# arXiv:2110.06991v1 [cs.LG] 13 Oct 2021

# Scalable Graph Embedding Learning On A Single GPU

Azita Nouri\*, Philip E. Davis<sup>†</sup>, Pradeep Subedi<sup>†</sup>, Manish Parashar<sup>†</sup>

\* School of Computer Science, Rutgers University, NJ, USA

azita.nouri@rutgers.edu

<sup>†</sup> Scientific Computing Imaging Institute, University of Utah, Salt Lake City, UT, USA philip.davis@sci.utah.edu, pradeep.subedi@utah.edu, parashar@sci.utah.edu

Abstract—Graph embedding techniques have attracted growing interest since they convert the graph data into continuous and low-dimensional space. Effective graph analytic provides users a deeper understanding of what is behind the data and thus can benefit a variety of machine learning tasks. With the current scale of real-world applications, most graph analytic methods suffer high computation and space costs. These methods and systems can process a network with thousands to a few million nodes. However, scaling to networks with billions of nodes remains a challenge. The complexity of training graph embedding system requires the use of existing accelerators. In this paper, we introduce a hybrid CPU-GPU framework that addresses the challenges of learning embedding of large-scale graphs. The performance of our method is compared qualitatively and quantitatively with existing embedding systems on common benchmarks. We also show that our system can scale training to datasets with an order of magnitude greater than a single machine's total memory capacity. The effectiveness of the learned embedding is evaluated within multiple downstream applications. The experimental results indicate the effectiveness of the learned embedding in terms of performance and accuracy.

### I. INTRODUCTION

In many real-world applications, graphs (a.k.a networks) have been widely used to demonstrate interactions between entities. Graph representation allows researchers to efficiently understand the structure of data in a systematic manner while they comprise many high-dimensional data to be processed (e.g., social networks[1], biology networks[2]). Due to the complexity of the data collected by various platforms and services, learning continuous low-dimensional vectors of graphs has attracted significant research interest. Moreover, with dynamically growing graphs, the high-dimensional data is not suitable for many machine learning approaches as they require vectors with low-dimensional representation for their computation. Among various approaches, graph embedding has attracted more attention in unsupervised learning of node representations in smaller space. Figure 1 illustrates the process of graph embedding in which low-dimensional vectors are learned through the training of samples that obtained from the graph. Later on, these d dimensional embeddings can be used as an input for many graph analytic methods (some of them are listed in Fig. 1). Representing nodes (originally in n dimensions) in low-dimensional space ( $d \ll n$ ) enables us to apply common machine learning techniques to find the hidden properties of the graph more efficiently, such as link

prediction [3], community detection [4], node classification [5], clustering, and graph visualization [6], [7]. Therefore, it is critical to have high-quality representations of nodes for these downstream machine learning tasks to accurately perform graph analytics.

Learning a graph embedding model can be a resource intensive process. First, training such a model requires a massive amount of computation [8] especially when the representation vectors have higher dimensions and graphs include many nodes and edges to be trained. The training of graph embeddings simply consists of many dot-product operations between various vectors, while higher dimensions and more number of edges in larger graphs pose a vast amount of computations in the training phase. Various graph embedding methods are suggested in the literature. However, these approaches rarely scale to large graphs. For example, DeepWalk[9], node2vec[10], and LINE[11] require hours of CPU training, even for smalland medium-scale graphs. Although these approaches can be parallelized, a parallel CPU implementation of DeepWalk takes over two hours on 26 CPU cores for a graph with 2 million vertices and 5 million edges. Traditional CPU-based methods are resource constraints. For example, training a large graph with billions of edges in vectors of size 100 using these methods is not feasible or in the best case takes hours of training, if not days. Therefore, with the rapidly growing size of graphs, it is essential for embedding methods to support the training of such large graphs in a reasonable time [8]. There are many studies that try to train large graphs using limited resources [12], [8]. In addition to that, with more availability of GPUs and other accelerators, new techniques have been done to utilize these resources to speed up the training phase of learning algorithms [13]. Thus, using the power of GPUs in a hybrid system is a popular method to achieve speedup for the computational part of embedding training. However, another challenge of these computations is related to memory requirements, mainly because we need to store a large graph in memory along with its representation vectors. For large graphs, the model parameters cannot be stored in the main memory, e.g., a graph with 100 million nodes represented in 256 dimensions requires around 400GB RAM, which is beyond the capacity available to oridinary users. Considering the increasing size of large graphs, we cannot fit the embedding vectors into CPU memory, while in the case of utilizing GPU,



Fig. 1: Graph embedding learning. Input graph, output of the training, and the applications.

this problem becomes significantly challenging because of the limited and even smaller GPU memory compared to CPU. There are efforts to increase graph embedding performance using accelerators such as GPU to handle large graphs. While existing methods that leverage GPUs are faster than running a CPU-based implementation, but their usage are limited by GPU memory and therefore they cannot embed a large graph on a single GPU. Motivated by the computation and memory requirement challenges of training large-scale graphs, we present a framework that utilizes the power of a hybrid CPU-GPU system to train an arbitrary size graph given a small CPU-GPU hardware. Our proposed framework aims to address the existing challenges by dividing the graph and parameter model into disjoint partitions and saving them on disk, then transferring these partitions in a small chunk to the GPU memory when needed for the training task. Our framwrok then learns to independently embed each partition by utilizing a pipeline that combines the core computation of a graph training on the GPU with the concurrent processing of data transfers from disk-to-CPU memory and CPU-to-GPU memory. Our pipeline training architecture allows us to overlap data access, transfer, and computation to achieve highperformance training. This pipeline maintains and updates node embedding parameters in CPU memory asynchronously, allowing to train graph embedding for a billion-edge graph on an order of magnitude faster than current hybrid CPU-GPU systems for the same level of accuracy.

