Triple Sparsification of Graph Convolutional Networks without Sacrificing the Accuracy

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ABSTRACT

Graph Neural Networks (GNNs) are widely used to perform different machine learning tasks on graphs. As the size of the graphs grows, and the GNNs get deeper, training and inference time become costly in addition to the memory requirement. Thus, without sacrificing accuracy, graph sparsification, or model compression becomes a viable approach for graph learning tasks. A few existing techniques only study the sparsification of graphs and GNN models. In this paper, we develop a SparseGCN pipeline to study all possible sparsification in GNN. We provide a theoretical analysis and empirically show that it can add up to 11.6% additional sparsity to the embedding matrix without sacrificing the accuracy of the commonly used benchmark graph datasets.

KEYWORDS

graph convolutional networks, classification, sparsification

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1 INTRODUCTION

In recent years, Graph Neural Networks (GNNs) have become popular for various learning tasks [1, 2] such as node classification [3] and link prediction [4]. Popular message-passing-based GNNs such as Graph Convolutional Network (GCN) [3] and GraphSAGE [5] learn the representation of a node by aggregating information from its neighbors. Dominant computations in such a GNN depend on the input graph, the hidden layer representation of nodes (embeddings), and weight matrices. Consequently, the computational complexity of GNN training and inference depends completely on the number of non-zero entries in these matrices. As graphs become bigger and GNNs become deeper, GNNs are increasingly demanding more computational resources. This paper aims to address this challenge by exploiting sparsity in all aspects of GNNs.

It is well known that GCN training and inference are computationally intensive for large-scale graphs. For example, You et al. [6] explained that a 2-layer GCN model with 32-dimensional embeddings in hidden layers may require 19 GFLOPs (FLOPs: floating point operations) on the Reddit graph with about 232K nodes and and 114M edges. In comparison, the popular ResNET50 model [7] requires 8 GFLOPs for a pass over ImageNet [8, 9]. Furthermore, the actual performance of GCN is significantly worse in practice because GCN requires sparse matrix multiplications that do not attain the peak performance of processors and GPUs [10]. As a result, it is extremely difficult to train a GCN with a graph with billions of nodes even with hundreds of GPUs.

A viable solution to GCN’s enormous computation demand is to sparsify input graphs, intermediate representations, and model parameters. Several prior work [6, 11, 12] have already showed that limited sparsification of the input graph and/or model weight does not reduce the accuracy of GCNs. Following on the footsteps of these pioneering work, we demonstrate that all aspects of data, features, embedding, and GCN weight matrices can be sparsified without sacrificing the performance of GCNs.

In each layer of a GCN (and most other GNNs), the hidden representation or embedding in a layer is determined by two matrix multiplications involving the adjacency matrix, the embedding matrix of the previous layer (input features being the starting embedding), and the weight matrix [3]. While the adjacency matrix almost always comes in sparse formats, the other matrices are usually dense in most GNNs. Given the involvement of three matrices in the computation of each layer, there are opportunities to sparsify all three matrices to bring down the computational requirements. However, all previous work on sparse GNNs considered sparsifying the input graph and/or model weights [6, 11, 12]. No previous work considered sparsifying the embedding matrices even though they often contain more non-zero elements than the adjacency and weight matrices. Thus, the sparsification of the embedding matrix is expected to bring down the computational requirement of GNNs significantly. In this paper, we consider sparsifying all three matrices involved in a GNN layer. We theoretically demonstrate that embedding sparsification accompanied by graph and weight sparsifications reduces the number of Multiply-Accumulate (MAC) operations needed to train a GNN model. The reduced computational requirement could be achieved without sacrificing the test accuracy. As with previous work, we demonstrate the impact of sparsity by counting the number of MAC operations needed for GNN training and inference. Our goal is not to show the actual reduction of runtime that depends on the implementation of sparse matrix multiplications and hardware platforms [10].

The main contributions of this paper are summarized below.

We study the impact of complete sparsification of all matrices (the input graphs, network weight matrices, and hidden layer representations) in the GCN model.
We use several sparsification techniques including Top-\(k\), Sorting, and Sensitivity-based methods. We derive theoretical bounds on the reduction of MAC operations for different induced sparsity.

