the adjacency matrix $A \in \{0, 1\}^{|V|\times|V|}$, and $\mathbb{R}^{|V|}$ is the domain of $\psi_i(A)$ for $i = 1, \ldots, K$. $X_k = H \psi_k(A)$ is the augmentation of node features by the k-hop operator, where $H \in \mathbb{R}^{d \times |V|}$ is a matrix of node features, and $d$ is the dimension of features. $X_k(k = 1, \ldots, K)$ are stacked into $X = [X_1; \ldots; X_K]$ by column. Then the GA-MLP training problem is formulated as follows [7].

Problem 1

\[
\begin{align*}
\min_{W_l, b_l, z_l} & \quad R(z_L; y) \\
\text{s.t.} & \quad z_l = W_l p_l + b_l, \quad p_{l+1} = f_l(z_l)(l = 1, \ldots, L-1)
\end{align*}
\]

where $p_l = X \in \mathbb{R}^{n_0 \times |V|}$ is the input of deep GA-MLP models, where $n_0 = Kd$ is the dimension of input and $y$ is a predefined label vector. $p_l \in \mathbb{R}^{n_l \times |V|}$ is the input for the $l$th layer, also the output for the $(l-1)$th layer, and $n_l$ is the number of neurons for the $l$th layer. $R(z_L; y)$ is a risk function for the $L$th layer, which is convex and continuous; $z_l = W_l p_l + b_l$ and $p_{l+1} = f_l(z_l)$ are linear and nonlinear mappings for the $l$th layer, respectively, and $W_l \in \mathbb{R}^{n_l \times n_{l-1}}$ and $b_l \in \mathbb{R}^{n_l}$ are the weight matrix and the intercept vector for the $l$th layer, respectively.

In Problem 1, $\Psi$ can be considered as a prepossessing step to augment node features via $A$, and hence it is predefined. One common choice can be $\Psi = \{I, A, A^2, \ldots, A^K\}$. Problem 1 can be addressed by deep learning ADMM (dADMM) [7]. However, parameters in one layer are dependent on its neighboring layers and hence cannot achieve parallelism. For example, the update of $p_{l+1}$ on the $(l+1)$th layer needs to wait before $z_l$ on the $l$th layer is updated. To address layer dependency, we relax Problem 1 to Problem 2 as follows.

Problem 2

\[
\begin{align*}
\min_{p, W, b, z, q} & \quad F(p, W, b, z, q) = R(z_L; y) + (v/2) \left( \sum_{l=1}^{L} ||z_l - W_l p_l - b_l||_2^2 + \sum_{l=1}^{L-1} ||q_l - f_l(z_l)||_2^2 \right) \\
\text{s.t.} & \quad p_{l+1} = q_l
\end{align*}
\]

where $p = \{p_l\}_{l=1}^{L}$, $W = \{W_l\}_{l=1}^{L}$, $b = \{b_l\}_{l=1}^{L}$, $z = \{z_l\}_{l=1}^{L}$, $q = \{q_l\}_{l=1}^{L-1}$, and $v > 0$ is a tuning parameter. As $v \rightarrow \infty$, Problem 2 approaches Problem 1. We reduce layer dependency by splitting the output of the $l$th layer and the input of the $(l+1)$th layer into two variables $p_{l+1}$ and $q_l$, respectively.

B. pdADMM-G Algorithm

The high-level overview of the pdADMM-G algorithm is shown in Fig. 1. Specifically, the inputs of GA-MLP models are augmented by $H \psi_k(A)$ for $k = 1, \ldots, K$, and then GA-MLP models are split into multiple layers, each of which can be optimized by an independent client. Therefore, layerwise training can be implemented in parallel. Moreover, the gradient vanishing problem can be avoided in this way. This is because the accumulated gradient calculated by the backpropagation algorithm is split into layerwise components.

Now we follow the ADMM routine to solve Problem 2. The augmented Lagrangian function is formulated mathematically as follows:

\[
L_p(p, W, b, z, q, u) = F(p, W, b, z, q) + \sum_{l=1}^{L} \left( u_l^T (p_{l+1} - q_l) + (\rho/2) ||p_{l+1} - q_l||_2^2 \right)
\]

\[
= R(z_L; y) + \phi(p_1, W_1, b_1, z_1) + \sum_{l=2}^{L} \phi(p_l, W_l, b_l, z_l, q_{l-1}, u_{l-1}) + (v/2) \sum_{l=1}^{L-1} ||q_l - f_l(z_l)||_2^2
\]

where $\phi(p_1, W_1, b_1, z_1) = (v/2) ||z_1 - W_1 p_1 - b_1||_2^2$, $\phi(p_l, W_l, b_l, z_l, q_{l-1}, u_{l-1}) = (v/2) ||z_l - W_l p_l - b_l||_2^2 + u_{l-1}^T (p_l - q_{l-1}) + (\rho/2) ||p_l - q_{l-1}||_2^2$, $u_l(l = 1, \ldots, L-1)$ are dual variables, $\rho > 0$ is a parameter, and $u = \{u_l\}_{l=1}^{L-1}$. The detail of the pdADMM-G algorithm is shown in Algorithm 1.