In the rest of this paper, in Section II, we provide a background and an overview of related graph embedding methods. Then, in Section III, we define our system design which composes of an optimized method for reading a graph, and a hybrid CPU-GPU system for training embedding. Finally, in Section IV, we evaluate our proposed system model

and various comparing methods using real data graphs. We conclude this paper in Section V and summarize our work with a discussion and future work.

### **II. BACKGROUND AND RELATED WORK**

In this section, we discuss the necessary background on graph embedding, related systems, and challenges for training large-scale graph embedding models. Since there exists a large body of literature as surveyed in [14], [15], we review the methods that are most relevant to our work.

A graph is G = (V, E), where  $v \in V$  is a set of nodes, each representing an entity in a network and  $e \in E$  is a set of edges between the nodes, each reflecting a relation between two nodes. Each edge  $e \in E$  is a pair of (u, v) with possible weights, indicating the strength relation. If G is directed, (u, v) = (v, u). If G is undirected,  $(u, v) \neq (v, u)$ . We have a set of node types and edge types, respectively, denoted by  $S_v$  and  $S_e$ . Each node  $v_i \in V$  belongs to one type of node, and  $e_i \in E$  is a particular type of edge. For homogeneous graphs, we have  $|S_v| = |S_e| = 1$ , meaning that all nodes belong to one type and similarly for all edges in the graph. For heterogeneous graphs, we have  $|S_v| > 1$  and/or  $|S_e| > 1$ , which results in having different types of nodes and/or edges. Given a graph G = (V, E), the goal of embedding is to learn a low-dimensional representation for each node. Such that these low-dimensional vectors preserve the structural information of the graph. For a graph G = (V, E), the embedding matrix consists of |V| vectors of d dimension. Each row of the embedding matrix corresponds to a node in the graph and each value in a d dimension vector captures a feature in the original graph. The mapping function is:

$$f: v_i \longrightarrow d_i \in \mathbb{R}^d, d \ll |V|, \tag{1}$$

where d is the dimension of the vector representation. The *first-order* proximity as defined in [11] is the pairwise proximity between two nodes. If there is no edge between two vertices, the first-order proximity between them is zero. If two vertices are linked by an edge with high weight, their embedding should be close in d dimensional space. This objective can be obtained by minimizing the distance between the two distributions for every vertex (vector space and empirical probability distribution of the graph). If we use the Kullback-Leibler (KL) divergence to calculate the distance, the objective function can be defined:

$$O_1 = -\sum_{(i,j)\in\mathbb{E}} w_{ij} \log p_1(v_i, v_j), \qquad (2)$$

where

$$p_1(v_i, v_j) = \frac{1}{1 + \exp(-\vec{u}_i^T \cdot \vec{u}_j)},$$
(3)

where  $\vec{u}_i$  is low dimensional vector representation of vertex  $v_i$  and  $w_{ij}$  is the weight. The *first-order* proximity is only applicable for undirected graphs. The *second-order* proximity [11] is applicable for both directed and undirected graphs. The *second-order* assumes a 2-step relationship between two vertices, where they share many connections but with no direct link between them. Consequently, the embedding for these two nodes needs to be close as they share similar neighborhood structures. In *second-order* proximity, each vertex is considered once for its actual connections and once for being a *context* for other nodes with similar structure. Therefore, we have two embedding representing two different roles for each vertex. The objective function for the *second-order* proximity is given by:

$$O_2 = -\sum_{(i,j)\in\mathbb{E}} w_{ij} \log p_2(v_j|v_i),\tag{4}$$

where

$$p_{2}(v_{j}|v_{i}) = \frac{\exp(\vec{u'_{j}}^{T}.\vec{u}_{i})}{\sum_{k=1}^{|V|} \exp(\vec{u'_{k}}^{T}.\vec{u}_{i})}$$
(5)

and where  $\vec{u}_i$  is vector representation of vertex  $v_i$  when we consider it as a vertex and  $\vec{u}'_j$  is embedding vector for  $v_j$  when it is considered as context for for vertex  $v_i$ . Computing the optimization in eq.4 is computationally expensive, since it sums over the entire set of vertices. To simplify the computation for large-scale graphs, negative sampling[16], [17] is adopted by recognizing the neighbors from others. This has been done by sampling multiple negative samples according to the noise distribution. Therefore, in the training process, each positive edge is trained with a set of negative samples.

Generally, the embedding learning process consists of traversing the graph and then performing training on the samples obtained from the graph. Once the graph is sampled, graph embeddings are trained on these samples. At first, the graph with all nodes and edges are [9], [10], [11] loaded into the main memory with O(V + E) space. Then sampling is done by various approaches, e.g. sequence-based learning methods [9], [10] or direct sampling [11]. In the first set of

