SERVING GRAPH COMPRESSION FOR GRAPH NEURAL NETWORKS

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ABSTRACT

Serving a GNN model online is challenging — in many applications when testing nodes are connected to training nodes, one has to propagate information from training nodes to testing nodes to achieve the best performance, and storing the whole training set (including training graph and node features) during inference stage is prohibitive for large-scale problems. In this paper, we study graph compression to reduce the storage requirement for GNN in serving. Given a GNN model to be served, we propose to construct a compressed graph with a smaller number of nodes. In serving time, one just needs to replace the original training set graph by this compressed graph, without the need of changing the actual GNN model and the forward pass. We carefully analyze the error in the forward pass and derive simple ways to construct the compressed graph to minimize the approximation error. Experimental results on semi-supervised node classification demonstrate that the proposed method can significantly reduce the serving space requirement for GNN inference.

1 INTRODUCTION

Graph Neural Networks (GNNs) (Kipf & Welling, 2016) have been widely used for graph-based applications, such as node property predictions (Kipf & Welling, 2016), link predictions (Zhang & Chen, 2018), and recommendation (Wu et al., 2020). Given a graph that encodes relationships between pairs of entities, the graph convolution operation in GNN iteratively refines entity representations by aggregating features from neighbors, which enables information to propagate through the graph and boosts the performance on uncertain nodes.

It has been well recognized that GNN training on large-scale input graphs is challenging, and many scalable training methods have been proposed (Hamilton et al., 2017; Chiang et al., 2019; Chen et al., 2018a; Zeng et al., 2019). However, the problem of how to efficiently **serve** a GNN model in online applications remain unsolved. In fact, for applications when testing nodes are connected with the training nodes, such as semi-supervised node classification, serving a GNN is very challenging and has hindered the deployment of GNN in real world. To conduct predictions on a batch of incoming testing nodes, GNN has to propagate information not only within the testing nodes but also from training nodes to testing nodes, which implies that the serving system needs to store graph and node features in memory. Unfortunately, it is almost impossible to store the training graph and node features in many real systems such as embedded and low-resource devices. For example, for the Reddit dataset with more than 150k training nodes, it needs 370.7MB storage for the training node features, 86.0MB for the graph, and only 7.6MB for the GNN model itself. In Table 1, we break down the serving space requirements for three public datasets (with statistics in the experiment section) with GNN model size, training graph space, and training node features size. From this table, we can see that the space bottleneck is on the training graph and node features. We define the problem of reducing the size of training graph and node features as **serving graph compression** for GNNs.

Unfortunately, naively discarding all or a large portion of training nodes will significantly hurt the inference performance, since GNN has extracted very powerful node representations of training nodes, and propagating those information to testing nodes is crucial for prediction. Figure 1 illustrates this problem, where we show that when discarding some part of training data, the performance of GNN will significantly reduce even on a standard node classification task.

Table 1: Model serving space

Datasets	Model size	Training graph size	Training feature size	Total serving size
Arxiv	1.4MB	5.9MB	46.5MB	53.8MB
Reddit	7.6MB	86.0MB	370.7MB	464.3MB
Product	4.8MB	87.2MB	78.6MB	170.6MB
Amazon2M	3.0MB	485.4MB	684.0MB	1.17GB

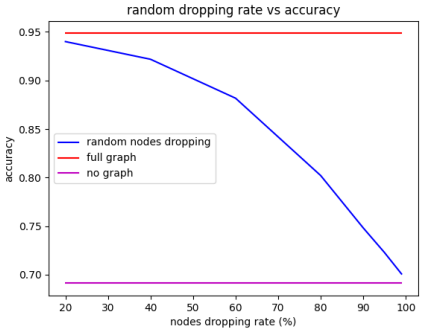


Figure 1: Random nodes dropping rate vs. accuracy on Reddit dataset. The red line is the accuracy of inference using the entire graph and features; purple line is the accuracy of inference without graph; blue line is accuracy for randomly dropping nodes in the graph with different dropping rate.

Although the problem of serving graph compression has not been formally studied before, at the first glance the problem seems to be solvable by adopting existing approaches. The first approach one can easily come up with is to treat training node features as a weight matrix and apply existing model compression techniques such as sparse or low-rank approximation (Han et al., 2015; Frankle & Carbin, 2018; Sainath et al., 2013; Chen et al., 2018b). However, existing model compression methods are not able to exploit graph information, and we will show in the experiments that they tend to perform poorly for serving graph compression. Another straightforward idea is to treat the problem as a core-set selection problem, where many algorithms have been developed to select a subset of important samples from massive data (Mirzasoleiman et al., 2020; Wang et al., 2018; Zhao et al., 2020). However, core-set selection methods are trying to obtain a small subset such that the model trained on the subset still achieves reasonable performance, and this goal is different from serving compression. For example, Jin et al. (2021) showed it's possible to extract a small synthesized graph for training, but they still require the whole training set in the inference phase to achieve good performance.

In this paper, we propose a simple and effective method for GNN serving graph compression via a virtual nodes graph (VNG). Given a GNN model to be served online, our method aims to construct a small set of **virtual nodes**, with artificially designed node features and adjacency matrix, to replace the original training graph. Without changing the model and the forward pass, users can just replace the original training set by the small representative set in the serving time to reduce the space requirement with small loss in testing accuracy. To construct the set of virtual nodes, we decompose the error of forward propagation into (1) the propagation error from training node features to testing nodes and (2) the propagation error from training to training nodes. Interestingly, the error in (1) can be bounded by a weighted kmeans objective, while the error in (2) can be minimized by solving a low-rank least-square problem to preserve consistency within a certain space constraint. These together lead to simple yet effective GNN serving graph compression that is easy to use in practice.

Our work makes the following contributions:

- To the best of our knowledge, this is the first work on the serving graph compression problem for GNN models, addressing the bottleneck when applying GNN in real world applications.
- By analyzing the error in forward propagation, we design a simple yet effective algorithm to construct a small virtual node set to replace the original huge training set for model serving.
- We show on multiple datasets that the proposed method significantly outperforms alternative ways of compressing the serving graph.

2 Related Work

Graph Neural Networks In this paper, we focus on GNN problems when there is a graph connecting entities of training and testing instances, including many important applications such as node classification, edge classification and recommendation systems. Note that there's another application of GNNs where each instance is a graph and we aim to predict properties of a new instance (graph), such as for molecular property prediction (Gilmer et al., 2017; Wu et al., 2018). Since in those

applications training and testing graphs (instances) are disjoint and there is no need to store training graphs for serving, they are out of the scope of this paper.

Many improvements have been made on GNNs in recent years. Based on the graph convolution operation, many different designs of graph neural networks have been proposed to achieve better performance (Veličković et al., 2017; Shi et al., 2020; Li et al., 2021; Chen et al., 2020; Xie et al., 2020). Also, although training GNNs with large networks is difficult, many scalable training algorithms have been developed (Hamilton et al., 2017; Chen et al., 2018a; 2017; Chiang et al., 2019; Zeng et al., 2019). In contrast to previous works, we study the inference phase of GNN which has been overlooked in the literature. In the serving phase of GNN, it requires storing both GNN model weights and training data (including node features and training graph) to achieve the best performance, since connections from training to testing nodes are crucial for feature propagation. Since the size of training data is often more than 40x larger than GNN model weights, we focus on shrinking the size of training data in this paper. Existing works on compressing GNNs focus on reducing or quantizing the model weights (Tailor et al., 2020; Yang et al., 2020; Kim et al., 2021), which is orthogonal to our work. Another recent work (Chen et al., 2021) tried to prune both model weights and graph by removing some edges. However, they do not reduce the size of training features so the serving space requirement will not be significantly reduced.

