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

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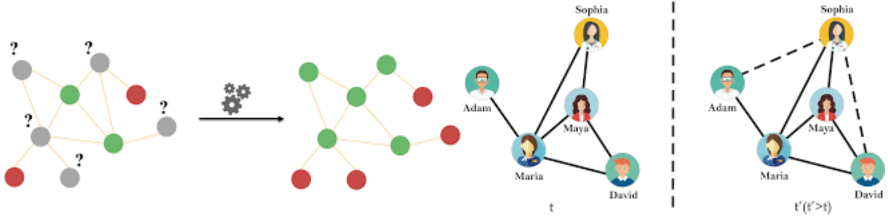
GNN Introduction

The Graph Neural Network (GNN) models achieve great performance on graph learning tasks such as node classification and link prediction. This is because they handle graph-structured data via aggregating neighbor information.



Node Classification

Link Prediction

Figure: Two applications of GNN models.

GA-MLP

Graph Augmented Multi-Layer Perceptron (GA-MLP) models have recently received fast increasing attention.

- GA-MLP models augment node representations of graphs and feed them into Multi-Layer Perceptron (MLP) models.
- GA-MLP models can be considered as an approximation of Graph Convolutional Network (GCN) models. For example, a two-layer GA-MLP approximates the performance of GCN models on multiple datasets [1].

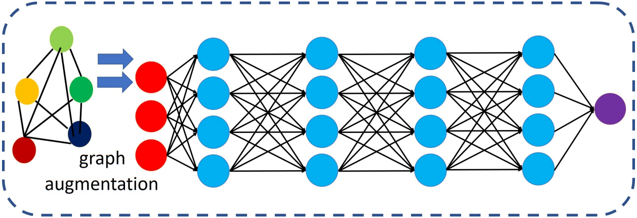


Figure: GA-MLP Models.

ADMM to Train Deep GA-MLP Models in Parallel

Because deeper GA-MLP models have more freedom of expressiveness than shallow ones, the goal of this talk is to devise a scalable training algorithm for training deep GA-MLP models in parallel.
While Stochastic Gradient Descent (SGD) is a state-of-the-art optimizer for deep learning models, we choose ADMM to achieve this goal because of its several advantages:

- The ADMM is a derivative-free algorithm, and can avoid the **gradient vanishing** issue of SGD (i.e. gradient signals vanish when they are transmitted to deep layers).
- The ADMM can address the **backward locking** problem of SGD, which means that the calculation of the gradient in one layer is dependent on its previous layers.

ADMM Introduction

The ADMM is a flexible framework to handle large-scale optimization problems, which splits a complex objective into multiple subproblems, each of which is easy to solve.

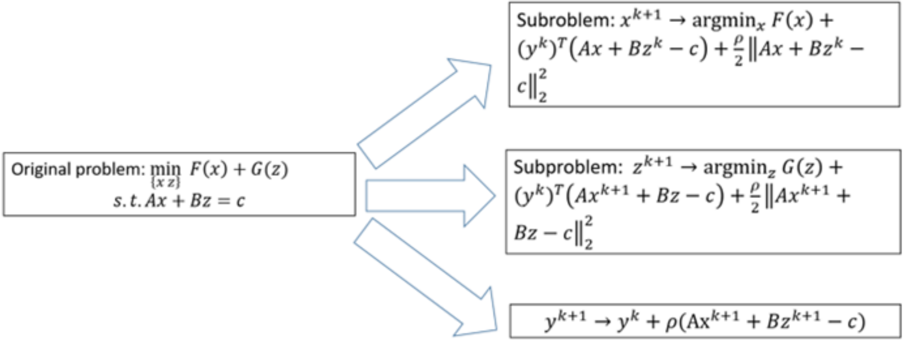


Figure: ADMM Framework.

GA-MLP Training Problem: Feature Augmentation

Consider a graph $G = (V, E)$, where V and E are sets of nodes and edges, respectively, let $\Psi = \{\psi_1(A), \cdots, \psi_K(A)\}$ be a set of (usually multi-hop) operators $\psi_i(A) : \mathbb{R}^{|V|} \rightarrow \mathbb{R}^{|V|} (i = 1, \cdots, K)$ that are functions of the adjacency matrix $A \in \mathbb{R}^{|V| \times |V|}$, where $\mathbb{R}^{|V|}$ is the domain. $X_k = H\psi_k(A)$ 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. Then the input is stacked into

$$X = [X_1; \cdots; X_K].$$

Ψ can be considered as a prepossessing step to augment node features via A, and hence it is predefined. One common choice can be $\Psi = \{I, A, A^2, \cdots, A^{K-1}\}$.