methods, a sequence of nodes is obtained by starting from a node and traversing its neighbors in a random manner (random walk). The sequence of nodes that appear in these random walks suggests that closer nodes in the graph will appear frequently together. Therefore, a machine learning algorithm can be utilized such that the closer nodes in random walks follow similar embedding. In the second approach, samples are obtained from a randomly picked edge (e.g. [11]) on the graph. For this approach, training node embedding includes computing the dot product of embedding for positive edges (actual samples) with some randomly negative edges (non-real links between nodes). For example in [11], we have two sets of embeddings, namely, the vertex embedding matrix and context embedding matrix. For an edge sample (u, v), the dot product of vertex[u] and context[v] is computed to predict whether the sample is a positive edge or drawn from negative samples. This encourages neighbor nodes to have close embeddings, whereas distant nodes will have very different embeddings. While these methods perform well on small graphs, they require hours or even days of training on larger graphs [18]. Thus it can be very challenging to adapt current node embedding methods to largescale graphs. The first limitation is the memory requirement for a large graph. The procedure of random walk (which is common in existing methods) poses a lot of random access memory. Therefore, to reduce the latency, the whole graph is maintained in the main memory while performing the random walk sampling. This is problematic when the graph is larger than the available memory for a CPU node. Subsequently, the augmented graph obtained from random walks along with the vector embedding and model parameters can exceed the memory capacity of a general computing server. Vector of node embedding for a graph with millions nodes is quite large for a single CPU's memory or a modern GPU's memory to hold. The next issue is the large amount of matrix computation that needs to be efficiently done in CPU. One way is to use the distributed setting to train large networks. However, extending the existing methods to distributed settings is a nontrivial task.

### A. Related Work

There are many algorithms in the literature on graph embedding learning. Our proposed framework follows the method that has been used in LINE [11]; a method which is parallelizable and consumes less memory compared to other methods. The memory requirement is bounded by the number of nodes which is O(V + E) in this work. When memory is not sufficient to hold this data in the available CPU memory, we perform partitioning to obtain a sub-graph where it can be maintained in CPU's main memory. Then in the training phase, we use two joint probability distributions for each pair of nodes (u, v), then minimize the KL divergence of the distributions (distance measure between two probability distributions). While our method tackles the memory usage bottleneck of training effectively, GPU capability becomes a good candidate for speeding up the compute-intensive part of the training. Our proposed embedding system allows working with large networks using a CPU with GPU. Thus, in our hybrid system, both CPU and GPU resources will be exploited effectively to achieve high performance computing.

Graph embedding aims to learn continuous feature representations of nodes by optimizing a neighborhood preserving likelihood objective. It iterates through all nodes in a graph, and for every node it aims to embed it such that its embedding can predict related edges to other nodes. To obtain such embedding, the node embedding method includes two stages: reading the graph and training. Generally, graphs are sparse, partially visible, or too large to be processed entirely. One way to achieve this is performing random walks over the graph to generate samples. Random walks are generated through running short random walks starting from each node on the graph. Training learns the node embedding through the model language that uses samples obtained in the previous phase as its input. The procedure of generating samples from edges or paths is widely adopted in existing methods, such as DeepWalk[9], LINE[11] and node2vec[10]. DeepWalk, and node2vec use random walks to expand the neighborhood of a vertex, with different strategies for sampling the paths. DeepWalk runs fixed-length, unbiased random walks starting from each vertex. Node2vec applies the same procedure as DeepWalk, with the difference of flexible, biased random walks being performed as a combination of breadth first search (BFS) and depth first search (DFS) to traverse the vertices of the graph. In a different approach, the embedding can be learned directly from the graph without any random walk, e.g. LINE [11] samples the edges independently and utilizes them as samples for training. As mentioned above, the second phase is to train the node embedding using the generated samples. In existing methods [10], [9], [11] node embedding are learned by optimizing the likelihood objective using SGD and the help of negative sampling/hierarchical softmax. The objective states that nodes within a structure tend to have similar embeddings. In DeepWalk, the probabilities of observing sequences of nodes (random walks) around a central node are maximized, which result in preserving the higher-order proximity between these nodes. In node2vec, the optimization is performed over the sum of log-likelihood for each sequence of nodes and can be regarded as an extension of DeepWalk. LINE defines two different functions, one for first-order proximity and one for second-order proximity. For each pair of nodes, the LINE calculates two joint probability distributions using the adjacency matrix and the dot product of the embedding, and then it tries to minimize the KL divergence of the two distributions.

Regarding to large-scale graphs, DeepWalk, node2Vec, and LINE are the most scalable among the proposed methods in the literature. These methods have a CPU parallel implementation for the node embedding training. Even with exploiting multiple threads in a CPU, the implementation of these methods does not scale to a graph with millions of nodes efficiently. The random-walk-based solutions suffer from immense computational costs, since they need to sample a large number of random walks and conduct expensive training processes, which can be prohibitive for large graphs. To alleviate the efficiency issue, massively parallel network embedding systems, e.g., GPU systems, e.g., in Graphvite[13], are developed to utilize a large system with multiple processing units. These frameworks adopt non-overlapping network partitioning methods to create smaller partitions with distinct vertices. They update the global parameter at each iteration of the learning phase. PyTorch-BigGraph (PBG) is a distributed system running on a cluster of machines with emphasis on scalability which is based on PyTorch. PBG uses ideas such as adjacency, matrix partitioning, and reusing examples within one batch to train models and applies different strategies for distributed training. It randomly divides the adjacency matrix of a graph into 2D blocks and assigns blocks to each machine based on a schedule that avoids conflicts with respect to the entity embedding. However, PBG uses a parameter server to synchronize embedding, in which all workers need to communicate with the parameter server, including synchronously sending the gradients and receiving the average gradient and the bottleneck is the bandwidth between the parameter server and workers. The other GPUSbased framework, GraphVite focuses on multi-GPUs singlenode machine training using the CPU as the parameter server and GPU for computation. When it trains a knowledge graph, it stores the node embedding parameters in CPU memory. It constructs a sub-graph, moves all data in the sub-graph to GPU memory, and performs many mini-batch training steps on the sub-graph. In GraphVite, training is performed synchronously and batches are formed and transferred on-demand. While synchronous training is beneficial for convergence, it is resource inefficient. The GPU will be idle while waiting for the batch to be formed and transferred. Moreover, gradient updates also need to be transferred from the GPU to CPU memory and applied to the embedding table, adding additional delays. As a result, GraphVite has largely improved the training time for medium size node embedding tasks. However, its design uses CPU as a parameter server to run random walk online and transfer embedding between GPUs, also the system lacks a pipeline design to properly overlap communication with computation. This method reduces the data movement between CPUs and GPUs at the cost of increasing the staleness of the embedding, which results in slower convergence. In addition, it cannot embed a graph when the total size of the embedding is larger than the total available GPU memory. With GPU memory size usually much smaller than the available RAM, this is a serious limitation. As the network size increases, the communication cost of updating the parameters over multiple iterations aggravates. In contrast, our hybrid framework utilizes a small CPU-GPU system for training large graph embeddings, with computation and data transfer overlapped between CPU and GPU. The CPU is responsible for loading, storing, and preparing the training inputs and model parameters while GPU independently is performing the computation on the assigned embedding vectors in a parallel manner.