Model compression Since the training feature matrix dominates the serving space, a straightforward method is to apply existing model compression techniques, such as pruning or low-rank approximation (Han et al., 2015; Frankle & Carbin, 2018; Sainath et al., 2013; Chen et al., 2018b), to the training feature matrix. However, we find those methods are not very effective in practice (see our experiments). This is because that standard compression methods to not consider feature matrix and graph jointly, and they do not really focus on reducing the forward pass error in GNN inference. Another commonly used compression method is quantization (Gholami et al., 2021). However, quantization is orthogonal to our method since we can also apply quantization after getting the virtual representative nodes with our method.

Coreset selection Since the bottleneck of GNN serving space is training data, it may seen natural to apply coreset selection methods here. However, most of the coreset selection methods such as k-means and k-median clustering (Har-Peled & Mazumdar, 2004), mixture models (Lucic et al., 2017), low-rank approximation (Cohen et al., 2017), and gradient matching methods (Mirzasoleiman et al., 2020) do not utilize the graph information. Furthermore, these methods are designed to select a coreset for efficient training, while our goal is to select a coreset to compress the serving space requirement. We will compare with some standard coreset selection methods in the experiments to demonstrate that they are not effective for our task. Further, although several recent works try to select coresets for graph data (Jin et al., 2021; Zhang et al., 2021), they still focus on selecting a coreset for training while utilizing the full training set in the inference phase.

Graph Coarsening Graph coarsening is widely used in the scalable graph clustering, with the aim to reduce the size of the graph or form some supernodes in the graph to represent the original graph (Liu et al., 2018; Chevalier & Safro, 2009). Most of them are trying to preserve some unsupervised properties of the graph, such as adjacency matrix or normalized Laplacian (Spielman & Teng, 2011; Bravo Hermsdorff & Gunderson, 2019). Graph coarsening method do not consider either model or the node features, and thus are not as effective for our task.

3 Proposed Method

3.1 Problem Definition

For simplicity, we will consider the canonical graph convolutional network (GCN) model (Kipf & Welling, 2016), but our method can also handle other GNN architectures. In the training phase, we are given the training graph $G = (\mathcal{V}, \mathcal{E})$ with $n = |\mathcal{V}|$ vertices and $|\mathcal{E}|$ edges. The corresponding training adjacency matrix, denoted as $A_{tr,tr} \in \mathbb{R}^{n\times n}$, is a sparse matrix with $(A_{tr,tr})_{ij} \neq 0$ if and only if there is an edge between node i and node j, and the value of $(A_{tr,tr})_{ij}$ denotes the weight of the edge. Note that standard GNN models usually conduct row normalization to the binary adjacency matrix and we directly assume $A_{tr,tr}$ is the normalized matrix here. Each node in the training graph is associated with a d-dimensional feature $\boldsymbol{x}_i \in \mathbb{R}^d$, and we use $X_{tr} \in \mathbb{R}^{n\times d}$ to denote the feature matrix. We use $X_{i\cdot}$ to denote the i-th row of a matrix X, so following this notation we have $(X_{tr})_{i\cdot} = \boldsymbol{x}_i$. Starting with $X^{(0)} = X_{tr}$, an L-layer GCN propagates node features layer-by-layer:

$$Z^{(\ell+1)} = A_{tr,tr}X^{(\ell)}W^{(\ell)}, \;\; X^{(\ell+1)} = \sigma(Z^{(\ell+1)}), \;\; \ell = 0, \ldots, L-1. \tag{1}$$

where $X^{(\ell)}$ is the feature matrix at the ℓ-th layer, $W^{(\ell)}$ is the weight matrix of a fully connected layer, and σ is nonlinear activation (usually element-wise ReLU). $A_{tr,tr}X^{(\ell)}$ is the graph convolution operation, which obtains a new representation of each node by a weighted average of its neighbors.

After L GCN layers, each node will obtain its final layer representation $X^{(L)}$, which will be associated with a loss function depending on the final task. A canonical application for GCN is semi-supervised node classification. In this application, each labeled node is associated with an observed label y_i, and we can use the standard cross-entropy loss to train the model. After training, we obtain the model weights $\mathcal{W} = \{W^{(0)}, \dots, W^{(L-1)}\}$.

In this paper, we focus on the **serving phase** of the GNN models. Depending on different scenarios, testing nodes can come one-by-one, batch-by-batch, or all together. For simplicity, we assume conducting GCN inference on a single node v with feature $\boldsymbol{x} \in \mathbb{R}^d$ and its connection to training nodes is represented by $\boldsymbol{a} \in \mathbb{R}^n$. In this case, GNN will conduct the following forward propagation to obtain node features

$$\begin{bmatrix} Z_{tr}^{(\ell+1)} \\ \boldsymbol{z}^{(\ell+1)} \end{bmatrix} = \begin{bmatrix} A_{tr,tr} & 0 \\ \boldsymbol{a} & \bar{a} \end{bmatrix} \begin{bmatrix} X_{tr}^{(\ell)} \\ \boldsymbol{x}^{(\ell)} \end{bmatrix} W^{(\ell)}, \ \begin{bmatrix} X_{tr}^{(\ell+1)} \\ \boldsymbol{x}^{(\ell+1)} \end{bmatrix} = \sigma(\begin{bmatrix} Z_{tr}^{(\ell+1)} \\ \boldsymbol{z}^{(\ell+1)} \end{bmatrix}), \ \boldsymbol{x}^{(0)} = \boldsymbol{x}, \tag{2}$$

where $\bar{a}$ is the constant depending how the GNN deals with the diagonal entries[1] Note that this can be easily generalized to cases with larger batch size m, where $\boldsymbol{x}$ will be replaced by an m-by-d feature matrix; $\boldsymbol{a}$ will become an m-by-n matrix representing the connections between testing and training nodes, and $\bar{a}$ will become the adjacency matrix between testing nodes.

We have demonstrated in Figure 1 that including training graph and node features in the serving phase is necessary. Intuitively, intermediate features for training nodes are very informative and propagating those information to testing nodes will significantly boost the performance. Also note that in (2) we assume there is no information flow from testing to training (0 in the top-right corner of joint adjacency matrix). This is because training nodes already have good features obtained in the training phase, so there is no need to propagate testing features to training nodes. This is adopted in several real GNN implementations (Chiang et al., 2019) and we found that setting the top-right corner of A as 0 or $\boldsymbol{a}^T$ have similar performance in practice.