GA-MLP Training Problem: Problem Formulation

The GA-MLP training problem is formulated as follows:

Problem

$$\min_{W_l,b_l,z_l,p_l} R(z_L; y),$$

$$s.t.\ z_l = W_l p_l + b_l,\ \ p_{l+1} = f_l(z_l)(l = 1, \cdots, L-1),$$

Notations	Descriptions
L	Number of layers.
W_l	The weight for the l-th layer.
b_l	The bias for the l-th layer.
z_l	The auxiliary variable of the linear mapping for the l-th layer.
$f_l(z_l)$	The nonlinear activation function for the l-th layer.
p_l	The input for the l-th layer ($p_0 = X$).
q_l	The output for the l-th layer.
X	The node representation of the graph.
A	The adjacency matrix of the graph.
y	The predefined label vector.
$R(z_L, y)$	The risk function for the L-th layer.
n_l	The number of neurons for the l-th layer.

Table: Important Notations

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pdADMM-G: Overview

The proposed parallel graph deep learning Alternating Direction Method of Multipliers (pdADMM-G) splits a GA-MLP model into layerwise components, each of which can be trained via an independent client.

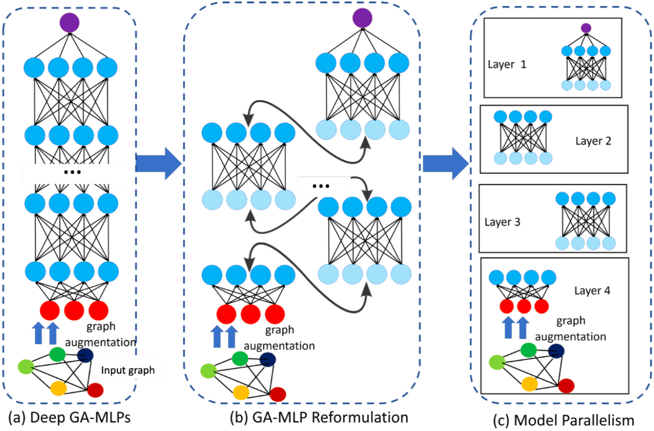

Figure: An Overview of the pdADMM-G.

pdADMM-G: Problem Relaxation

In order to address layer dependency, we relax GA-MLP training problem to the following:

Problem (Relaxed Problem)

$$\min_{\mathbf{p},\mathbf{W},\mathbf{b},\mathbf{z},\mathbf{q}} F(\mathbf{p},\mathbf{W},\mathbf{b},\mathbf{z},\mathbf{q}) = R(z_L; y)$$
$$+ (\nu/2)(\sum\nolimits_{l=1}^{L} \|z_l - W_l p_l - b_l\|_2^2 + \sum\nolimits_{l=1}^{L-1} \|q_l - f_l(z_l)\|_2^2),$$
$$s.t.\ p_{l+1} = q_l,$$

where $\mathbf{p} = \{p_l\}_{l=1}^{L}$, $\mathbf{W} = \{W_l\}_{l=1}^{L}$, $\mathbf{b} = \{b_l\}_{l=1}^{L}$, $\mathbf{z} = \{z_l\}_{l=1}^{L}$, $\mathbf{q} = \{q_l\}_{l=1}^{L-1}$, and $\nu > 0$ is a tuning parameter. 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.

pdADMM-G: The Augmented Lagrangian

The Augmented Lagrangian is formulated mathematically as follows:

$$
\begin{aligned}
&L_\rho(\mathbf{p}, \mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{q}, \mathbf{u}) \\
&= F(\mathbf{p}, \mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{q}) + \sum\nolimits_{l=1}^{L-1} (u_l^T (p_{l+1} - q_l) + (\rho/2)\|p_{l+1} - q_l\|_2^2) \\
&= R(z_L; y) + \phi(p_1, W_1, b_1, z_1) + \sum\nolimits_{l=2}^{L} \phi(p_l, W_l, b_l, z_l, q_{l-1}, u_{l-1}) \\
&+ (\nu/2) \sum\nolimits_{l=1}^{L-1} \|q_l - f_l(z_l)\|_2^2,
\end{aligned}
$$

where $\phi(p_1, W_1, b_1, z_1) = (\nu/2)\|z_1 - W_1 p_1 - b_1\|_2^2$,
$\phi(p_l, W_l, b_l, z_l, q_{l-1}, u_{l-1}) = (\nu/2)\|z_l - W_l p_l - b_l\|_2^2 + u_{l-1}^T (p_l - q_{l-1})$
$+(\rho/2)\|p_l - q_{l-1}\|_2^2 (l = 2, \cdots, L)$, $u_l (l = 1, \cdots, L-1)$ are dual variables,
$\rho > 0$ is a hyperparameter, and $\mathbf{u} = \{u_l\}_{l=1}^{L-1}$.