Specifically, Lines 5–9 update primal variables $p, W, b, z, q$, respectively, while Line 11 updates the dual variable $u$.

Due to space limit, the details of all subproblems are shown in Section A in the Supplementary Material.

Our proposed pdADMM-G algorithm can be efficient for training deep GA-MLP models via the greedy layerwise training strategy [31]. Specifically, we begin by training a
shallow GA-MLP model. Next, more layers are increased to the GA-MLP model and their parameters are trained, then we introduce even more layers and iterate this process until the whole deep GA-MLP model is included. The pdADMM-G algorithm can achieve excellent performance as well as reduce training costs by this strategy.

Last but not least, we compare the computational costs of the proposed pdADMM-G algorithm with the state-of-the-art backpropagation algorithm, on which the GD is based. We show that they share the same level of computational costs. For the backpropagation algorithm, the most costly operation is the matrix multiplication $z_l = W_l p_l + b_l$ in the forward pass, where $W_l \in \mathbb{R}^{n_l \times n_{l-1}}$ and $p_l \in \mathbb{R}^{n_{l-1} \times |V|}$, which requires a time complexity of $O(n_l n_{l-1} |V|)$ [32]; for the proposed pdADMM-G algorithm, the most costly operation is to compute the derivative $\nabla W \phi$, and it also involves the matrix multiplication, and hence its time complexity is again $O(|n_{l-1}| |V|)$. However, the proposed pdADMM-G algorithm trains the whole GA-MLP model in a model parallelism fashion [33], and therefore all computational costs can be split into different independent clients for parallel training; whereas the backpropagation algorithm is implemented sequentially, and thus it is less efficient than the proposed pdADMM-G algorithm.

C. Quantization Extension of pdADMM-G

In the proposed pdADMM-G algorithm, $p_l$ and $q_l$ are transmitted back and forth among layers (i.e., clients). However, the communication overheads of $p_l$ and $q_l$ surge for a large-scale graph $G$ with millions of nodes. To alleviate this challenge, the quantization technique is commonly utilized to reduce communication costs by mapping continuous values into a discrete set [34]. In other words, $p_l$ is required to fit into a countable set $\Delta$, which is shown as follows.

Problem 3

$$
\min_{p, W, b, z, q} F(p, W, b, z, q) = R(z_L; y) + \frac{v}{2} \left( \sum_{l=1}^{L} \| z_l - W_l p_l - b_l \|_2^2 \right) + \sum_{l=1}^{L-1} \| q_l - f_l(z_l) \|_2^2 \\
\text{s.t. } p_{l+1} = q_l, \ p_l \in \Delta = \{ \delta_1, \ldots, \delta_m \}
$$

where $\delta_i (i = 1, \ldots, m) \in \Delta$ are quantized values, which can be integers or low-precision values. $m = |\Delta|$ is the cardinality of $\Delta$. To address Problem 3, we rewrite it into the following form:

$$
\min_{p, W, b, z, q} R(z_L; y) + \sum_{l=1}^{L} \| p_l \|_2 \\
+ \frac{v}{2} \left( \sum_{l=1}^{L} \| z_l - W_l p_l - b_l \|_2^2 \right) + \sum_{l=1}^{L-1} \| q_l - f_l(z_l) \|_2^2 \\
\text{s.t. } p_{l+1} = q_l
$$

where the indicator function $\mathbb{I}(p_l)$ is defined as follows: $\mathbb{I}(p_l) = 0$ if $p_l \in \Delta$, and $\mathbb{I}(p_l) = +\infty$ if $p_l \notin \Delta$. The augmented Lagrangian of Problem 3 is shown as follows:

$$
\beta_d(p, W, b, z, q, u) = L_\rho(p, W, b, z, q, u) + \sum_{l=2}^{L} \mathbb{I}(p_l)
$$

where $L_\rho$ is the augmented Lagrangian of Problem 2. The extended pdADMM-G-Q algorithm follows the same routine as the pdADMM-G algorithm, where $L_\rho$ is replaced with $\beta_d$. Due to space limit, the solutions to all subproblems generated by two proposed algorithms are shown in Section B in the Supplementary Material.
IV. CONVERGENCE ANALYSIS

In this section, the theoretical convergence of the proposed pdADMM-G algorithm and the pdADMM-G-Q algorithm is provided. Due to space limit, we only provide sketches of proofs in this section, and their details are available in Section C in the Supplementary Material. Our problem formulations are more difficult than existing ADMM literature: the term $\|q_l - f_l(z_l)\|^2$ is coupled in the objective, while it is separable in the existing ADMM formulations. To address this, we impose a mild condition that $\tilde{c}_l(z_l)$ is bounded in Assumption 1, and prove that $u_l$ is controlled via $q_l$ and $z_l$ in Lemma 5 in Section C in the Supplementary Material.