Fig. 2: System architecture. The process consists of various stages: pre-processing, data preparation, data movement, and computation in GPU. First stage is responsible for data and node partitioning regarding available CPU and GPU memory. Then, multiple threads form the next batch of data by populating edges in multiple queues. These queues will be transferred to the GPU memory. When the GPU becomes available, the computation for one of the available queues will be started. Then gradient updates will be applied to the node embedding partition that resides in GPU memory. This process continues until all partitions are traversed.

# III. OUR HYBRID CPU-GPU METHOD

There are many efforts on graph embedding, which mainly perform well on small-size graphs. However, real graphs pose an extra challenge to the standard embedding methods by including millions of nodes and billions of edges, where each edge represents a connection between nodes. In existing methods, the first step of graph embedding training is to sample the graphs by random walks. Therefore, the original graph needs to be placed into the main memory to mitigate the effect of random-access memory caused by random walks. The resulted graphs, namely, the augmented graph, are usually in the order of magnitude larger than the original graph's size. Thus, it is impossible to load large-scale graphs into the main memory if the original graph is already very large. To support largescale graph training with GPU memory constraints, we store the embedding parameters in CPU memory and partially send parts of it to GPU memory. Uniform partitioning is used to split up node embedding parameters into n disjoint partitions that are calculated based on the available GPU memory and then store them on a disk. This requires training examples for each node partition, which are essentially edges of the graph, to be transferred between CPU and GPU frequently. Edges are then divided into  $n^2$  edge buckets, according to their source and destination. For each edge in bucket (i, j), the source belongs to i - th partition and destination located in j - thpartition. Each epoch in our training involves iterating over all edges in a partition. After performing the training on each bucket, the node embedding related to the next bucket will be swapped in GPU memory. Mini-batch training is performed synchronously while batches are formed and transferred on demand. When GPU is processing the current batch, the CPU is preparing the future batches simultaneously that ensure the GPU will not be idle while waiting for the next batch to be formed. Although the performance of GPU is superior compared to CPU, it requires an approach to synchronize the call execution and transfer pattern between CPU and GPU while properly managing CPU-GPU communication to hide the communication overhead. Thus, we design a system that utilizes the distinct advantages of CPU and GPU and use them collaboratively to hide communication and memory bottlenecks. By using the data movement pipeline, we overlap the computation with data movement, which improves the utilization of CPU and GPU resources. Finally, our method is not limited by the size of the CPU and GPU memory, which is essential for training large graph embedding models.

## A. Pipeline

We now describe the pipeline of our hybrid system model, which includes pre-processing, preparing inputs, data movement, and computation in GPU. The pipeline includes multiple threads that pre-process training edges in parallel and populate them in multiple queues. Consequently, all full capacity queues will be transferred to the GPU for the next batch of training. On the GPU side, batches of training data will be waiting for the GPU to become available for training. By keeping multiple queues populated with new batches of data, we ensure the maximum utilization of the GPU. Except the pre-processing step, all other stages have a configurable number of threads that can collaborate in parallel, while in-GPU computation consists of thousands of threads performing training on various edges. Here is a detailed explanation of our pipeline:

1) *Pre-processing:* The process (left side of Fig. 2) starts with reading the graph (number of nodes, edges), followed by calculating the degree of each node and storing the information in the memory required for the training. Then, with respect

to the available CPU memory, a portion of edges from the original graph is loaded to CPU memory. If size of the embedding model is larger than the size of GPU memory (that is true for most large-scale graphs), the node embeddings will be partitioned into a p-disjoint set of vertices. For each edge (i, j), the source and destination can be in any of the p partitions. Thus, all entries (i.e., edges) of the graph correspond to  $p^2$ different partitions. In summary, for each of  $p^2$  bucket, all edges from the graph will be collected in the main memory, while the node embedding for this bucket will be transferred to the GPU memory. Moreover, following the method that used in LINE, we have two sets of vertices for one-hop and twohop connectivity (vertex and context embeddings). For onehop computation, the embedding for source and destination is the same, whereas for two-hop embedding for destination is different.

2) Preparation: This stage (middle part of Fig. 2) is responsible for populating edges into multiple queues. In an online parallel manner, each thread is assigned to an equal-size portion of the graph stored in memory. Threads independently access the memory, retrieve edges to form the next batch of data that corresponds to the node embedding partitions that reside in GPU memory. Threads also prepare the negative (non-real) edges along with positive ones (non-real) and place them in smaller queues. These queues are part of larger queues that eventually will be distributed to the GPU memory whenever they become full. On GPU, a kernel is launched to process each batch of training inputs. When performing GPU computation, the worker threads at this stage prepare the next batch of training inputs. When GPU completes the execution, these threads redistribute a new batch of data for the next round of computation. This procedure is replicated by all threads available on the CPU for a number of epochs.