pdADMM-G: Pseudocode

Algorithm The pdADMM-G Algorithm

Require: y, $p_1 = X$, ρ, ν.
Ensure: $\mathbf{p}, \mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{q}$.

Initialize $k = 0$.
while $\mathbf{p}^k, \mathbf{W}^k, \mathbf{b}^k, \mathbf{z}^k, \mathbf{q}^k$ not converged **do**
  Update p_l^{k+1} of different l in parallel.
  Update W_l^{k+1} of different l in parallel.
  Update b_l^{k+1} of different l in parallel.
  Update z_l^{k+1} of different l in parallel.
  Update q_l^{k+1} of different l in parallel.
  $r_l^k \leftarrow p_{l+1}^{k+1} - q_l^{k+1} (l = 1, \cdots, L)$ in parallel # Compute residuals.
  Update u_l^{k+1} of different l in parallel.
  $k \leftarrow k + 1$.
end while
Output $\mathbf{p}, \mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{q}$.

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Motivation: Heavy Communication Overheads

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 surge for a large-scale graph G.

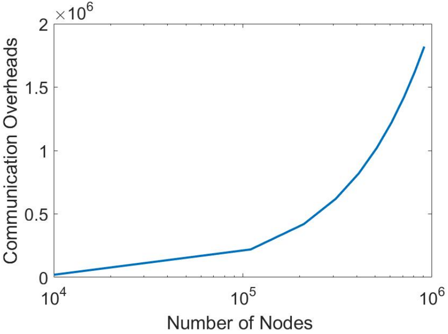

Figure: Heavy communication overheads for millions of nodes.

Solution: Quantization Technique

The quantization technique is commonly utilized to reduce communication overheads by mapping continuous values into a discrete set. To achieve this, p_l is required to fit into a countable set Δ, which is shown as follows:

Problem (Quantized GA-MLP Training Problem)

$$\min_{\mathbf{p},\mathbf{W},\mathbf{b},\mathbf{z},\mathbf{q}} F(\mathbf{p},\mathbf{W},\mathbf{b},\mathbf{z},\mathbf{q}) = R(z_L; y)$$
$$+ (\nu/2)(\sum\nolimits_{l=1}^{L} \|z_l - W_l p_l - b_l\|_2^2 + \sum\nolimits_{l=1}^{L-1} \|q_l - f_l(z_l)\|_2^2),$$
$$s.t.\ p_{l+1} = q_l,\ \ p_l \in \Delta = \{\delta_1, \cdots, \delta_m\},$$

where $\delta_i (i = 1, \cdots, m) \in \Delta$ are quantized values, which can be integers or low-precision values. $m = |\Delta|$ is the cardinality of Δ.

pdADMM-G-Q: Problem Transformation and Algorithm

To address this problem, we rewrite it into the following form:

$$\min_{\mathbf{p},\mathbf{W},\mathbf{b},\mathbf{z},\mathbf{q}} R(z_L; y) + \sum\nolimits_{l=2}^{L} \mathbb{I}(p_l)$$
$$+ (\nu/2)(\sum\nolimits_{l=1}^{L} \|z_l - W_l p_l - b_l\|_2^2 + \sum\nolimits_{l=1}^{L-1} \|q_l - f_l(z_l)\|_2^2),$$
$$s.t.\ p_{l+1} = q_l,$$

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 the pdADMM-G-Q is shown as follows:

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

where L_ρ is the augmented Lagrangian of the pdADMM-G algorithm. The pdADMM-G-Q algorithm follows the same routine of the pdADMM-G algorithm.

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Several Definitions

Definition (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 (Coercivity)

A function $h(x)$ is coerce over the feasible set $\mathscr{F}$ means that $h(x) \to \infty$ if $x \in \mathscr{F}$ and $\|x\| \to \infty$.

Definition (Quantized Stationary Point)

The p_l is a quantized stationary point of of the quantized GA-MLP training problem if there exists $\tau > 0$ such that

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

Convergence Assumptions

Convergence assumptions are so mild that common losses and activations satisfy our assumptions.