First, the proper function, Lipschitz continuity, and coercivity are defined as follows.

Definition 1 (Proper Functions [35]): For a convex function $g(x): \mathbb{R} \rightarrow \mathbb{R} \cup \{\pm \infty\}$, $g$ is called proper if $\forall x \in \mathbb{R}$, $g(x) > -\infty$, and $\exists x_0 \in \mathbb{R}$ such that $g(x_0) < +\infty$.

Definition 2 (Lipschitz Continuity): A function $g(x)$ is Lipschitz continuous if there exists a constant $D > 0$ such that $\forall x_1, x_2$, the following holds:

$$\|g(x_1) - g(x_2)\| \leq D\|x_1 - x_2\|.$$ 

Definition 3 (Coercivity): A function $h(x)$ is coercive over the feasible set $\mathcal{F}$ means that $h(x) \rightarrow \infty$ as $x \rightarrow \infty$ in $\mathcal{F}$, and $\|x\| \rightarrow \infty$.

Next, the definition of a quantized stationary point [34] is shown as follows.

Definition 4 (Quantized Stationary Point): The $p_l$ is a quantized stationary point of Problem 3 if there exists $\tau > 0$ such that

$$p_l \in \arg \min_{\delta \in \Delta} \|\delta - (p_l - \nabla_{p_l} F(p, W, b, z, q))/\tau\|.$$ 

The quantized stationary point is an extension of the stationary point in the discrete setting, and any global solution $p_l$ to Problem 3 is a quantized stationary point to Problem 3 (see [34, Lemma 3.7]). Then the following assumption is required for convergence analysis.

Assumption 1: $f_l(z_l)$ is Lipschitz continuous with coefficient $S > 0$, $R(Z_l; y)$ is proper, and $F(p, W, b, z, q)$ is coercive. Moreover, $\tilde{c}_l(z_l)$ is bounded, i.e., there exists $M > 0$ such that $\|\tilde{c}_l(z_l)\| \leq M$.

Assumption 1 is mild to satisfy: most common activation functions such as rectified linear unit (ReLU) [33] and leaky ReLU [36] satisfy Assumption 1. The risk function $R(Z_l; y)$ is only required to be proper, which shows that the convergence condition of our proposed pdADMM-G is milder than that of the dADMM, which requires $R(Z_l; y)$ to be Lipschitz differentiable [7]. Due to the space limit, detailed proofs are provided in Section C in the Supplementary Material. The technical proofs follow a similar routine as dADMM [7]. The difference consists in the fact that the dual variable $u_l$ is controlled by $q_l$ and $z_l$ (see Lemma 6 in Section C in the Supplementary Material), which holds under Assumption 1, while $u_l$ can be controlled only by $z_l$ in the convergence proof of dADMM. The first lemma shows that the objective keeps decreasing when $\rho$ is sufficiently large:

Lemma 1 (Objective Decrease): For both the pdADMM-G algorithm and the pdADMM-G-Q algorithm, if $\rho > \max(4V^2, \sqrt{\frac{1}{17}} + 1)v/2$, there exist $C_1 = v/2 - 2\nu^2/\rho > 0$ and $C_2 = \rho - 2\nu^2/\rho - 2v/\rho > 0$ such that it holds for any $k \in \mathbb{N}$ that

$$L_{p_l}(p_{l+1}, W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1}, u_{l+1}) - L_{p_l}(p_l, W_l, b_l, z_l, q_l, u_l) \leq C_1 + C_2,$$

where $L_{p_l}(p_{l+1}, W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1}, u_{l+1})$ is the objective function of the pdADMM-G algorithm.

Sketch of Proof: They can be proven via the optimality conditions of all subproblems, and Assumption 1.

Lemma 2 shows that the objective is bounded from below when $\rho$ is large enough, and all variables are bounded.

Lemma 2 (Bounded Objective): 1) For the pdADMM-G algorithm, if $\rho > \nu$, then $L_{p_l}(p_{l+1}, W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1}, u_{l+1})$ is lower bounded. Moreover, $p_{l+1}, W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1}, u_{l+1}$ are bounded, i.e., there exist $N_p, N_W, N_b, N_z, N_q,$ and $N_u > 0$ such that $\|p_{l+1}\| \leq N_p$, $\|W_{l+1}\| \leq N_W$, $\|b_{l+1}\| \leq N_b$, $\|z_{l+1}\| \leq N_z$, $\|q_{l+1}\| \leq N_q,$ and $\|u_{l+1}\| \leq N_u$.

2) For the pdADMM-G-Q algorithm, if $\rho > \nu$, then $L_{p_l}(p_{l+1}, W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1}, u_{l+1})$ is lower bounded. Moreover, $W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1}, u_{l+1}$ are bounded, i.e., there exist $N_W, N_b, N_z, N_q,$ and $N_u > 0$ such that $\|W_{l+1}\| \leq N_W$, $\|b_{l+1}\| \leq N_b$, $\|z_{l+1}\| \leq N_z$, $\|q_{l+1}\| \leq N_q,$ and $\|u_{l+1}\| \leq N_u$.