Our experimental results show that SparseGCN can attain a higher percentage of overall sparsity than the existing methods without sacrificing the baseline accuracy.

2 BACKGROUND

2.1 Notations

Let \(G(V, E)\) be a directed graph, where \(V = \{v_1, \ldots, v_n\}\) is the set of vertices and \(E = \{e_1, \ldots, e_m\}\) is the set of edges such that \(|V| = n\) and \(|E| = m\). Let \(X \in \mathbb{R}^{n \times d}\) store \(d\)-dimensional input features of \(n\) vertices. A denotes the adjacency matrix of \(G\) where \(A_{ij} = 1\) if \((v_i, v_j) \in E\), otherwise \(A_{ij} = 0\). The core computation at the \(l\)-th layer of GCN [3] is:

\[
H^l = \sigma(\hat{A}H^{l-1}W^{l-1})
\]

where, \(W\) is the neural network weight matrix, \(\sigma\) is the activation function and \(H\) is the hidden representation of corresponding convolutional layer such that \(H^0 = X\). In Eqn. 1, \(\hat{A}\) is the renormalized graph Laplacian matrix such that \(\hat{A} = \hat{D}^{-\frac{1}{2}} \hat{A} \hat{D}^{-\frac{1}{2}}\), \(\hat{A} = I + A\), where \(I\) is the identity matrix, and \(\hat{D}_{ii} = \sum_j \hat{A}_{ij}\). We optimize the GCN model using the negative log-likelihood loss function.

2.2 Related Work

Graph Neural Networks. Over the last decade, hundreds of GNN methods, libraries, and software have been developed for semi-supervised, unsupervised, and self-supervised learning on graphs [1, 13–18]. Their success in graph learning tasks and their limitations such as over-smoothing and neighborhood explosion problems are also well-documented in the literature [19–21]. Here, our focus is the computational challenges arising in GNN training due to the size of different matrices in Eqn. 1.

Table 1: Papers discussing pruning strategy of a GNN.

| Paper(s)          | Prune A? | Prune W? | Prune H? |
|-------------------|----------|----------|----------|
| SGCN [12], FastGCN [22] | ✔        | ✗        | ✗        |
| ULTH [11], GEBT [6] | ✔ ✔      | ✔        | ✗        |
| SparseGCN (Ours)  | ✔ ✔ ✔    | ✔ ✔ ✔    | ✔ ✔ ✔    |

Sparsifications in GNNs. In GNNs, three matrices are involved (see Eqn. 1) that can be sparsified jointly or separately. In the literature, the sparsification of GNNs has been tackled by researchers considering two directions: (i) input graph or adjacency matrix sparsification, and (ii) model weight sparsification. The former has been studied much in the GNN literature [22, 23]; however, the latter has not been explored that much. There are a handful of studies in the literature that discuss such sparsifications of graphs [12, 24]. We observe a few studies in the literature for GNN model compression. The quantization or binarization technique can compress the GNN model too [25–27]. In recent years, Unified lottery Ticket Hypothesis (ULTH) [11] and early-bird ticket [6] are the two noticeable works for both graph and model weight sparsifications in GNNs. However, the embedding matrix sparsification has not been explored previously except random dropout for regularization. We summarize the pruning or sparsification related papers of GNN in Table 1. In this paper, we study the fully sparse GCN by analyzing the sensitivity of different sparse matrices in Eqn. 1.

3 METHODS

We use GCN as a representative model to induce triple sparsity in three different matrices and call this approach SparseGCN.

3.1 Algorithmic Workflow

Our training strategy, after adding sparsity to the model, is similar to most of the methods in the literature [11, 12]. We followed the protocol used in the unified lottery ticket hypothesis paper [11]. We assume that \(m^l_w\) and \(m^l_h\) are two differential binary masks of weights and embedding matrices, respectively, on the \(l\)-th layer.