As evident from (2), the serving phase of GNN requires storing model weights $\mathcal{W}$, training node features X_{tr} and training graph $A_{tr,tr}$. Storing X_{tr} and $A_{tr,tr}$ requires $O(nd)$ and $O(|\mathcal{E}|)$ space respectively, and both of these are much larger than the size of $\mathcal{W}$ which consists of L $O(d^2)$-sized matrices, with the corresponding storage requirement being independent of n. Taking a standard Reddit dataset as example, there are $n = 153,932$ training samples and $d = 602$ features, X_{tr}'s size is 370.7MB, $A_{tr,tr}$'s size is 86.0MB, and $\mathcal{W}$ is only 7.6MB size.

Accordingly, for GNNs, we define the task of reducing the space requirement for serving by primarily compressing X_{tr} and $A_{tr,tr}$ as the **serving graph compression** problem.

3.2 The Virtual Node Graph (VNG) method

We propose the virtual node graph (VNG) method in this section. The main idea is to replace n training nodes by a small number of c **virtual (VR) nodes**, with $c \ll n$. Let $X_{vr} \in \mathbb{R}^{c \times d}$ be the features and $A_{vr,vr} \in \mathbb{R}^{c \times c}$ be the adjacency matrix of the VR nodes, we aim to obtain those matrices by minimizing the forward propagation error. With the training nodes replaced by VR nodes, the graph convolution operation (first equation of (2)) will be replaced by

$$\begin{bmatrix} Z_{vr}^{(\ell+1)} \\ \boldsymbol{z}^{(\ell+1)} \end{bmatrix} = \begin{bmatrix} A_{vr,vr} & 0 \\ \boldsymbol{a}_{vr} & \bar{a} \end{bmatrix} \begin{bmatrix} X_{vr}^{(\ell)} \\ \boldsymbol{x}^{(\ell)} \end{bmatrix} W^{(\ell)}. \tag{3}$$

Note that $\boldsymbol{a}_{vr}$ in (3) represents the connection from node v to the VR nodes, which cannot be a fixed vector since it will depend on the the original $\boldsymbol{a}$ (the connections between node v and training nodes). We thus assume each original training node is represented by one of the VR nodes, and the mapping is defined as $\pi : \{1, \dots, n\} \to \{1, \dots c\}$. We thus have

$$\boldsymbol{a}_{vr} = \boldsymbol{a}\, \Pi, \tag{4}$$

[1] Can be 0 or 1 depending on the implementation, while some others methods add small constants to diagonal.

where $\Pi \in \{0,1\}^{n\times c}$ is the assignment matrix of the bipartite graph between training nodes and VR nodes. Specifically, Π is a 0/1 matrix with $\Pi_{i,j} = 1$ if and only if $\pi(i) = j$.

With these setups, VR nodes will involve in two computations when computing the features for a given node v: 1) The propagation from VR nodes to v 2) The propagation between VR nodes which will impact testing nodes in the next GNN layer. In the following, we will consider these two parts separately: in Sec 3.2.1 we consider 1) to obtain a solution for Π and X_{vr}, and in 3.2.2 we consider the 2) to obtain a solution for $A_{vr,vr}$. We show with this two-step decomposition, all the components can be solved by simple closed form solutions which leads to an efficient and easy-to-implement algorithm. Although the solution can be potentially improved by solving the whole problem jointly, we leave it to the future work.

3.2.1 Propagation from virtual representative nodes to testing nodes

Propagation from VR nodes to node v is the bottom row of the forward propagation in (3) and (2), where we want the resulting $\boldsymbol{z}^{(\ell+1)}$ to have minimal error. Therefore we want to have $\boldsymbol{a}X_{tr}^{(\ell)}W^{(\ell)} \approx \boldsymbol{a}_{vr}X_{vr}^{(\ell)}W^{(\ell)} = \boldsymbol{a}\Pi X_{vr}^{(\ell)}W^{(\ell)}$ which can be achieved if

$$\boldsymbol{a}X_{tr}^{(\ell)} \approx \boldsymbol{a}\Pi X_{vr}^{(\ell)}. \tag{5}$$

Since the testing nodes are unseen in the compression phase, we hope the compressed model to at least preserve the latent embedding when given every training node. If v is the i-th training node, then $\boldsymbol{a} = (A_{tr,tr})_{i,\cdot}$. Therefore, based on the spirit of empirical risk minimization, we aim to construct the Π matrix to minimize the following averaged square error:

$$\begin{aligned}\sum_{i\in[n]} \|(A_{tr,tr})_{i\cdot}X_{tr}^{(\ell)} - (A_{tr,tr})_{i\cdot}\Pi X_{vr}^{(\ell)}\|_2^2 &= \sum_{i\in[n]} \| \sum_{j\in[n]} (A_{tr,tr})_{ij}(X_{tr}^{(\ell)})_{j\cdot} - (A_{tr,tr})_{ij}(X_{vr}^{(\ell)})_{\pi(j)\cdot}\|_2^2 \\ &\leq \sum\nolimits_{i\in[n]}\sum\nolimits_{j\in[n]} (A_{tr,tr})_{ij}\|(X_{tr}^{(\ell)})_{j\cdot} - (X_{vr}^{(\ell)})_{\pi(j)\cdot}\|_2^2 \\ &= \sum\nolimits_{j\in[n]}(\sum\nolimits_{i\in[n]}(A_{tr,tr})_{ij})\|(X_{tr}^{(\ell)})_{j\cdot} - (X_{vr}^{(\ell)})_{\pi(j)\cdot}\|_2^2. \end{aligned} \tag{6}$$

Let $\gamma_j = \sum_{i\in[n]}(A_{tr,tr})_{ij}$ being the column sum of $A_{tr,tr}$, finding the VR nodes' features $X_{vr}^{(\ell)}$ and mapping $\pi(\cdot)$ is then equivalent to the weighted kmeans objective, with weight γ_j for training node j.

As we aim to minimize the error for all layers, we can bound the sum of (6) over all layers. If we define the concatenation of features from all layers as

$$\bar{X}_{tr} = [X_{tr}^{(0)}, \ldots, X_{tr}^{(L-1)}], \tag{7}$$

since the weights are independent to layers, we can lower bound the sum of loss over layers per (6):

$$\sum\nolimits_{\ell\in[L]}\sum\nolimits_{i\in[n]} \|(A_{tr,tr})_{i\cdot}X_{tr}^{(\ell)} - (A_{tr,tr})_{i\cdot}\Pi X_{vr}^{(\ell)}\|_2^2 \leq \sum\nolimits_{j\in[n]} v_j\|(\bar{X}_{tr})_{j\cdot} - (\bar{X}_{vr})_{\pi(j)\cdot}\|_2^2. \tag{8}$$

As the right hand side is equivalent to the weighted kmeans objective on $\bar{X}_{tr}$, we can apply the well-known EM-style weighted kmeans algorithm to (approximately) optimize the upper bound, where it iteratively updates the cluster centers $\bar{X}_{vr}$ and the cluster assignment π. After running weighted kmeans, we will obtain the assignment π^*, and the cluster centers are weighted average of training features within each cluster, so ideally we would like VR nodes' features at layer ℓ to be

$$X_{vr}^{(\ell)} = EX_{tr}^{(\ell)}, \text{ where } E_{ij} = \begin{cases} \frac{v_j}{\sum_{q:\pi^*(q)=i} v_q} & \text{if } \pi(j) = i, \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

Intuitively, E can be viewed as edges from training nodes to VR nodes, where each training node is only linked to one VR node. Since we only have freedom to assign the input features for virtual representative nodes, we set $X_{vr}^{(0)} = EX_{tr}^{(0)}$, and since beyond first layer the features are computed by propagating previous layers feature with $A_{vr,vr}$, we will discuss how to assign $A_{vr,vr}$ to best preserve this property for other layers. Note that we assume all layers share the same Π, which means each virtual node in different layers correspond to the same set of training nodes. Having different Π for each layer requires different $A_{vr,vr}$ for each layer, significantly increasing the space complexity.