Sketch of Proof: We only show the sketch proof of (1) because (2) follows the same routine as (1). To prove the boundedness of $L_{p_l}$, we should prove the following:

$$L_{p_l}(p_{l+1}, W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1}, u_{l+1}) \geq F(p_{l+1}, W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1}) + ((\rho - \nu)/2)\|p_{l+1} - q_{l+1}\|_2^2 > -\infty,$$

where $\|p_{l+1} - q_{l+1}\|_2^2 < q_l^2$. Therefore, $F(p_{l+1}, W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1})$ and $((\rho - \nu)/2)\|p_{l+1} - q_{l+1}\|_2^2$ are upper bounded by $L_{p_l}(p_l, W_l, b_l, z_l, q_l, u_l)$ and hence $L_{p_l}(p_{l+1}, W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1}, u_{l+1})$ (see Lemma 1). The boundedness of variables can be obtained via Assumption 1.

Based on Lemmas 1 and 2, the following theorem ensures that the objective is convergent.

Theorem 1 (Convergent Objective): 1) For the pdADMM-G algorithm, if $\rho > \max(4V^2, \sqrt{\frac{1}{17}} + 1)v/2$, then $L_{p_l}(p_{l+1}, W_{l+1}, b_{l+1}, z_{l+1}, q_{l+1}, u_{l+1})$ is convergent. Moreover, $\lim_{k \to \infty} \|p_{l+1} - p_l\|_2^2 = 0$, $\|w_{l+1} - w_l\|_2^2 = 0$. We refer to [34] for the proof of this theorem.
Theorem 2 (Convergence of the pdADMM-G Algorithm): If \( \rho > \max(4vS^2, (\sqrt{T} + 1)v/2) \), then for the variables \((p^k, \bar{W}^k, b^k, z^k, q^k, u^k)\) starting from any \((p^0, \bar{W}^0, b^0, z^0, q^0, u^0)\), \((p^k, \bar{W}^k, b^k, z^k, q^k, u^k)\) has at least a limit point \((p^*, \bar{W}^*, b^*, z^*, q^*, u^*)\), and any limit point is a stationary point of Problem 2. That is, \( p^*_t = q^*_t \), \( \nabla_p L_{\rho}(p^*, \bar{W}^*, b^*, z^*, q^*, u^*) = 0 \)

\[
\nabla_{b^*} \beta_p(p^*, \bar{W}^*, b^*, z^*, q^*, u^*) = 0
\]

\( 0 \in \partial_\rho L_{\rho}(p^*, \bar{W}^*, b^*, z^*, q^*, u^*) = 0 \)

Sketch of Proof: This theorem can be derived directly from Lemmas 2 and 3.

Theorem 3 (Convergence of the pdADMM-G-Q Algorithm): If \( \rho > \max(4vS^2, (\sqrt{T} + 1)v/2) \), then for the variables \((p^k, \bar{W}^k, b^k, z^k, q^k, u^k)\) starting from any \((p^0, \bar{W}^0, b^0, z^0, q^0, u^0)\), \((p^k, \bar{W}^k, b^k, z^k, q^k, u^k)\) has at least a limit point \((p^*, \bar{W}^*, b^*, z^*, q^*, u^*)\), and any limit point \((W^*, b^*, z^*, q^*, u^*)\) is a stationary point of Problem 3. Moreover, if \( t^*_k \) is bounded, then \( p^k \) is a quantized stationary point of Problem 3. That is,

\[
p^*_t = q^*_t,
\]

\[
\nabla_p L_{\rho}(p^*, \bar{W}^*, b^*, z^*, q^*, u^*) = 0
\]

\( 0 \in \partial_\rho L_{\rho}(p^*, \bar{W}^*, b^*, z^*, q^*, u^*) = 0 \)

\( p^*_t \in \arg\min_{\delta \in \Delta} \left( p^*_t - \nabla_\rho F(p^*, \bar{W}^*, b^*, z^*, q^*)/t^*_k \right) \)

Sketch of Proof: This theorem is proven using a similar procedure as Theorem 2, and the definition of the quantized stationary point.

The only difference between Theorems 2 and 3 is that \( p^* \) is a stationary point in Problem 2 and a quantized stationary point in Problem 3. Next, the following theorem ensures the sublinear convergence rate \( o(1/k) \) of the proposed pdADMM-G algorithm and the pdADMM-G-Q algorithm.

Theorem 4 (Convergence Rate):

1. For the pdADMM-G algorithm and a sequence \((p^k, \bar{W}^k, b^k, z^k, q^k, u^k)\), define \( c_k = \min_{0 \leq l \leq k} \left( \sum_{j=0}^l (\zeta_j/2^j) + \sum_{j=0}^l \|b^j-b^0\|^2 + \sum_{j=0}^l \|\bar{W}^j-\bar{W}^0\|^2 + \sum_{j=0}^l \|\bar{W}^j-\bar{W}^0\|^2 \right) \).