Graph Sparsification. To add sparsity to the graph or adjacency matrix, we remove a subset of edges from the graph. In Fig. 1(a), we show the removed edges by dotted lines. Since the sparsified graph is used in all layers, we do not create additional masks for different layers. In this step, we remove a% edges from the weighted adjacency matrix \(A\) using a chosen sparsification technique.

Embedding Sparsification. Unlike previous work, we also sparsify the embedding matrix shown in the schematic diagram 1(b). To sparsify it, we select h% non-zero entries and set them to 0. We perform this sparsification step with a Boolean mask \(m^l_h\) and then masking entries from the embedding matrix using \(m^l_h \odot \hat{H}^l\).

Weight Sparsification. Similar to previous studies [6, 11], we also sparsify model weights of GCN in different layers as shown in Fig. 1(c). We mask out a fraction of non-zero entries from the weight matrix using the operation \(m^l_w \odot \hat{W}^l\).

In the workflow, as shown in Fig. 1(d), we train the GCN model for the input graph with associated node features to obtain the baseline accuracy for the node classification problem. After that, we sparsify the graph, embedding matrix, and weight matrix using a sparsification technique described in Section 3.2. Then, we retrain the model with sparsified matrices and compare the accuracy level. If it is similar to the baseline accuracy, we sparsify the sparse matrices again and re-train the model. We continue this process until the accuracy level drops compared to the baseline. Finally, we report the highest sparsity level for which the sparsed model can retain the baseline accuracy.

3.2 Sparsification Techniques

For our experiments analyses, we used three pruning strategies: (i) Random-a naive and straightforward approach for the sparsification of any matrices in Eqn. 1. We pick \(p\%\) entries from the non-zero elements of the matrices and mask them out by assigning zero to them. (ii) Sorting-based-a global sparsification technique where we sort all the non-zero entries of the matrices based on the absolute values. Then, we pick the smaller \(p\%\) entries and mask them out by assigning zero. The rationale for this technique is that we can remove more insignificant entries globally which will have less computational effect. (iii) Top-\(k\)-a local sparsification technique where each row of the matrix is sorted based on the absolute value of the non-zero entries. Then, we select the smaller \(k\) entries...
from each row and mask them out by assigning zero. The intuition behind this approach is that the absolute smaller non-zero entries contribute less to the matrix multiplication.

3.3 Theoretical Analysis

We focus on the computation in the $l$-th layer of a GNN, but the obtained bounds are extendable to other layers. We assume that the graph is stored in the compressed sparse row (CSR) format so that the memory requirement is $O(m)$, and the number of Floating-point Operations (FLOPs) in sparse-dense matrix multiplication meets its lower bound [28]. Suppose, the dimensions of $\mathbf{H}^l$, and $\mathbf{W}^l$ matrices in the $l$-th convolutional layer of GCN are $n \times d$, and $d \times f$, respectively. Then, we can deduce the following bounds.

**Lemma 3.1.** The total number of MAC operations on the $l$-th layer is $(f m + d f n - f n)$, where $d > f$.

**Proof.** For $d > f$, the right ordered multiplications (i.e., $\hat{\mathbf{A}} (\mathbf{H}^l \mathbf{W}^l)$) in Eqn. 1 would cost less computations than the left ordered (i.e., $(\hat{\mathbf{A}} \mathbf{H}^l) \mathbf{W}^l$). The total number of FLOPs for $T = \mathbf{H}^l \mathbf{W}^l$ are $2 d f n - f n$, where $T \in \mathbb{R}^{n \times f}$ is a temporary matrix. The number of FLOPs for $\hat{\mathbf{A}} \mathbf{T}$ are $f m + f (m - n)$, or $2 f m - f n$. Plugging $\text{MACs} = \frac{\text{FLOPs}}{2}$ (same as ULTH for GCN [11]), the total number of MAC operations on $l$-th layer are $\frac{2 d f n - f n + 2 f m - f n}{2}$, or $(f m + d f n - f n)$. □

**Lemma 3.2.** If we introduce $a\%$, $h\%$, and $w\%$ sparsity to $\hat{\mathbf{A}}$, $\mathbf{H}^l$, and $\mathbf{W}^l$, respectively, then the total MAC operations are bounded by $(1 - w)(1 - w')f m + d f n - f n$, where $d > f$ and $a \approx h = h'$.