3.2.2 PROPAGATION BETWEEN VIRTUAL REPRESENTATIVE NODES

Note that the E matrix obtained by weighted kmeans captures the transformation from training nodes to virtual nodes, and we have enforced (9) in the input layer. We will then study how to set the propagation among VR nodes or *equivalently* define the matrix $A_{vr,vr}$ such that it preserves the property of (9) for other layers.

Towards this, assume that $X_{vr}^{(\ell)} = EX_{tr}^{(\ell)}$ holds at layer ℓ. We then want to make sure that conducting a graph convolution on both VR nodes and training nodes will preserve this relationship, i.e.,

$$A_{vr,vr}X_{vr}^{(\ell)} = A_{vr,vr}EX_{tr}^{(\ell)} \approx EA_{tr,tr}X_{tr}^{(\ell)}, \tag{10}$$

where the left hand side is the propagation of VR nodes and the right hand side is the propagation of original training nodes, with an additional projection operator to map the features back to VR nodes.

Note that we want the above approximation to hold for all layers $\ell \in [0, L-2]$. Thus, summing the approximation error for each layer leads to the following optimization problem:

$$A_{vr,vr} = \arg\min_H \|HE\bar{X}_{tr} - EA_{tr,tr}\bar{X}_{tr}\|_F^2, \tag{11}$$

where $\bar{X}$ is defined in (7). Note that (11) can be easily solved by a standard least square solver. However, this will lead to a dense $c \times c$ matrix, which leads to storage bottleneck when c is large. Therefore, we propose to obtain a low-rank solution of (11) by requiring H to have a rank at most $c < k$. Such a low-rank matrix can then be stored with only $O(ck)$ memory overhead. With the rank constraint our optimization problem to solve for $A_{vr,vr}$ takes the form:

$$A_{vr,vr} = \arg\min_H \|HP - Q\|_F^2 \quad \text{s.t.} \quad \text{rank}(H) \leq k, \tag{12}$$

where $P = E\bar{X}_{tr}$ and $Q = EA_{tr,tr}\bar{X}_{tr}$. We now present a closed-form optimal solution for (12).

Theorem 1 *Assume $P = U_p\Sigma_pV_p^T$ and $Q = U_Q\Sigma_QV_Q^T$ are the thin-SVD of P and Q, respectively. Then the solution of (12) is $(QV_p)_k\Sigma_p^{-1}U_p^T$, where $(\cdot)_k$ denotes the rank-k truncated SVD of a matrix.*

The proof is deferred to the appendix. With this closed form solution, it is straightforward to solve (12). Note that the closed form solution requires to compute the thin-SVD of P and Q. These are c-by-d matrices where c is the number of virtual nodes and d is the hidden dimension size (sum over all layers). As d is usually small (e.g., less than $3,000$ in all our cases) and the complexity of SVD is $O(\min(c,d)^2\max(c,d))$, thin-SVD will be efficient (see Appendix C for details). In practice, this can be done within 1 minutes on standard CPU, even without GPU. Note that it is necessary to store rank-k matrix $A_{vr,vr}$ in a factorized form to realize the aforementioned $O(ck)$ storage cost during inference, and our closed form solution in the above theorem naturally provide such a factorization.

3.3 OVERALL ALGORITHM

Here we summarize the proposed Virtual Node Graph (VNG) algorithm from Section 3.2. Given the original GNN model and training data, we will first compute the collection of training node features before graph convolution $\bar{X}_{tr} = [X_{tr}^{(0)}, \ldots X_{tr}^{(L-1)}]$. For general GNN, these are features before one-hop propagation or mathematically, left-multiplying with the adjacency matrix. We then compute the column sum of the $A_{tr,tr}$ to get $\{\gamma_1, \ldots, \gamma_n\}$; subsequently we run weighted kmeans on $\bar{X}_{tr}$ using these weights (cf. (8)). Given the clustering assignment π obtained from the weighted kmeans, we form an E matrix based on (9) and set features for VR nodes as $X_{vr}^{(0)} = EX_{tr}^{(0)}$. We then solve (12) with $P = E\bar{X}_{tr}$ and $Q = EA_{tr,tr}\bar{X}_{tr}$ to obtain $A_{vr,vr}$ (stored in the factorized form). At the inference time, the forward propagation is conducted by (2), where we only store virtual nodes instead of training nodes. The algorithm reduces the space complexity from the original $O(n + |\mathcal{E}| + nd)$ to $O(ck + cd)$, where $c \ll n$ is the number of virtual representative nodes and k is a low-rank factor in (12). Please see Algorithm 1 for the description of the algorithm.

4 EXPERIMENTAL RESULTS

In this section, we empirically test our proposed method on four real datasets:

Algorithm 1 The Virtual Node Graph (VNG) algorithm

Input: Training adjacency matrix $A_{tr,tr}$ and features X_{tr}, GNN weights $\mathcal{W}$, number of virtual nodes c, rank of virtual adjacency matrix k.

1: Compute $\bar{X}_{tr} = [X_{tr}^{(0)}, \ldots, X_{tr}^{(L-1)}]$ by GNN forward pass with training data $A_{tr,tr}$ and X_{tr}.
2: Compute weights $\gamma_j = \sum_i (A_{tr,tr})_{ij}$ for all j.
3: $\pi \leftarrow$ weighted_kmeans$(\bar{X}_{tr}, c, \{\gamma_i\}_{i=1}^n)$.
4: Get E matrix based on (4).
5: Compute $X_{vr} = EX_{tr}$ (X_{tr} is the raw feature for training nodes).
6: Solve $A_{vr,vr}$ based on (12).

Output: $A_{vr,vr}$ and X_{vr}

Table 2: The statistics of Arxiv, Reddit, Product, and Amazon2M datasets.