2. For the pdADMM-G-Q algorithm and a sequence \((W^k, b^k, z^k, q^k, u^k)\), define \( d_k = \min_{0 \leq l \leq k} \left( \sum_{j=0}^l (\zeta_j/2^j) + \sum_{j=0}^l \|b^j-b^0\|^2 + \sum_{j=0}^l \|\bar{W}^j-\bar{W}^0\|^2 \right) \).

Sketch of Proof:

1. Prove the convergence rate \( o(1/k) \), \( c_k \) satisfies three conditions: (a) \( c_k \geq c_{k+1} \), (b) \( \sum_{k=0}^\infty c_k \) is bounded, and (c) \( c_k \geq 0 \).

2. \( d_k \) can be proven using a similar procedure as (1).
In this section, we evaluate the performance of the proposed pdADMM-G algorithm and the proposed pdADMM-G-Q algorithm on GA-MLP models using nine benchmark datasets. Convergence and computational overheads are demonstrated on different datasets. Speedup and test performance are compared with several state-of-the-art optimizers. All experiments were conducted on the Amazon Web Services (AWS) p2.16xlarge instance, with 16 NVIDIA K80 GPUs, 64vCPUs, and 732 GiB of RAM.

### A. Datasets and Settings

Nine benchmark datasets were used for experimental evaluation, whose statistics are shown in Table II. Each dataset is split into a training set, a validation set, and a test set. Due to space limit, their details can be found in Section D1 in the Supplementary Material.

When it comes to experimental settings, we set $K = 4$ for the multihop operator $\Psi$, and defined a diagonal degree matrix $D$ where $D_{ii} = \sum_{j=1}^{V} A_{ij}$, and a renormalized adjacency matrix $\tilde{A} = (D + I)^{-1/2}(A + I)(D + I)^{-1/2} \in \mathbb{R}^{V \times V}$ [1]. Moreover, we set $\Psi = \{I, \tilde{A}, \tilde{A}^2, \tilde{A}^3\}$ [2]. For all GA-MLP models, the activation function was set to ReLU. The loss function was set to the cross-entropy loss. For the pdADMM-G-Q algorithm, $\Delta = \{-1, 0, 1, \ldots, 20\}$ in Problem 3, and $p$ was quantized by default.

### B. Comparison Methods

GD and its variants are state-of-the-art optimizers and hence served as comparison methods. For GD-based methods, all datasets were used for training models in a full-batch fashion. All hyperparameters were chosen by maximizing the performance of validation sets. Due to space limit, hyperparameter settings of all methods are shown in Section D2 in the Supplementary Material. The following are their brief introductions.

1) **GD** [37]: The GD and its variants are the most popular deep learning optimizers. The GD updates parameters simply based on their gradients.

2) **Adaptive Learning Rate Method (Adadelta)** [38]: The Adadelta is proposed to overcome the sensitivity to hyperparameter selection.

3) **Adaptive Gradient Algorithm (Adagrad)** [39]: Adagrad is an improved version of GD: rather than fixing the learning rate during training, it adapts the learning rate to the hyperparameter.

4) **Adaptive Momentum Estimation (Adam)** [40]: Adam is the most popular optimization method for deep learning models. It estimates the first and second momentum to correct the biased gradient, and thus accelerates empirical convergence.

### C. Convergence

First, to validate the convergence of two proposed algorithms, we set up a GA-MLP model with ten layers, each of which has 1000 neurons. The number of epochs was set to 100. $\nu$ and $\rho$ were set to 0.01 and 1, respectively.

Fig. 2 demonstrates objectives and residuals of two proposed algorithms on four datasets. Overall, the objectives and residuals of the two proposed algorithms are convergent. From Fig. 2(a) and (c), the objectives of the two proposed algorithms decrease drastically at the first 50 epochs and then drop smoothly to the end. The objectives on the PubMed dataset achieve the lowest among all four datasets, whereas these on the Coauthor Computer Science (CS) dataset are the highest, which still reach near $10^7$ at the 100th epoch. As for residuals, even though the residuals of the pdADMM-G-Q algorithm are higher than these of the pdADMM-G algorithm initially, they both converge sublinearly to 0, which is consistent with Theorem 2 and Theorem 3. Specifically, as shown in Fig. 2(b) and (d), the residuals on the Cora dataset decrease more slowly with fluctuation than these on other datasets, while residuals on the Amazon Computers and Amazon Photo datasets demonstrate the fastest decreasing speed at the first 40 epochs before reaching a plateau less than $10^{-6}$. The residuals on the PubMed dataset accomplish the lowest values among all four datasets again with a value of less than $10^{-7}$.

### D. Speedup

Next, we investigate the speedup of the pdADMM-G algorithm in the large deep GA-MLP models. The running time per epoch was an average of ten epochs. $\nu$ and $\rho$ were both set to $10^{-3}$. We investigate the speedup concerning two factors: the number of layers and the number of GPUs.