**Proof.** For simplicity of the computations, we distribute the percentage of sparsity across matrix dimensions. Then, an $a\%$ sparsity of graph would leave $(1 - a)m$ non-zero elements in $\hat{\mathbf{A}}$, an $h\%$ sparsity of embedding would leave $n \times (1 - h)d$ non-zero elements in $\mathbf{H}$, and a $w\%$ sparsity of weight matrix would leave $(1 - h)d \times (1 - w)f$ non-zero elements in $\mathbf{W}$. The right to left order multiplication would cost $(1 - h)(1 - w)d f n + (1 - w)(d - dh - 1)f n$ FLOPs for $T = \hat{\mathbf{A}} \mathbf{H}^l \mathbf{W}^l$, where $T \in \mathbb{R}^{n \times (1 - w)f}$ is a temporary matrix. Similarly, the number of FLOPs for $\hat{\mathbf{A}} \mathbf{T}$ are $(1 - a)(1 - w)f m + (1 - a)(1 - w)(m - n)f$.

Then, the total number of FLOPs on the $l$-th layer are as follows:

\begin{align*}
&= 2(1 - h)(1 - w)f n - (1 - w)f n + 2(1 - a)(1 - w)f m - (1 - a)(1 - w)f n \\
&= 2(1 - h)(1 - w)f n - 2(1 - a)(1 - w)f m - 2(1 - a)(1 - w)f n \\
&= 2(1 - w)(1 - h')(f m + d f n - f n)
\end{align*}

From the above computational bound, we can derive that the MACs on the $l$-th layer are bounded by $(1 - w)(1 - h')(f m + d f n - f n)$. □

**Theorem 3.3.** For $a\%$, $h\%$, and $w\%$ sparsity to $\hat{\mathbf{A}}$, $\mathbf{H}^l$, and $\mathbf{W}^l$ matrices, the total reduction factor of MAC operations in GCN is bounded by $\frac{1}{(1 - w)(1 - h')}$, where $a \approx h = h'$.

**Proof.** We can infer it by taking the ratio of the result of Lemma 3.1 to Lemma 3.2 that the reduction is bounded by $\frac{1}{(1 - w)(1 - h')}$.

**Complexity.** From Lemma 3.2, we can deduce that the asymptotic time complexity of the sparse training procedure for a $L$-layered GCN would be $O((1 - w)(1 - h')(m + f n)L)$, where $f = d$, and $|E| = m$. Similarly, the asymptotic memory complexity would be $O(L f ((1 - h'n + (1 - w)f) + (1 - h'm))$.

4 EXPERIMENTS

4.1 Experimental Setup

**Overview.** The goal of our experiments is to explore the sparsity of different matrices in Eqn. 1 without sacrificing the baseline accuracy. We primarily aim to address the following two key Research Questions (RQs): RQ1: How does the performance of node classification vary with individual sparsity techniques? RQ2: What would be the achievable combined sparsity for benchmark graphs?

| Graphs | Nodes | Edges | Classes | Features | Avg. Deg. |
|--------|-------|-------|---------|----------|-----------|
| Cora   | 2,708 | 10,556| 7       | 1,433    | 3.89      |
| Citeseer| 3,327 | 9,104 | 6       | 3,703    | 2.74      |
| Pubmed | 19,717| 88,648| 3       | 500      | 4.5       |

Table 2: Summary of the Graph Datasets.
4.2 Results and Analysis

Individual Sparsity Analysis. We report the sparsity of different graphs in Fig. 2. Here, we show the test accuracy for three different sparsification techniques, namely, (i) Random, (ii) Top-$k$, and (iii) Sorting-based. The x-axis shows different percentages of sparsity.

Observation 4.2.1. The Top-$k$ approach can retain the baseline accuracy with a higher percentage of sparsity in the embedding matrix.