Datasets	#Training Nodes	#Validate Nodes	#Labels	#Features
Arxiv	90,941	29,799	40	128
Reddit	153,932	23,699	41	602
Product	196,615	39,323	47	100
Amazon2M	1,709,997	739,032	47	100

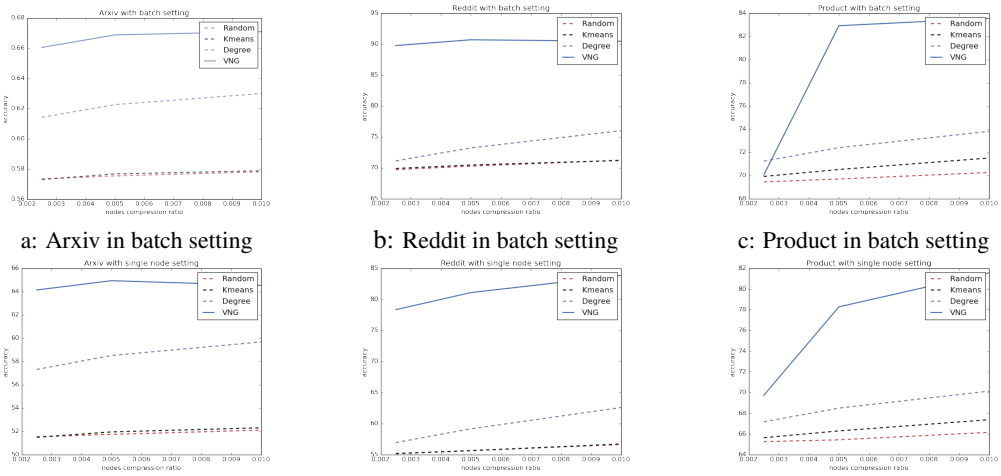
- **Arxiv**: A multi-class node classification dataset used for predicting the category of a paper. We use the same dataset and partition as in (Hu et al., 2020).
- **Reddit**: A multi-class node classification dataset used for predicting the communities of online posts. We use the same dataset and partition as in (Chiang et al., 2019).
- **Product**: A multi-class classification dataset that is similar to Amazon2M , with a key difference that it is based on a different preprocessing and split by Hu et al. (2020).
- **Amazon2M**: A multi-class classification dataset, where the graph has products co-purchase history, data features have each product's information, and the label is the category of the product.

All above datasets are publicly available and are commonly used for benchmarking the performance of GNNs on node classification tasks. The statistics of these datasets are summarized in Table 2. As this is the first paper considering the serving graph compression problem for GNN, we mainly compare our method against standard model compression methods (for compressing training node features) and core-set selection methods (selecting a subset of nodes for serving). Specifically, we include the following methods in the comparison:

- **Sparse**: Sparsifying the training nodes' features by sorting the values and removing small values in the features. For this method, the connection graph does not change. The serving space is controlled by the pruning ratio.
- **SVD**: Performing SVD over the training nodes' features to save the serving space. The serving space is controlled by the rank used in performing low-rank approximation via SVD. Also, note that the original graph remains unchanged for this method.
- **Random**: Randomly selecting some training nodes and their corresponding subgraph.
- **Degree**: Selecting the training nodes by sorting the degree of training nodes and picking the nodes with the highest degrees.
- **Kmeans**: Performing kmeans over the training nodes features, and selecting the training nodes closest to the kmeans centroids.
- **VNG** (our proposed method): Constructing the virtual nodes graph which is much smaller than the original graph based on the GNN forward pass reconstruct error (cf. Algorithm 1).

We use GCN model as example model to test above methods. Note that these methods are also applicable to other GNN models. In Appendix, we include the results of applying VNG on GraphSAGE model. Also in Appendix, we show different variations of our method such as replacing weighted kmeans with vanilla kmeans or choosing different ranks during low-rank step, etc. (see Appendix A for details). We use ClusterGCN's tensorflow implementation [2] for GCN model training. As for architecture, on all datasets, we consider a 4-layer GCN model with hidden dimensions 512, 256, and 512 for Product, Arxiv, and Reddit, respectively, and the mean aggregator from Hamilton et al. (2017). To test each model, we first train a GCN model and freeze the model, then we run each method to

[2] https://github.com/google-research/google-research/tree/master/cluster_gcn



a: Arxiv in batch setting b: Reddit in batch setting c: Product in batch setting

d: Arxiv in single node setting e: Reddit in single node setting f: Product in single node setting

Figure 2: Comparisons of graph compression for GCN inference methods. The x-axis shows the node compression ratio for our proposal. Other methods' graph is chosen to be of the same size as our method. The y-axis corresponds to the accuracy for the node classification tasks. The graph sizes for Sparse and SVD are too large and they cannot realize the compression ratios considered in the figure.

generate a compressed graph for efficient inference on the new testing nodes. The process of graph compression and subsequent inference with the compressed graph does not involve retraining the GCN model.

Here we consider two settings of inference. The first setting is batch inference, where we are given a batch of testing nodes at each time, with their node features and interconnections. The connection from the testing nodes to training nodes are also given. This is the typical setting for GNN model inference. The second setting is single node inference, where we assume the testing nodes appear one-by-one in an on-line fashion. In this setting, we only know the testing node features and the connections from this testing node to the training nodes.

4.1 Batch Inference Setting

As explained previously, in batch inference setting, we assume the testing data become available in batches. Since the edges connecting training nodes to testing nodes and the connections among testing nodes are given, each testing node's features will be updated using the information from the training nodes and other testing nodes. We show the compression results in Table 3, where the graph size (including nodes' features and adjacency graph size) are shown in the brackets following the accuracy. We construct the compressed graph with only 1% and 5% of total training nodes for our method. Note that Kmeans, Degree, and Random generate the graphs that have the same number of nodes as VNG.

From Table 3, we observe that our method is able to achieve very high compression rate (e.g., the compressed graph contains 1% of the total of nodes in the original graph) for the serving space– 37.5x on Arxiv, 41.0x on Reddit, and 70.3x on Product. Other methods will suffer from a significant performance loss when using such a compression rate. Note that Sparse and SVD both operate on nodes features, while maintaining the original adjacency graph. Thus, the compressed graph is still as large as the original graph . Random is not aware of information in the graph and features. Kmeans only uses node features and is not aware of adjacency graph information. Degree considers adjacency graph and does not take features into consideration. Therefore, all the methods except our proposed method consider either adjacency graph or node features. Furthermore, these methods are model agnostic as the GNN model itself does not play a role in the compression. In contrast, our proposed method considers all three factors: adjacency graph, node features, and GNN model; consequently, performing better than other baselines. Note that Figure 2[a-c] shows the accuracy when we vary the compression ratio, and our method always performs best in comparison with the other methods. Note that, besides reducing the inference serving size, VNG can also speed up the inference. In Table 7 in the appendix, we can observe VNG can speed up original GCN model's inference.

Table 3: Accuracy% (Size) on four datasets for batch setting where test data appears in batches. The brackets next to accuracy show the compressed graph size including both adjacency matrix and node features. 'Full' corresponds to using the original adjacency graph and nodes features. For 'Random', 'Degree', 'Kmeans', 'VNG', we show the results under different number of distilled nodes–1% or 5% means the compressed graph contains 1% or 5% of the total number of nodes in the original graph. *For Amazon2M the number of nodes in the compressed graph is 0.1% or 0.5% of the original graph.