3) Data Movement: To avoid memory access conflict between multiple workers in the preparation stage, each worker thread is assigned to a smaller queue (middle part of Fig. 2). When all threads finish their tasks, one thread worker will concatenate all small-size queues and form a larger queue that is proportion to the compute capability of the GPU. This thread is responsible for moving the batch data to GPU memory and waiting for the GPU to become available for the training of the next batch. Each parallel queue is assigned to one CUDA stream in a GPU. Each batch queue waits for the previous kernel call to finish the processing and then initiates the next kernel call. When GPU execution is completed, the next kernel execution starts using the batch already waiting to be processed. If all queues are full at the current time, threads in the previous stage stop reading the edges until activativating again. By starting the next batch of data in GPU, one of the large queues will be available for threads in CPU to be populated again. When a bucket from  $p^2$  partition is trained, the node embedding model will be moved from GPU to CPU and finally saved to the disk. This sequence of tasks continues until the last batch of data from the last bucket is processed.

4) Computation: GPU (right side of Fig. 2) is performing parallel computations by thousands of light-weight threads

for training the embedding of assigned samples.GPU works on learning the embedding of different nodes by iterating on thousands of samples. Due to the limited GPU memory and the size of real graphs, the entire embedding vectors cannot be stored on GPU. As mentioned before, the problem of limited GPU memory is solved as GPU stores only a subset of embeddings corresponding to the current samples. During the training, both vertex and context embedding matrices should be transferred to the GPU in a small chunk. Therefore, upon completion of the training for each chunk, the GPU copies the embedding vectors to the CPU memory and continues with the next stream of samples if available. The embedding model for the next partition of nodes will be pulled from the GPU memory. This collaborative training allows GPU to train node embedding efficiently, with only synchronization required after training each partition of graph. The size of queues is obtained with respect to the memory of GPU and how frequently synchronization is needed. Thus, instead of storing the whole embedding vectors on a GPU memory, we transfer a portion of them by a small granularity.

A major limitation of GPU is the bus bandwidth. The computations of GPU happen much faster than the transfer of data between CPU-GPU. To keep GPU well fed to training operations, greater parallelism is required. Therefore, threads in a multi-core CPU parse the input file and generate batches of training samples in multiple queues. To reduce the idle time and latency in both CPU and GPU, we leverage multiple online queues for GPU that are ready to transfer the next batch of training data from CPU to GPU. Threads in a multi-core CPU do this parsing at the same time that the GPU is using its floating-point units to process training batches. CPU threads fill up a queue and when each GPU is available, the training data is iteratively passed to it. Our method requires more data transfer to the GPU, but it allows the multi-core CPU to handle the parsing of inputs while the GPU need only handle floating point operations, which are still the bulk of the work (90%) in this application. The CPU to GPU memory transfer latency is hidden and overlapped by the amount of time it takes to complete the floating-point operations.

### **IV. EXPERIMENTS**

In this section, we report our experimental findings on the performance and accuracy of the embedding vectors obtained using our system model compared to other relevant methods (node2vec, DeepWalk, LINE, Graphvite). To test the effectiveness of our proposed framework, we deploy a link prediction task. The main idea is how well a given method can predict the missing links between various nodes using small graphs, i.e. Email-EuAll, WikiVote, Com-dblp, medium size graphs i.e. Web-Google, Youtube, Soc-LiveJournal1. Summaries and description of all graphs are provided in Table I. As for large-scale graphs which are computationally expensive and impossible to train on the baseline models, we employ large-scale embedding framework. The details of these frameworks are described in the compared methods. We perform a comparative speed evaluation on all methods while having small

Dataset	V	E	Description
Wiki-Vote	7,115	103,689	Wikipedia who-votes-on-whom network
Email-EuAll	265,214	420,045	Email network from a EU research institution
Com-dblp	317,080	1,049,866	DBLP collaboration network
Web-Google	875,713	5,105,039	Web graph from Google
Youtube	1,138,499	4,945,382	Youtube online social network
Soc-LiveJournal1	4,847,571	68,993,773	LiveJournal online social network
Hyperlink	39,497,204	623,056,313	Hyperlink network from web
Twitter	41,652,230	1,468,365,182	Twitter online social network
FRIENDSTER	65,608,376	1,806,067,142	Friendster online social network

TABLE I: Properties of small, medium, and large graphs used in the experiments

and medium graphs. Our hyperparameters are set according to the settings similar to Graphvite. We train each model with the default values of each methods' optimal configurations suggested by their authors in their original papers or repositories per each dataset. We treat graphs as undirected graphs. For DeepWalk, during the network augmentation stage, we use random walks with a length of 20 edges to meet the constraint of time. For this method, we reduced the value of parameters because with the recommended configuration, the execution time passed the 24 hours limitation in our system. All experiments are conducted on identical hardware (CPU and GPU instances) using a single node on a Linux-based server running Ubuntu 18.04. The configuration consists of one compute node with 1-26 cores and a clock speed of 2.10GHzpowered by an NVIDIA Tesla k80. We used CUDA 10.0 runtime and driver APIs as a C/C++ extension for using the GPU. Our system program includes two main parts: CPUcode and GPU-code. CPU code is a regular C/C++ code with CUDA run-time library and it is able to call device functions (kernel function) in GPU-code. The GPU-code contains the functions required for kernel execution, and several device functions to copy and transfer data/results between CPU cores and the GPU devices. We tune the length of the queue for GPU to maximize the speed of our hybrid system. During the embedding training stage, negative samples are sampled with a probability proportional to the 3/4 power of the node degrees. For each positive sample, we draw 5 negative samples to match the gradient scale in LINE and Graphvite. We follow the initial learning rate of 0.025 and the linear learning rate decrease mechanism in LINE, DeepWalk, and Graphvite. We define a training epoch as training |E| positive edge samples. For a fair comparison, we report the training time of all methods with the same number of training epochs. For all methods except DeepWalk, the total number of training epochs is set to 2.000. The dimension of node embedding is set to 128except otherwise noted. We omit the result of a method on a dataset, if the algorithm cannot handle the dataset with the issue of memory limit, or the algorithm cannot finish within 24 hours.