Assumption

$f_l(z_l)$ is Lipschitz continuous with coefficient $S > 0$ and $F(\mathbf{p}, \mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{q})$ is coercive.

Common loss functions such as the cross-entropy loss and the least square loss satisfy it.

Assumption

$\partial f_l(z_l)$ is bounded, i.e. there exists $M > 0$ such that $\|\partial f_l(z_l)\| \leq M$.

Common activations such as ReLU, leaky ReLU, sigmoid and tanh satisfy it.

Convergence Properties

Theorem (Convergence of the pdADMM-G algorithm)

If $\rho > \max(4\nu S^2, (\sqrt{17}+1)\nu/2)$*, then for the variables* $(\mathbf{p}, \mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{q}, \mathbf{u})$*, starting from any* $(\mathbf{p}^0, \mathbf{W}^0, \mathbf{b}^0, \mathbf{z}^0, \mathbf{q}^0, \mathbf{u}^0)$*,* $(\mathbf{p}^k, \mathbf{W}^k, \mathbf{b}^k, \mathbf{z}^k, \mathbf{q}^k, \mathbf{u}^k)$ *has at least a limit point* $(\mathbf{p}^*, \mathbf{W}^*, \mathbf{b}^*, \mathbf{z}^*, \mathbf{q}^*, \mathbf{u}^*)$*, and any limit point is a stationary point. That is,* $0 \in \partial L_\rho(\mathbf{p}^*, \mathbf{W}^*, \mathbf{b}^*, \mathbf{z}^*, \mathbf{q}^*, \mathbf{u}^*)$*.*

Theorem (Convergence of the pdADMM-G-Q algorithm)

If $\rho > \max(4\nu S^2, (\sqrt{17}+1)\nu/2)$*, then for the variables* $(\mathbf{p}, \mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{q}, \mathbf{u})$*, starting from any* $(\mathbf{p}^0, \mathbf{W}^0, \mathbf{b}^0, \mathbf{z}^0, \mathbf{q}^0, \mathbf{u}^0)$*,* $(\mathbf{p}^k, \mathbf{W}^k, \mathbf{b}^k, \mathbf{z}^k, \mathbf{q}^k, \mathbf{u}^k)$ *has at least a limit point* $(\mathbf{p}^*, \mathbf{W}^*, \mathbf{b}^*, \mathbf{z}^*, \mathbf{q}^*, \mathbf{u}^*)$*, and any limit point* $(\mathbf{W}^*, \mathbf{b}^*, \mathbf{z}^*, \mathbf{q}^*, \mathbf{u}^*)$ *is a stationary point. Moreover, if* τ_l^{k+1} *is bounded, then* $\mathbf{p}^*$ *is a quantized stationary point. where* τ_l^* *is a limit point of* τ_l^k*.*

The convergence rates of the proposed pdADMM-G and pdADMM-G-Q are $o(1/k)$, where k is the number of iterations.

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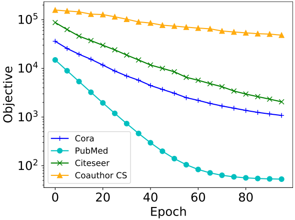
Datasets

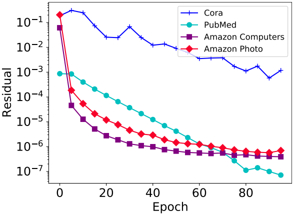
Dataset	Node#	Training Sample#	Test Sample#	Class#	Feature#
Cora	2708	140	1000	7	1433
PubMed	19717	60	1000	3	500
Citeseer	3327	120	1000	6	3703
Amazon Computers	13752	200	1000	10	767
Amazon Photo	7650	160	1000	8	745
Coauthor CS	18333	300	1000	15	6805

Table: Six benchmark datasets

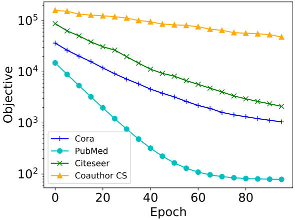
Convergence



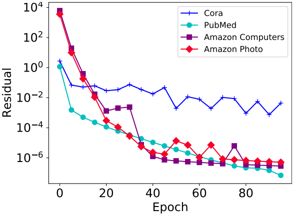
(a). pdADMM-G Objective.



(b). pdADMM-G Residual.



(c). pdADMM-G-Q Objective.



(d). pdADMM-G-Q Residual.