Model		Arxiv	Reddit	Product	Amazon2M*
Full		69.94 (52.4MB)	94.85 (456.6MB)	87.51 (165.8MB)	89.15 (1.17GB)
SVD		58.69 (8.1MB)	88.35 (104.5MB)	40.82 (91.1MB)	68.08 (512.7MB)
Sparse		56.90 (6.0MB)	68.27 (93.4MB)	64.75 (88.7MB)	66.45 (486.1MB)
Random	1%	58.32 (2.3MB)	71.23 (11.2MB)	70.26 (2.5MB)	77.80 (2.1MB)
	5%	62.85 (12.0MB)	77.91 (57.5MB)	74.57 (13.7MB)	77.98 (10.4MB)
Degree	1%	63.63 (3.2MB)	76.00 (15.5MB)	73.81 (3.8MB)	78.99 (2.8MB)
	5%	66.42 (14.8MB)	86.62 (78.1MB)	79.36 (24.5MB)	81.71 (38.4MB)
Kmeans	1%	58.09 (2.4MB)	71.93 (11.4MB)	69.73 (2.5MB)	77.75 (2.1MB)
	5%	61.93 (12.00MB)	80.31 (60.3MB)	72.83 (14.3MB)	78.33 (20.95MB)
VNG (ours)	1%	67.07 (1.4MB)	90.51 (11.1MB)	83.11 (2.4MB)	83.12 (2.1MB)
	5%	68.64 (7.0MB)	91.00 (55.6MB)	85.60 (11.8MB)	84.23 (10.2MB)

Table 4: Accuracy% (Size) on four datasets for batch setting where testing data appears in batches. In the brackets next to accuracy, we show the compressed graph size including both adjacency matrix and node features. 'Full' corresponds to using the original adjacency graph and nodes features. For 'Random', 'Degree', 'Kmeans', 'VNG', we show the results under different number of distilled nodes–1% or 5% means the compressed graph contains 1% or 5% of the total number of nodes in the original graph. *For Amazon2M, #nodes in the compressed graph is 0.1% or 0.5% of original graph.

Model		Arxiv	Reddit	Product	Amazon2M*
Full		68.35 (52.4MB)	92.75 (456.6MB)	86.95 (165.8MB)	87.79 (1.17GB)
SVD		55.37 (8.1MB)	81.46 (104.5MB)	39.64 (91.1MB)	54.72 (512.7MB)
Sparse		51.54 (6.8MB)	54.55 (93.4MB)	60.81 (88.8MB)	61.32 (499.0MB)
Random	1%	52.71(2.3MB)	5662 (11.2MB)	66.15 (2.4MB)	61.01 (2.1MB)
	5%	58.57 (12.0MB)	69.22 (57.7MB)	71.18 (13.7MB)	61.34 (10.4MB)
Degree	1%	60.58 (3.2MB)	62.58 (15.4MB)	7013 (3.8MB)	63.53 (2.8MB)
	5%	63.95 (14.8MB)	77.18 (78.1MB)	76.77 (24.9MB)	67.64 (17.3MB)
Kmeans	1%	52.51 (2.3MB)	57.42 (11.4MB)	65.57 (2.5MB)	60.99 (2.1MB))
	5%	57.75 (12.0MB)	67.53 (60.3MB)	69.31 (14.4MB)	61.94 (21.0MB)
VNG (ours)	1%	66.73 (1.4MB)	90.51 (11.1MB)	83.04 (2.4MB)	82.53 (2.1MB)
	5%	67.84 (7.0MB)	91.40 (55.6MB)	85.08 (11.8MB)	84.26 (10.2MB)

4.2 Single Node Inference Setting

In the single node inference setting, each testing node appears one-by-one. Unlike the batch setting, no connections among testing nodes are given. Therefore, how to effectively utilize the information from training data becomes even more crucial. We compare our method with all the baselines in this setting and present the results in Table 4. Since our method is able to better utilize the information of training graph and features, the accuracy gap between our method and baselines becomes larger in this setting. Also, Figure 2[d-f] shows the accuracy when we vary the compression ratio for this setting, and our method always performs best as compared to the other baseline methods.

5 Conclusion

Although GNNs achieve promising performance handling graph data, they require storing training graph and features to perform inference, leading to a high serving space requirement. In this paper, we propose a novel method for serving graph compression, where we replace the training features and graph by a small set of virtual nodes. The features and adjacency matrix of virtual nodes are designed to minimize the forward propagation error of GNN and can be simply adapted to any GNN structure. Our empirical results demonstrate that the proposed method can significantly reduce the GNN serving size while maintaining a reasonable predictive performance. As one of the limitations of our method, it may suffer from higher performance loss if a larger compression rate (e.g., 50x) is desired, but it is possible to further improve by combining it with pruning or quantization approaches.

REFERENCES

Gecia Bravo Hermsdorff and Lee Gunderson. A unifying framework for spectrum-preserving graph sparsification and coarsening. *Advances in Neural Information Processing Systems*, 32, 2019.

Jianfei Chen, Jun Zhu, and Le Song. Stochastic training of graph convolutional networks with variance reduction. *arXiv preprint arXiv:1710.10568*, 2017.

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

Patrick Chen, Si Si, Yang Li, Ciprian Chelba, and Cho-Jui Hsieh. Groupreduce: Block-wise low-rank approximation for neural language model shrinking. *Advances in Neural Information Processing Systems*, 31, 2018b.

Tianlong Chen, Yongduo Sui, Xuxi Chen, Aston Zhang, and Zhangyang Wang. A unified lottery ticket hypothesis for graph neural networks. In *International Conference on Machine Learning*, pp. 1695–1706. PMLR, 2021.

Yu Chen, Lingfei Wu, and Mohammed Zaki. Iterative deep graph learning for graph neural networks: Better and robust node embeddings. *Advances in Neural Information Processing Systems*, 33: 19314–19326, 2020.

Cédric Chevalier and Ilya Safro. Comparison of coarsening schemes for multilevel graph partitioning. In *International Conference on Learning and Intelligent Optimization*, pp. 191–205. Springer, 2009.

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

Michael B Cohen, Cameron Musco, and Christopher Musco. Input sparsity time low-rank approximation via ridge leverage score sampling. In *Proceedings of the Twenty-Eighth Annual ACM-SIAM Symposium on Discrete Algorithms*, pp. 1758–1777. SIAM, 2017.

Jonathan Frankle and Michael Carbin. The lottery ticket hypothesis: Finding sparse, trainable neural networks. *arXiv preprint arXiv:1803.03635*, 2018.

Amir Gholami, Sehoon Kim, Zhen Dong, Zhewei Yao, Michael W Mahoney, and Kurt Keutzer. A survey of quantization methods for efficient neural network inference. *arXiv preprint arXiv:2103.13630*, 2021.

Justin Gilmer, Samuel S Schoenholz, Patrick F Riley, Oriol Vinyals, and George E Dahl. Neural message passing for quantum chemistry. In *International conference on machine learning*, pp. 1263–1272. PMLR, 2017.

William L. Hamilton, Rex Ying, and Jure Leskovec. Inductive representation learning on large graphs. In *Advances in Neural Information Processing Systems*, 2017.

Song Han, Huizi Mao, and William J Dally. Deep compression: Compressing deep neural networks with pruning, trained quantization and huffman coding. *arXiv preprint arXiv:1510.00149*, 2015.

Sariel Har-Peled and Soham Mazumdar. On coresets for k-means and k-median clustering. In *Proceedings of the thirty-sixth annual ACM symposium on Theory of computing*, pp. 291–300, 2004.

Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. Open graph benchmark: Datasets for machine learning on graphs. *arXiv preprint arXiv:2005.00687*, 2020.

Wei Jin, Lingxiao Zhao, Shichang Zhang, Yozen Liu, Jiliang Tang, and Neil Shah. Graph condensation for graph neural networks. *arXiv preprint arXiv:2110.07580*, 2021.

Junghun Kim, Jinhong Jung, and U Kang. Compressing deep graph convolution network with multi-staged knowledge distillation. *Plos one*, 16(8):e0256187, 2021.

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

Guohao Li, Matthias Müller, Bernard Ghanem, and Vladlen Koltun. Training graph neural networks with 1000 layers. In *International conference on machine learning*, pp. 6437–6449. PMLR, 2021.

Yike Liu, Tara Safavi, Abhilash Dighe, and Danai Koutra. Graph summarization methods and applications: A survey. *ACM computing surveys (CSUR)*, 51(3):1–34, 2018.

Mario Lucic, Matthew Faulkner, Andreas Krause, and Dan Feldman. Training gaussian mixture models at scale via coresets. *The Journal of Machine Learning Research*, 18(1):5885–5909, 2017.

Baharan Mirzasoleiman, Jeff Bilmes, and Jure Leskovec. Coresets for data-efficient training of machine learning models. In *International Conference on Machine Learning*, pp. 6950–6960. PMLR, 2020.

Tara N Sainath, Brian Kingsbury, Vikas Sindhwani, Ebru Arisoy, and Bhuvana Ramabhadran. Low-rank matrix factorization for deep neural network training with high-dimensional output targets. In *2013 IEEE international conference on acoustics, speech and signal processing*, pp. 6655–6659. IEEE, 2013.

Yunsheng Shi, Zhengjie Huang, Shikun Feng, Hui Zhong, Wenjin Wang, and Yu Sun. Masked label prediction: Unified message passing model for semi-supervised classification. *arXiv preprint arXiv:2009.03509*, 2020.

Daniel A Spielman and Shang-Hua Teng. Spectral sparsification of graphs. *SIAM Journal on Computing*, 40(4):981–1025, 2011.

Shyam A Tailor, Javier Fernandez-Marques, and Nicholas D Lane. Degree-quant: Quantization-aware training for graph neural networks. *arXiv preprint arXiv:2008.05000*, 2020.

Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. Graph attention networks. *arXiv preprint arXiv:1710.10903*, 2017.

Tongzhou Wang, Jun-Yan Zhu, Antonio Torralba, and Alexei A Efros. Dataset distillation. *arXiv preprint arXiv:1811.10959*, 2018.

Shiwen Wu, Fei Sun, Wentao Zhang, Xu Xie, and Bin Cui. Graph neural networks in recommender systems: a survey. *ACM Computing Surveys (CSUR)*, 2020.

Zhenqin Wu, Bharath Ramsundar, Evan N Feinberg, Joseph Gomes, Caleb Geniesse, Aneesh S Pappu, Karl Leswing, and Vijay Pande. Moleculenet: a benchmark for molecular machine learning. *Chemical science*, 9(2):513–530, 2018.

Yiqing Xie, Sha Li, Carl Yang, Raymond Chi Wing Wong, and Jiawei Han. When do gnns work: Understanding and improving neighborhood aggregation. In *IJCAI International Joint Conference on Artificial Intelligence*, 2020.

Yiding Yang, Jiayan Qiu, Mingli Song, Dacheng Tao, and Xinchao Wang. Distilling knowledge from graph convolutional networks. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 7074–7083, 2020.

Hanqing Zeng, Hongkuan Zhou, Ajitesh Srivastava, Rajgopal Kannan, and Viktor Prasanna. Graph-saint: Graph sampling based inductive learning method. *arXiv preprint arXiv:1907.04931*, 2019.

Muhan Zhang and Yixin Chen. Link prediction based on graph neural networks. *arXiv preprint arXiv:1802.09691*, 2018.

Wentao Zhang, Zhi Yang, Yexin Wang, Yu Shen, Yang Li, Liang Wang, and Bin Cui. Grain: Improving data efficiency of graph neural networks via diversified influence maximization. *arXiv preprint arXiv:2108.00219*, 2021.

Bo Zhao, Konda Reddy Mopuri, and Hakan Bilen. Dataset condensation with gradient matching. *arXiv preprint arXiv:2006.05929*, 2020.

A ABLATION STUDY

Here we show the ablation study over our method. Our proposed method contains two components: weighted kmeans to construct features for VR nodes $\bar{X}_{vr}$ using Eq 9 and computing propagation matrix $A_{vr,vr}$ using Eq 11. In Table 5, we show different variations of our method: VNG-kmeans is using normal kmeans to replace weighted kmeans; VNG-weighted-kmeans without using SVD and using least square instead to get $A_{vr,vr}$; then using different ranks when solving Eq 12 in VNG: VNG (rank=512), VNG (rank=128), VNG (rank=32) and VNG (rank=8). We learn from this table that weighted kmeans is performing better than kmeans (this verifies the usefulness of weighted kmeans to find $\bar{X}_{vr}$), and reducing the rank in VNG will decrease the performance but results in smaller graph size. So it is a trade-off when choosing the rank when approximating $A_{vr,vr}$ using low-rank method.

In Table 6, we conducted another ablation study that instead of solving a low-rank $A_{vr,vr}$, we use a sparse structure to reduce memory consumption. In this experiment, we compute the unconstrained optimal $A_{vr,vr}$ first and then prune part of its elements based on the absolute values. We observe that with 40% sparsity, the accuracy of VNG already reduces to 62.77% (compared with the original 67.14% accuracy). This suggests that low-rank compression works better than sparsity when we want to reduce the memory consumption of $A_{vr,vr}$.

Table 5: Ablation study on Arxiv dataset (in terms of accuracy).

VNG-kmeans	VNG-weighted-kmeans	VNG (rank=512)	VNG (rank=128)	VNG (rank=32)	VNG (rank=8)
66.57%(4.2MB)	67.15%(4.2MB)	67.14%(4.6MB)	67.07%(1.4MB)	66.48%(1.1MB)	66.25%(1.0MB)

B PROOF OF THEOREM 1

Theorem 1 Assume $P = U_p \Sigma_p V_p^T$ and $Q = U_Q \Sigma_Q V_Q^T$ are the thin-SVD of$P$ and Q, respectively. Then the solution of

$$A_{vr,vr} = \arg\min_{H} \|HP - Q\|_F^2 \quad \text{s.t.} \quad \text{rank}(H) \leq k, \tag{13}$$

is $(QV_p)_k \Sigma_p^{-1} U_p^T$, where $(\cdot)_k$ denotes the rank-k truncated SVD of the matrix.