For the relationship between the speedup and the number of layers, the pdADMM-G algorithm in the GA-MLP models with 4000 neurons was tested. The number of layers ranged from 8 to 17. The speedup on small datasets and large datasets are shown in Fig. 3(a) and (b), respectively. Overall, the speedup of the proposed pdADMM-G increases linearly with the number of layers. For example, the speedups on the Cora dataset and the Amazon Computers dataset rise from 3 and 3.5 gradually to 4 and 4.5, respectively. The speedup on the PubMed dataset achieves the lowest with a value of less than 3, whereas that on the Coauthor CS dataset at least doubles that on any other small dataset, with a peak of 6. Moreover, the speedup is more obvious on large datasets. For example, when the slopes of speedups are compared, the slope on the Flickr dataset is at least five times much steeper than that on the

### Table II: Dataset Statistics

| Dataset         | Nodes | Edges | Class | Train | Test | Validation | Train | Test | Validation | Train | Test | Validation | Val. | Test | Validation |
|-----------------|-------|-------|-------|-------|------|------------|-------|------|------------|-------|------|------------|------|------|------------|
| Cora            | 2,486 | 10,566| 7     | 1,433 | 149  | 600        | 1000  | 1000 | 1000       | 1000  | 1000 | 1000       |      |      |            |
| PubMD           | 19,727| 88,648| 6     | 3,506 | 60   | 500        | 1000  | 1000 | 1000       | 1000  | 1000 | 1000       |      |      |            |
| Citeseer        | 2,110 | 3,002 | 6     | 3,506 | 60   | 500        | 1000  | 1000 | 1000       | 1000  | 1000 | 1000       |      |      |            |
| Amazon Computer | 13,383| 491,722| 10    | 767   | 60   | 500        | 1000  | 1000 | 1000       | 1000  | 1000 | 1000       |      |      |            |
| Amazon Photo    | 7,167 | 218,162| 8     | 765   | 60   | 500        | 1000  | 1000 | 1000       | 1000  | 1000 | 1000       |      |      |            |
| Citeseer        | 18,333| 163,744| 15    | 6,865 | 60   | 500        | 1000  | 1000 | 1000       | 1000  | 1000 | 1000       |      |      |            |
| Amazon Physics  | 34,493| 695,924| 5     | 8,115 | 60   | 500        | 1000  | 1000 | 1000       | 1000  | 1000 | 1000       |      |      |            |
| Citeseer        | 33,753| 699,776| 7     | 3,506 | 60   | 500        | 1000  | 1000 | 1000       | 1000  | 1000 | 1000       |      |      |            |
| Amazon Movie    | 199,143| 1,168,225| 40    | 129  | 60   | 500        | 1000  | 1000 | 1000       | 1000  | 1000 | 1000       |      |      |            |

1Registered trademark.
Coauthor CS dataset. The same trend is applied to the Ogbn-Arxiv dataset. This means that our proposed pdADMM-G algorithm is more suitable for large datasets.

For the relationship between the speedup and the number of GPUs, we set up a large GA-MLP model with 16 layers and 4000 neurons and kept all hyperparameters in the previous experiment. The speedup of our proposed pdADMM-G algorithm was compared with all comparison methods. Fig. 4 shows all speedups on two large datasets. The proposed pdADMM-G algorithm achieves a higher speedup than any GD-based method. For example, the speedups of eight GPUs are nearly 8 on the Flickr dataset and the Ogbn-Arxiv dataset, while the best speedups achieved via comparison methods are in the vicinity of 6 and 5 on two datasets, respectively. We also observe that while speedups of all methods scale linearly with the number of GPUs, the slopes of our proposed pdADMM-G algorithm are steeper than these of any comparison method. For example, the slope of our proposed pdADMM-G algorithm on the Flickr dataset is more than ten times steeper than that of Adam. All comparison methods show similar flat slopes, and they achieve a higher slope of the speedup on the Ogbn-Arxiv dataset than that on the Flickr dataset.

In summary, the speedup of our proposed pdADMM-G algorithm scales linearly with the number of layers and the number of GPUs. Moreover, its speedup is superior to any other comparison method significantly by more than ten times.