Figure: Convergence curves of the pdADMM-G and the pdADMM-G-Q on four datasets: they both converge.

Speedup

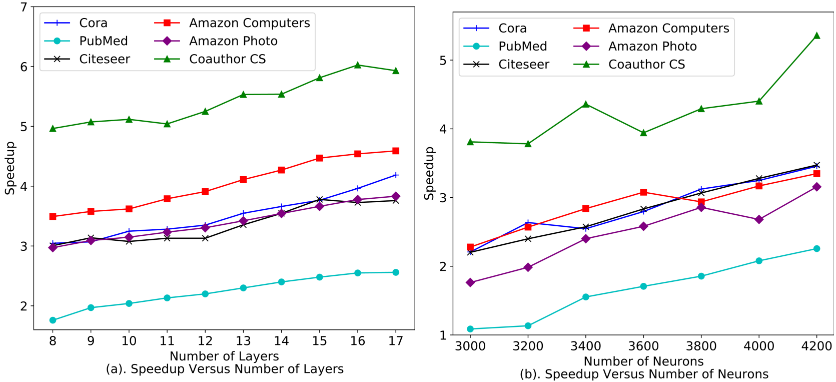
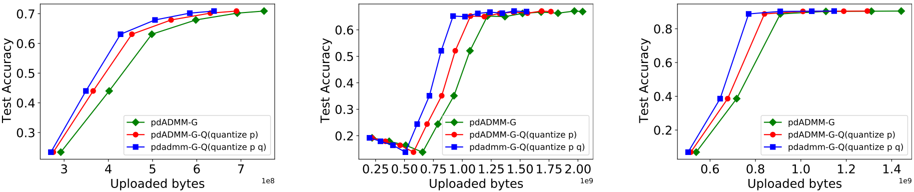


Figure: The relationships between speedup and: (a) the number of layers; (b) the number of neurons in six datasets: the speedup increases linearly with the number of layers and the number of neurons.

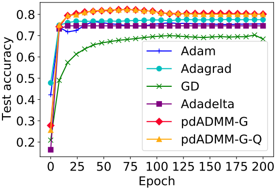
Communication Overheads



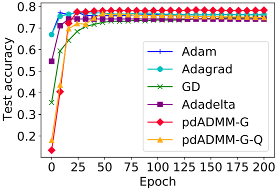
(a). Citeseer (b). Amazon Computers (c). Coauthor CS

Figure: Communication overheads of the pdADMM-G algorithm and the pdADMM-G-Q algorithm in three datasets: the application of the quantization technique on **p** and **q** reduces the communication overheads by 25% without loss of performance.

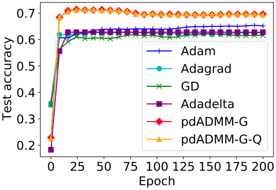
Performance



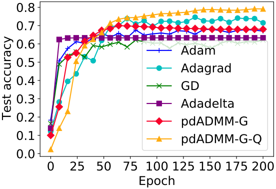
(a). Cora



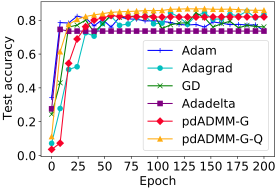
(b). PubMed



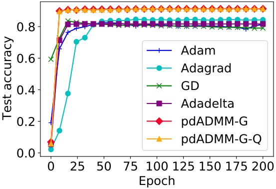
(c). Citeseer



(d). Amazon Computers



(e). Amazon Photo



(f). Coauthor CS

Figure: Test accuracy of all methods: the pdADMM-G algorithm and the pdADMM-G-Q algorithm outperform other comparison methods in six datasets.

Summary

- We propose a novel pdADMM-G framework to train a GA-MLP model in parallel. The extended pdADMM-G-Q algorithm reduces communication costs using the quantization technique.
- The proposed pdADMM-G algorithm and the pdADMM-G-Q algorithm theoretically converge to a stationary point of GA-MLP models with sublinear convergence rates $o(1/k)$.
- Extensive experiments have been conducted to show the convergence, outstanding performance, and the massive speedup of the proposed pdADMM-G algorithm and the pdADMM-G-Q algorithm.

Code Release

pdADMM-G: `https://github.com/xianggebenben/pdADMM-G`

Thank you for your attention!

Reference

F. Wu, A. Souza, T. Zhang, C. Fifty, T. Yu, and K. Weinberger, "Simplifying graph convolutional networks," in *International conference on machine learning*. PMLR, 2019, pp. 6861–6871.