In the sparsity results of embedding matrix (see Fig. 2, left column), we observe that the Top-$k$ method can retain the baseline accuracy level with a higher percentage of sparsity compared to the random and sorting-based techniques. The Top-$k$ approach is a local sparsification technique that prunes the same number of entries from each row of the embedding matrix based on the absolute value. The impact of the Top-$k$ pruning is similar to reducing the hidden dimension (assuming $k < d$ and $k < f$).

Observation 4.2.2. The Sorting-based approach can retain the baseline accuracy with a higher percentage of sparsity in the weight matrix and adjacency matrix than the other sparsification techniques.

In the experiments of neural network weight sparsity (see Fig. 2, middle column), we add the same percentage of sparsity to both layers of the GCN. We observe that it is similar to previous studies, which suggests that the sorting-based method can retain the baseline accuracy better than others with a higher percentage of sparsity [11]. Notice that the Top-$k$ method can be competitive to the Sorting-based method. The average degree of Cora and Citeseer is comparatively low i.e., they are already very sparse. Making these graphs sparser may disconnect some vertices, which prevents information propagation from neighbors. Thus, even with a small percentage of sparsity in Cora and Citeseer, test accuracy tends to drop. On the other hand, the Pubmed graph is comparatively bigger. Thus, pruning some edges does not affect the test accuracy significantly. For example, the Sorting-based approach can retain the baseline accuracy with up to 40% graph sparsity, whereas test accuracy drops above 20% graph sparsity for Cora and Citeseer.

Comparison with Unified Lotter Ticket Hypothesis. We compare our results with ULTH [11] which is a state-of-the-art approach to introduce sparsity to the adjacency matrix and model weights in GNNs. To introduce sparsity using SparseGCN, we use the Top-$k$ approach for the embedding matrix, $\hat{A}$ (Observation 4.2.1) and the Sorting-based approach for other matrices. We run both ULTH and SparseGCN for 64-dimensional embedding and report the results in Table 3. We use a grid search technique to find the highest possible sparsity in different matrices retaining a similar level of test accuracy compared to the baseline. We observe that both ULTH and SparseGCN attain a similar level of test accuracy with similar percentages of sparsity in $\hat{A}$ and $W$; however,
SparseGCN introduces additional sparsity to the embedding matrix. More specifically, SparseGCN can introduce 8.4% to 11.5% more sparsity to the embedding matrix for these datasets retaining a similar level of test accuracy. For the Pubmed graph, the level of sparsity, as well as test accuracy, outperform ULTH. These empirical results show that a sparsity can be introduced to all matrices of GCN for optimal resource utilization.

Table 3: Comparison of combined sparsity and test accuracy between ULTH and SparseGCN. The sparsity in each row of columns Â, W, and H, are used combined.

| Graphs | Methods     | A   | W   | H   | Accuracy |
|--------|-------------|-----|-----|-----|----------|
| Cora   | ULTH [11]   | 14.8%| 59.1%| 0.0%| 80.0%    |
|        | SparseGCN   | 14.5%| 61.0%| 8.4%| 80.0%    |
| Citeese | ULTH [11]   | 19.0%| 70.1%| 0.0%| 71.5%    |
|        | SparseGCN   | 19.1%| 70.8%| 9.8%| 71.4%    |
| Pubmed | ULTH [11]   | 20.6%| 70.0%| 0.0%| 77.8%    |
|        | SparseGCN   | 23.0%| 75.0%|11.5%| 80.0%    |

5 CONCLUSIONS

In this paper, we study the sparsification of the embedding matrix of any GNN for the first time. We also explore one new sparsification technique, namely, the Top-k approach. Using the SparseGCN pipeline, we explore the viability of full sparsification of GCN. We demonstrate that sparsifying all matrices simultaneously reduces the computational cost more than prior methods that sparsified a subset of matrices. Our theoretical analysis shows that a fully sparse GNN could attain similar baseline performance with fewer computations (additional sparsity reduces MACs in Theorem 3.3). In the existing GNN models of popular graph learning frameworks, the sparse gradient computation is not explicitly supported. Thus, we aim to implement a fully sparse framework for GNN with efficient sparse-sparse-matrix multiplication (SpGEMM) [31, 32].

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