Proof:

$$\begin{aligned} A_{vr,vr} &= \arg\min_{H:\text{rank}(H)\leq k} \|HP - Q\|_F^2 \\ &= \arg\min_{H:\text{rank}(H)\leq k} \|(HP - Q)V_p V_p^T\|_F^2 + \|(HP - Q)(I - V_p V_p^T)\|_F^2 \\ &= \arg\min_{H:\text{rank}(H)\leq k} \|(HP - Q)V_p V_p^T\|_F^2 \\ &= \arg\min_{H:\text{rank}(H)\leq k} \|(HP - Q)V_p\|_F^2 \\ &= \arg\min_{H:\text{rank}(H)\leq k} \|HU_p\Sigma_p - QV_p\|_F^2 \\ &= (QV_p)_k \Sigma_p^{-1} U_p^T \end{aligned} \tag{14}$$

C TIME COMPLEXITY FOR IMPLEMENTING THEOREM 1

We show a closed form solution for (12) in Theorem 1. Here we anlayze the time complexity and show the run time for achieving such low-rank closed form solution. The main computation in Theorem 1 is the SVD of two tall and thin matrices P and Q which are c-by-d matrices (where c is the number of compressed nodes and d is the hidden dimensions times the number of GNN layers plus input dimension). In practice, the size of c depends on the desired compression rate, and d is fixed based on the GNN architecture. The time complexity for computing the SVD of a c-by-d matrix is $O(\min(c, d)^2 \max(c, d))$, which will be fast if one of the c, d is small. For example, when

Table 6: Ablation study on Arxiv dataset (in terms of accuracy) using sparse vs low-rank for $A_{vr,vr}$.

VNG (rank=512)	VNG (rank=8)	VNG-Sparse (sp: 90%)	VNG-Sparse (sp: 40%)	VNG-Sparse (sp: 10%)
67.14%(4.6MB)	66.25%(1.0MB)	58.89%(1.4MB)	62.70%(4.4MB)	66.72%(6.4MB)

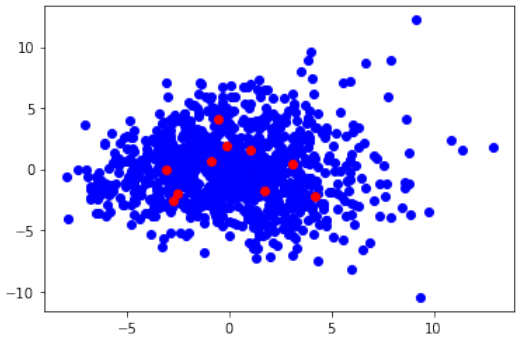


Figure 3: 2-D projection of the virtual nodes (red dots) and training nodes (blue dots) using PCA over their node features on the Reddit dataset.

$d < c$, the time complexity for computing SVD of P (or Q) will be $O(d^2c + d^3)$ which is linear to c. This is using the fact that since $P = USV^T$, then $P^TP = VS^2V^T$, so they share the same right singular vectors. Therefore, we can compute SVD of P^TP (d-by-d matrix) instead of P. More specifically, the procedure will be 1) Compute $H = P^TP$ which takes $O(d^2c)$ time, 2) Compute SVD of $H = V\Sigma V^T$ which takes $O(d^3)$ time. 3) Compute $S = \Sigma^{1/2}$ which is a diagonal matrix and this costs $O(d)$ time; 4) Compute $U = PVS^{-1}$ which takes $O(d^2c)$ time.

Typically in GNN d is small. For example, $d = 2648$ for Reddit. If we use 5% compression rate on Reddit, then $c = 7696$. In this case, running the computation we mentioned above for SVD computation will take only 4 seconds on a CPU, even without using a GPU.

Table 7: Inference time (in seconds). Since ClusterGCN's inference is on CPU, the below numbers are based on CPU time. *For Amazon2M, #nodes in the compressed graph is 0.1% or 0.5% of original graph.

Datasets		Arxiv	Reddit	Product	Amazon2M*
Full		1.28	20.6	8.351	65.24
VNG	1%	0.57	1.64	2.95	13.88
	5%	1.17	12.08	7.64	16.38

D VIRTUALIZATION OF VIRTUAL NODES

In Figure 3, we show the 2-D projection of the virtual nodes (red dots) and training nodes (blue dots) using PCA over graph node features. This figure is based on the data in the Reddit dataset, where we generate 10 virtual nodes with our algorithm VNG, and randomly select 1000 training nodes for visualization purpose.

E EXPERIMENTAL RESULT ON GRAPHSAGE MODEL

Besides GCN model, our method can also be applied to other GNN models to reduce inference model serving size. In Table 8, we show the performance of various graph compression methods on GraphSAGE model (Hamilton et al., 2017) with mean aggregator over Arxiv dataset. The results show that our method is still consistently better than the baselines.

Table 8: Results on GraphSAGE model on Arxiv dataset. We construct the compressed graph with only 1% of total training nodes for our method. We use the graph size of our proposed method (VNG) as the baseline (1x), and other methods' graph sizes are evaluated w.r.t. this baseline. For example, 10x means using 10 times more space as compared to our method. 'Full' means using the original adjacency graph and nodes features.

Full	SVD	Sparse	Random	Degree	Kmeans	VNG
69.59(37.5x)	59.1(5.8x)	56.3(4.5x)	57.2(1.0x)	62.6(1.3x)	57.6(1.0x)	65.9(1.0x)

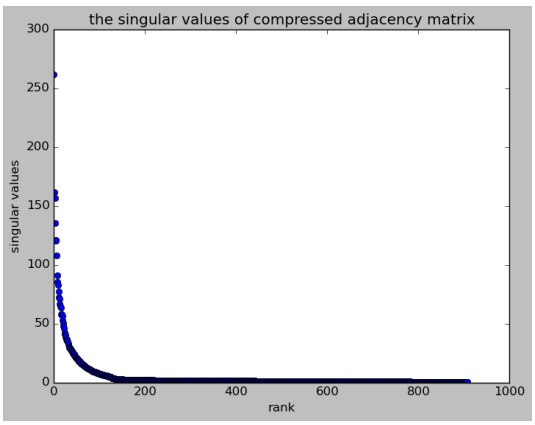


Figure 4: The singular values plot of learned $A_{vr,vr}$. We can see when the rank increases, the singular values will decrease dramatically, which shows that some low-rank structure exists in $A_{vr,vr}$.

F Singular values of $A_{vr,vr}$

In Figure 4, we show the singular values of $A_{vr,vr}$, where $A_{vr,vr}$ is the unconstrained optimal. We compute $A_{vr,vr}$ on Arxiv dataset with 1% VR nodes. We observe that the $A_{vr,vr}$ matrix has a low-rank structure, validating why our low-rank approach works well in practice.

G Inference Speed

Although we focus on reducing the space complexity in this paper, our method will not sacrifice inference speed. Instead of storing full $A_{vr,vr}$, we store it in the factorization form where $A_{vr,vr} = UV^T$ and U, V are obtained by Theorem 1. Let k be the rank, c be the number of VR nodes and d be the feature dimension, our method $A_{vr,vr}X_{vr} = U(V^T X_{vr})$ takes $O(cdk)$ flops while the original propagation $A_{tr,tr}X_{tr}$ takes $O(\text{nnz}(A)d)$ flops. In most of the experiments in our paper, we achieve a better or at least comparable inference speed. To compare the inference speed, we run it on a standard CPU with full-batch inference on the whole testing set, and report the numbers in Table 7.