# A. Compared Methods

To evaluate the performance of our framework, we consider the following state-of-the-art graph embedding methods/systems for comparison. We use the recommended parameters as mentioned in their paper. Except otherwise noted, the representation dimension for all algorithms is d = 128 and the number of threads per CPU is 26.

- LINE [11]: is a CPU based embedding learning system. It can train the embedding in a parallel fashion by optimizing the objective function of edge reconstruction. We use the configuration of the YouTube dataset from the author repository for embedding this dataset. The parameters were set the same as the original paper, namely,  $\rho 0 = 0.025$ , negative sampling K = 5 and sample size T = 10000. We concatenate the embedding obtained from first-order and second-order as recommended by the authors.
- **Graphvite** [13]: is a hybrid CPU-GPU implementation for learning embedding running on a single machine node, which is the existing fastest system to train graph node embedding. However, this framework cannot embed graphs with embeddings larger than a single GPU memory capacity. The default value for the parameters is used as recommended by the authors and LINE is chosen as the base embedding method.
- **DeepWalk** [9]: is a CPU parallel system running on one machine using multiple threads, written in Python. This method samples the graphs through random walks obtained from each node (DFS). Then it applies word2vecbased[19] learning on those walks. We tried to use the default parameters described in the paper, i.e., walk length t = 80, numbers of walks per node  $\gamma = 80$ . However, none of the experiments could finish in 24 hours (time limitation). Thus, we updated the parameters as following: The window size win = 10, walk length t = 20, and walk per node  $\gamma = 10$ .
- Node2Vec [10]: is a CPU based learning method, written in Python and can perform in parallel. This approach extends DeepWalk by adding two parameters, p and q



Fig. 3: Results of various method's runtime on small size graphs.

Fig. 4: Runtime for medium scale graphs on compared methods.



Fig. 5: Results of link prediction on small and medium size graphs, as compared with state-of-the-art embedding methods

to control the sampling of random walks. We used the original author configuration on the set of graphs we had. None of the executions finished in 24 hours, either by the time limit exceeded or the program's issues.

# B. Datasets

We use several graphs to evaluate and compare the performance of our method with other tools in terms of performance and quality. These datasets are obtained from real networks and have different number of vertices (spanning from small, medium-sized, and large), and origin. These datasets are standard benchmarks for evaluating graph embedding methods. Table 1 shows the properties and statistics of these graphs.

- WikiVote [20]: is a network obtained from Wikipedia voting data from the inception of Wikipedia. Nodes in the network represent Wikipedia users and a directed edge from node i to node j represents that user i voted on user j.
- Email-EuAll [21]: is a directed email network generated using email data from a large European research



Fig. 6: Effect of embedding dimension on training time for large-scale graphs

institution. Given a set of email messages, each node corresponds to an email address.

- **Com-dblp** [22]: is DBLP collaboration network where two authors are connected if they publish at least one paper together.
- Web-Google [23]: is a web graph obtained from Google where nodes represent web pages and directed edges represent hyperlinks between them. The data was part of Google Programming Contest in 2002.
- Youtube [24]: is a directed social network among users of YouTube, including over 1.1 million nodes and about 4.9 million edges. The labels of these nodes represent the type of videos watched by each group of users.
- **Soc-LiveJournal1** [25]: is a directed network obtained from LiveJournal; a free online community with almost 10 million members.
- **Hyperlink** [26]: is a hyperlink network generated from the Web with 43 million nodes and 623 million edges.
- **Twitter** [27]: is a network of follower relationships from a snapshot of Twitter in 2010. An edge from i to j indicates that j is a follower of i.
- **FRIENDSTER** [22]: is an online social networking site where users can form a friendship edge with each other.

# C. Metric Evaluation

We conduct several experiments to measure the efficiency of different methods in terms of runtime for small, medium, and large graphs. To standardize the experiments, we execute all CPU-based implementations with 26 parallel threads and run with similar sample size similarly for hybrid CPU-GPU methods. For measuring the efficiency of hybrid systems, we assign one GPU to a CPU node, and we further measure the performance of CPU and GPU (if available) in each system model. We evaluate the quality of the embedding via link prediction that uses the embedding vectors generated from each method. Link prediction is commonly used for the evaluation of graph embedding frameworks. Therefore, we implemented the well-known logistic regression method as a baseline for link prediction. We measure the accuracy of the prediction by reporting the average number of accurate predictions. Following the suggested evaluation paradigm, we split the input graph into train and test with 70% and 30% of the edges respectively. We split the experiments to include positive and negative edges for both train and test parts during the evaluation. For link prediction, we evaluated each individual embedding 6 times. We report the average values over the runs.