E. Communication Overheads

Then, it is necessary to explore how many communication overheads can be reduced using the proposed quantization technique on different quantization levels. To achieve this, we established a large GA-MLP model with ten layers, each of which consists of 1000 neurons. We set up three quantization cases: no quantization, the quantization concerning \( p \) only, and the quantization concerning both \( p \) and \( q \). For every quantization case, we also set up two different quantization sizes: 8 bits and 16 bits. Fig. 5 demonstrates the relationship between the test accuracy and communication overheads for different quantization cases and sizes on three datasets. Overall, communication overheads can be reduced significantly by the proposed quantization technique. The amount of reduction depends on different quantization cases and sizes. Generally speaking, the more variables are quantized and the fewer bits are compressed, then the more savings in communications can be achieved. Take the Citeseer dataset as an example, while all algorithms reach the same test accuracy above 70%, the proposed pdADMM-G (i.e., no quantization) consumes the most communication costs with the value of around \( 1.4 \times 10^9 \) bytes. If the variable \( p \) is quantized using 16 bits, the communication overhead drops by 10%, and then using 8 bits saves another 5%. When variables \( p \) and \( q \) are both quantized, the communication overhead tumbles down to \( 1.2 \times 10^9 \) bytes, which means decreases by 16.7% when it is compared with the case where only \( p \) is quantized. When variables are compressed to 8 bits instead of 16 bits, the communication overhead slips further to \( 1.1 \times 10^9 \), a nearly 30% decline. The same trend is applied to the other two datasets, and they accomplish a shrink of communication overheads by 33% and 45%, respectively. This demonstrates that our proposed quantization technique is effective for reducing unnecessary communication costs without loss of performance. We also observe that the
Communication overheads of two proposed algorithms on three datasets: the quantization concerning both $p$ and $q$ using eight bits reduces the communication overheads by up to 45% without loss of performance. (a) Citeseer. (b) Amazon computers. (c) Coauthor CS.

Table III demonstrates the performance of all methods when the number of neurons is 100. In summary, the two proposed algorithms outperform all comparison methods slightly: they occupy the best algorithms on eight datasets out of the total nine datasets. For example, they both achieve 78% test accuracy on the Cora dataset, whereas the best comparison method is GD, which only reaches 73% test accuracy, and is at least 6% lower than the two proposed algorithms. As another example, two proposed algorithms accomplish 78% test accuracy on the PubMed dataset, 4% better than that achieved by Adagrad, whose performance is the best aside from the two proposed algorithms. The Citeseer dataset shows the largest performance gap between the two proposed algorithms and all comparison methods. Two proposed algorithms reach the level of 70% test accuracy, whereas all comparison methods fall in the vicinity of 60% test accuracy. In other words, the two proposed algorithms outperform all comparison methods by more than 10%. For two proposed algorithms, the proposed pdADMM-G-Q algorithm outperforms marginally the proposed pdADMM-G algorithm due to the quantization technique. Their largest performance gap is 5%, which is achieved on the Amazon Computers dataset. The Adam is the best comparison method overall, and it serves as the best algorithm on the

Coauthor CS dataset is the largest dataset among the three, and it accomplishes the greatest communication reduction.

F. Performance

Finally, we evaluate the performance of two proposed algorithms against all comparison methods on nine benchmark datasets. We set up two standard GA-MLP models with ten layers but different neurons: the first model has 100 neurons, while the second model has 500 neurons. Following the greedy layerwise training strategy [31], we first trained a two-layer GA-MLP model, and then three more layers were added to training, and finally, all ten layers were involved. The number of epochs was set to 200. We repeated all experiments five times and reported their means and the standard deviations. Due to space limit, hyperparameter settings and the performance of validation sets are shown in Section D2 and D3 in the Supplementary Material, respectively.

Table IV demonstrates the performance of all methods when the number of neurons is 500. In summary, the two proposed algorithms outperform all comparison methods slightly: they occupy the best algorithms on eight datasets out of the total nine datasets. For example, they both achieve 78% test accuracy on the Cora dataset, whereas the best comparison method is GD, which only reaches 73% test accuracy, and is at least 6% lower than the two proposed algorithms. As another example, two proposed algorithms accomplish 78% test accuracy on the PubMed dataset, 4% better than that achieved by Adagrad, whose performance is the best aside from the two proposed algorithms. The Citeseer dataset shows the largest performance gap between the two proposed algorithms and all comparison methods. Two proposed algorithms reach the level of 70% test accuracy, whereas all comparison methods fall in the vicinity of 60% test accuracy. In other words, the two proposed algorithms outperform all comparison methods by more than 10%. For two proposed algorithms, the proposed pdADMM-G-Q algorithm outperforms marginally the proposed pdADMM-G algorithm due to the quantization technique. Their largest performance gap is 5%, which is achieved on the Amazon Computers dataset. The Adam is the best comparison method overall, and it serves as the best algorithm on the

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Ogbn-Arxiv dataset. The Adadelta performs the worst among all comparison methods, whose performance is significantly lower than any other method on several datasets such as the Amazon Computers dataset, the Amazon Photo dataset, and the Coauthor CS dataset. Last but not least, the standard deviations of all methods remain low, and this shows that they are robust to different initializations.

Table IV shows the performance of all methods when the number of neurons is 500. In general, two proposed algorithms still reach a better performance than all comparison methods, but the gap is more narrow. For example, in Table III, the proposed pdADMM-G algorithm achieves the best on the Amazon Computers dataset. However, it is surpassed by Adagrad slightly in Table IV. We also observe that a GA-MLP model with 500 neurons performs better than that with 100 neurons, which are trained by the same algorithm. This makes sense since the wider a model is, the more expressive it is equipped with.