# D. Results

1) samll- and medium-size dataset: Fig. 3, and Fig. 4 represent the experiment on the running time of each algorithm on small and medium size datasets resepctivly, where 2 of these datasets have more than one million of nodes. As shown in Figure Fig. 3, our model is able to handle small datasets and outperforms all other methods. For speedup comparison, we considered LINE as a baseline since we followed the algorithm of this work. Compared to LINE, our method in small graphs achieves 100X - 500X speedup, while this acceleration even increases regarding Deepwalk. Graphvite as a hybrid CPU-GPU implementation of LINE shows slower performance compared to our model across these datasets, where our model shows an acceleration of 15X - 75X over this method. Similarly, the results of medium-size graphs (Fig. 4) verify above discussion, where our method only needs 10 seconds to train 2000 epochs on youtube data. In particular, our model runtime is 342X and 75X faster than LINE and Graphvite, respectively, which demonstrates the superiority of our computing approach compared with the single-machine ones. Based on these results, our method is the most efficient method for running on both small- and medium-sized graphs. On one GPU, our system finishes training node embedding on a million-scale network in the order of seconds for 2000 epochs. Besides, the result of node2vec is missing on all graphs due to timeout (24 hours limit). This is because of the



Fig. 7: Effect of CPU-threads on runtime

high cost of matrix manipulations that cause the issue of memory overflow, rendering them difficult to handle large graphs. Furthermore, the result of DeepWalk on the Soc-LiveJournal1 dataset is missing, since it cannot finish within 24 hours, which is caused by the similar memory problem of Node2vec. To measure the quality of node embedding learned by various methods, we use the standard task of link prediction. We follow the pipeline of widely adopted link prediction methods [10], [11]: graph embedding are first learned and then used as feature inputs to build a binary classifier (e.g., Logistic Regression, SVM, MLP) to predict the unobserved links. Area under ROC curve (AUC) is used to different embedding methods performance. Fig. 5 shows the AUC score used to evaluate the performance of different embedding methods. It is observed that our system achieves comparable AUC scores in most settings, showing that it does not sacrifice much quality over the runtime. There is a negligible difference regarding the performance of the embedding generated by our framework compared to others. This is predictable due to the fact that we tried to achieve the maximum parallelism on GPU. Thus, we load as many edge samples as possible to be computed at the same time on the GPU, which causes the overlap of the update parameters to expand which which means some of the computation results will not be applied to the model parameters. This has a direct effect on accuracy. Therefore, to achieve higher accuracy, one can reduce the maximum level of parallelism on GPU to obtain a higher score. Among the baseline methods, DeepWalk achieves the highest accuracy and the fastest convergence, because it uses both hierarchical softmax and negative sampling, while its algorithm considers a higher order of connectivity compared to the LINE. Therefore, our model and Graphvite show the same pattern because of using one-hop and two-hop connectivity that introduced in LINE. As the results show, our method reaches a similar accuracy while our model significantly reduces the training complexity with negligible accuracy loss in small and medium size scale compared to the GPU-based method, which also can be recovered by reducing the maximum parallelism on GPU.

2) Large-scale dataset: To demonstrate the scalability of our method, we test it on larger graphs of Friendster, Hyperlink-PLD, and Twitter on 1 GPU. The training times of baseline systems are not reported here, as all compared systems cannot solve such a large graph with/without one GPU. In the case of Graphvite, the embedding matrices for these datasets cannot fit into the memory of a single GPU, therefore it is not able to produce any results. Fig. 6 shows the performance of our model versus various dimensions of embeddings obtained for three large datasets. It is observed that our model computes embedding in a fast time on all these datasets. Using the Hyperlink-PLD, we obtain an embedding from the dimension of 32 to 256 around 30-500 seconds. For Twitter and Friendster, the performance shows an increase in runtime due to the larger number of edges to be computed the same as the number of nodes. The above observations verify the performance of our system on large-scale datasets. Our method takes less than 5 minutes to train node embedding on the Friendster with 1.8 billion edges with a dimension of 128, showing that our tool can be an efficient tool for analyzing billion-scale graphs on a single GPU. Fig. 7 presents the parallel training time relative to various numbers of CPU threads used in our method on large datasets with a dimension of 128 for one epoch. In this experiment, we measure their training

time in GPU and preparation time in CPU, including memory access and populating queues. As this figure illustrates, more number of CPU threads corresponds to better performance of CPU-side pipeline, thus decreasing the overall time of execution. However, more number of threads does not change the GPU's execution time, where GPU exploits thousands of parallel threads for the computation. The training time of GPU includes the data transfer time between CPU and GPU.

### V. DISCUSSION AND FUTURE DIRECTIONS

In this paper, we present a framework that performs a parallel computation on a single GPU for training the embedding. This framework improves the performance of existing graph embedding systems by introducing memory-aware edge traversal model, partitioning-based embedding for GPUmemory constraints, and a pipeline to minimize the transfer time between disk to CPU-memory and CPU-memory to GPU-memory. The tool is fast and accurate that can train arbitrary-size graphs on a single CPU-GPU system. When using GPU, we perform the embedding in multi-steps regarding the available GPU memory. Through this process, the graph is partially read in a parallel manner while trying to avoid generating/holding massive vertex embeddings during training. With this technique, the initial graph is iteratively read into multiple queues corresponding to GPU computation capability. Then, starting from the first tier of nodes in the graph, unsupervised training is performed on a GPU device. The embedding obtained from the current set of nodes will be transferred to CPU's main memory before starting the new set of vertices. The process continues with the embedding of the next set of vertices until the original graph is processed on the GPU and the final embedding is obtained. We introduce a highperformance CPU-GPUs hybrid system that provides highquality, fast graph embedding. In addition to this, we provide concurrency techniques between CPU-GPU to minimize the overhead of transferring data to GPU and thus maximizing GPU utilization during training. Our experiments demonstrate the effectiveness of our method on various sizes of graphs. In the future, we will extend our method to the multi-GPU version.

### REFERENCES

- [1] L. C. Freeman, "Visualizing social networks," *Journal of social structure*, vol. 1, no. 1, p. 4, 2000.
- [2] A. Theocharidis, S. Van Dongen, A. J. Enright, and T. C. Freeman, "Network visualization and analysis of gene expression data using biolayout express 3d," *Nature protocols*, vol. 4, no. 10, pp. 1535–1550, 2009.
- [3] D. Liben-Nowell and J. Kleinberg, "The link-prediction problem for social networks," *Journal of the American society for information science and technology*, vol. 58, no. 7, pp. 1019–1031, 2007.
- [4] S. Cavallari, V. W. Zheng, H. Cai, K. C.-C. Chang, and E. Cambria, "Learning community embedding with community detection and node embedding on graphs," in *Proceedings of the 2017 ACM on Conference* on Information and Knowledge Management, pp. 377–386, 2017.
- [5] W. L. Hamilton, R. Ying, and J. Leskovec, "Representation learning on graphs: Methods and applications," arXiv preprint arXiv:1709.05584, 2017.
- [6] P. Goyal and E. Ferrara, "Graph embedding techniques, applications, and performance: A survey," *Knowledge-Based Systems*, vol. 151, pp. 78–94, 2018.

- [7] J. Tang, J. Liu, M. Zhang, and Q. Mei, "Visualizing large-scale and highdimensional data," in *Proceedings of the 25th international conference* on world wide web, pp. 287–297, 2016.
- [8] A. Lerer, L. Wu, J. Shen, T. Lacroix, L. Wehrstedt, A. Bose, and A. Peysakhovich, "Pytorch-biggraph: A large-scale graph embedding system," arXiv preprint arXiv:1903.12287, 2019.
- [9] B. Perozzi, R. Al-Rfou, and S. Skiena, "Deepwalk: Online learning of social representations," in *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 701–710, 2014.
- [10] A. Grover and J. Leskovec, "node2vec: Scalable feature learning for networks," in *Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 855–864, 2016.
- [11] J. Tang, M. Qu, M. Wang, M. Zhang, J. Yan, and Q. Mei, "Line: Large-scale information network embedding," in *Proceedings of the 24th international conference on world wide web*, pp. 1067–1077, 2015.
- [12] C. Deng, Z. Zhao, Y. Wang, Z. Zhang, and Z. Feng, "Graphzoom: A multi-level spectral approach for accurate and scalable graph embedding," arXiv preprint arXiv:1910.02370, 2019.
- [13] Z. Zhu, S. Xu, J. Tang, and M. Qu, "Graphvite: A high-performance cpu-gpu hybrid system for node embedding," in *The World Wide Web Conference*, pp. 2494–2504, 2019.
- [14] H. Cai, V. W. Zheng, and K. C.-C. Chang, "A comprehensive survey of graph embedding: Problems, techniques, and applications," *IEEE Transactions on Knowledge and Data Engineering*, vol. 30, no. 9, pp. 1616–1637, 2018.
- [15] D. Zhang, J. Yin, X. Zhu, and C. Zhang, "Network representation learning: A survey," *IEEE transactions on Big Data*, vol. 6, no. 1, pp. 3– 28, 2018.
- [16] T. Mikolov, I. Sutskever, K. Chen, G. S. Corrado, and J. Dean, "Distributed representations of words and phrases and their compositionality," in Advances in neural information processing systems, pp. 3111– 3119, 2013.
- [17] M. F. Møller, "A scaled conjugate gradient algorithm for fast supervised learning," *Neural networks*, vol. 6, no. 4, pp. 525–533, 1993.
- [18] B. Rychalska, P. Bąbel, K. Gołuchowski, A. Michałowski, and J. Dąbrowski, "Cleora: A simple, strong and scalable graph embedding scheme," arXiv preprint arXiv:2102.02302, 2021.
- [19] T. Mikolov, K. Chen, G. Corrado, and J. Dean, "Efficient estimation of word representations in vector space," *arXiv preprint arXiv:1301.3781*, 2013.
- [20] J. Leskovec, D. Huttenlocher, and J. Kleinberg, "Signed networks in social media," in *Proceedings of the SIGCHI conference on human factors in computing systems*, pp. 1361–1370, 2010.
- [21] J. Leskovec, J. Kleinberg, and C. Faloutsos, "Graph evolution: Densification and shrinking diameters," ACM transactions on Knowledge Discovery from Data (TKDD), vol. 1, no. 1, pp. 2–es, 2007.
- [22] J. Yang and J. Leskovec, "Defining and evaluating network communities based on ground-truth," *Knowledge and Information Systems*, vol. 42, no. 1, pp. 181–213, 2015.
- [23] J. Leskovec, K. J. Lang, A. Dasgupta, and M. W. Mahoney, "Community structure in large networks: Natural cluster sizes and the absence of large well-defined clusters," *Internet Mathematics*, vol. 6, no. 1, pp. 29–123, 2009.
- [24] A. Mislove, M. Marcon, K. P. Gummadi, P. Druschel, and B. Bhattacharjee, "Measurement and analysis of online social networks," in *Proceedings of the 7th ACM SIGCOMM conference on Internet measurement*, pp. 29–42, 2007.
- [25] L. Backstrom, D. Huttenlocher, J. Kleinberg, and X. Lan, "Group formation in large social networks: membership, growth, and evolution," in *Proceedings of the 12th ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 44–54, 2006.
- [26] R. Meusel, S. Vigna, O. Lehmberg, and C. Bizer, "The graph structure in the web-analyzed on different aggregation levels," *The Journal of Web Science*, vol. 1, 2015.
- [27] H. Kwak, C. Lee, H. Park, and S. Moon, "What is twitter, a social network or a news media?," in *Proceedings of the 19th international* conference on World wide web, pp. 591–600, 2010.