VI. CONCLUSION

The GA-MLP models are attractive to the deep learning community due to potential resistance to some problems of GNNs such as over-smoothing and over-squashing. In this article, we propose a novel pdADMM-G algorithm to achieve parallel training of GA-MLP models, which is accomplished by breaking the layer dependency. The extended pdADMM-G-Q algorithm reduces communication overheads by the introduction of the quantization technique. Their theoretical convergence to a (quantized) stationary point of the problem is guaranteed with a sublinear convergence rate $\alpha(1/k)$, where $k$ is the number of iterations. Extensive experiments verify that the two proposed algorithms not only converge in terms of objectives and residuals, and accelerate the training of deep GA-MLP models, but also stand out among all the existing state-of-the-art optimizers on nine benchmark datasets. Moreover, the pdADMM-G-Q algorithm reduces communication overheads by up to 45% without loss of performance.

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Junxiang Wang received the bachelor’s degree from East China Normal University, Shanghai, China, in 2012, the master’s degree from George Mason University, Fairfax, VA, USA, in 2016, and the Ph.D. degree from the Department of Computer Science, Emory University, Atlanta, GA, USA, in 2019.

He is currently an Incoming Researcher with NEC Laboratories America. He has published various research papers in top-tier conferences and journals, such as ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), IEEE International Conference on Data Mining (ICDM), International World Wide Web Conference (WWW), Association for the Advancement of Artificial Intelligence (AAAI), PROCEEDINGS OF THE IEEE, and ACM Computing Surveys. His research interests include data mining in social media, inverse problems on graphs, and nonconvex optimization in deep learning.

Hongyi Li received the B.E. degree in telecommunication engineering from Xidian University, Xi’an, China, in 2019, where she is currently pursuing the Ph.D. degree with the State Key Laboratory of Integrated Services Networks (ISN). Her research interests include graph learning, optimization algorithms, and their applications in wireless communication systems.

Zheng Chai received the master’s degree from Georgetown University, Washington, DC, USA, in 2018. He is currently pursuing the Ph.D. degree with the Department of Computer Science, University of Virginia, Charlottesville, VA, USA, under the supervision of Prof. Yue Cheng. His research interests include distributed machine learning, federated learning, and high-performance computing.

Yongchao Wang received the B.E. degree in communication engineering from Xidian University, Xi’an, China, in 1998, 2004, and 2006, respectively. He has been a one-year Visiting Scholar and then a Post-Doctoral Fellow with the Department of Electronics and Communication Engineering, University of Minnesota, Minneapolis, MN, USA. From March 2016 to March 2017, he was a Visiting Scholar with Purdue University, West Lafayette, IN, USA. Since 2012, he has been a Professor with the State Key Laboratory of Integrated Services Networks (ISN), Xidian University. His research works have been applied to several real telecommunication systems.

Dr. Wang was a recipient of several awards, such as the Prize in Progress of Science and Technology from the Ministry of Education of the People’s Republic of China, Shaanxi Government, and Xidian University.

Dr. Zhao has received the NSF CAREER Award in 2020. He has also received the Outstanding Doctoral Student in the Department of Computer Science at Virginia Tech in 2017, the NSF CRII Award in 2018, the Jeffress Trust Award in 2019, the Amazon Research Award in 2020, and the Meta Research Award in 2022. He was ranked as one of the “Top 20 Rising Star in Data Mining” by Microsoft Search in 2016. He has won the Best Paper Award, the Best Poster Runner-Up, and the Best Paper Candidates in top-tier venues, such as ICDM 2021, ICDM 2019, WWW 2021, and ACM SIGSPATIAL 2022. He is recognized as a “Computing Innovative Fellow Mento” in 2021 by Computing Research Association.

Yue Cheng received the Ph.D. degree in computer science from Virginia Tech, Blacksburg, VA, USA, in 2017.

He is currently an Assistant Professor of data science and computer science with the University of Virginia (UVA), Charlottesville, VA, USA. His research interests include distributed systems, cloud and serverless computing, and high-performance computing. His current research interests focuses on the systems support for cloud- and HPC-scale data-intensive computing, such as deep learning and data analytics. His research results have been published at major conferences, such as International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), International ACM Symposium on High-Performance Parallel and Distributed Computing (HPDC), EuroSys, USENIX Annual Technical Conference (ATC), ACM Symposium on Cloud Computing (SoCC), and IEEE International Conference on Data Mining (ICDM). He has developed a set of new techniques that make stateful serverless computing efficient, scalable, and easy to program. His work on serverless data analytics has been used by tech giants, including Alibaba, Sunnyvale, CA, USA, Microsoft, Redmond, WA, USA, and Adobe, San Jose, CA, USA.

Dr. Cheng was a recipient of the NSF CAREER Award, the Meta Research Award, the Amazon Research Award, and the IEEE CS Technical Community on High Performance Computing (TCHPC) Early Career Researchers Award for excellence in high-performance computing.

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