DGL-KE: Training Knowledge Graph Embeddings at Scale

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ABSTRACT

Knowledge graphs have emerged as a key abstraction for organizing information in diverse domains and their embeddings are increasingly used to harness their information in various information retrieval and machine learning tasks. However, the ever growing size of knowledge graphs requires computationally efficient algorithms capable of scaling to graphs with millions of nodes and billions of edges. This paper presents DGL-KE, an open-source package to efficiently compute knowledge graph embeddings. DGL-KE introduces various novel optimizations that accelerate training on knowledge graphs with millions of nodes and billions of edges using multi-processing, multi-GPU, and distributed parallelism. These optimizations are designed to increase data locality, reduce communication overhead, overlap computations with memory accesses, and achieve high operation efficiency. Experiments on knowledge graphs consisting of over 86M nodes and 338M edges show that DGL-KE can compute embeddings in 100 minutes on a EC2 instance with 8 GPUs and 30 minutes on an EC2 cluster with 4 machines with 48 cores/machine. These results represent a $2\times \sim 5\times$ speedup over the best competing approaches. DGL-KE is available on https://github.com/awslabs/dgl-ke.

CCS CONCEPTS

• **Information systems** → **Data mining**; *Retrieval models and ranking*; *Web searching and information discovery*.

KEYWORDS

knowledge graph embeddings, large scale, distributed training

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1 INTRODUCTION

Knowledge graphs (KGs) are data structures that store information about different entities (nodes) and their relations (edges). They are used to organize information in many domains such as music, movies, (e-)commerce, and sciences. A common approach of using KGs in various information retrieval and machine learning tasks is to compute knowledge graph embeddings (KGE) [4, 18]. These approaches embed a KG's entities and relation types into a d-dimensional space such that the embedding vectors associated with the entities and the relation types of each edge satisfy a pre-determined mathematical model. Numerous models for computing knowledge graph embeddings have been developed, such as TransE [2], TransR [10] and DistMult [20].

As the size of KGs has grown, so has the time required to compute their embeddings. As a result, a number of approaches and software packages have been developed that exploit concurrency in order to accelerate the computations. Among them are GraphVite [21], which parallelizes the computations using multi-GPU training and Pytorch-BigGraph (PBG) [9], which uses distributed training to split the computations across a cluster of machines. However, these approaches suffer from high data-transfer overheads and low computational efficiency. As a result, the time required to compute embeddings for large KGs is high.

In this paper we present various optimizations that accelerate KGE training on knowledge graphs with millions of nodes and billions of edges using multi-processing, multi-GPU, and distributed parallelism. These optimizations are designed to increase data locality, reduce communication overhead, overlap computations with memory accesses, and achieve high operation efficiency.

We introduce novel approaches of decomposing the computations across different computing units (cores, GPUs, machines) that enable massive parallelization while reducing write conflicts and communication overhead. The write conflicts are reduced by partitioning the processing associated with different relation types

across the computing units as well as reducing data communication on multi-GPU training. The communication overhead is reduced by using a min-cut-based graph partitioning algorithm (METIS [6]) to distribute the knowledge graph across the machines. For entity embeddings, we introduce massive asynchronicity by having separate processes to compute the gradients of embeddings independently as well as allowing entity embedding updates overlapped with mini-batch computation. Finally, we use various negative sampling strategies to construct mini-batches with a small number of embeddings involved in a batch, which reduces data movement from memory to computing units (e.g., CPUs and GPUs).

We implement an open-source KGE package called DGL-KE that incorporates all of the optimization strategies to train KG embeddings on large KGs efficiently. The package is implemented with Python on top of Deep Graph Library (DGL) [19] along with a C++-based distributed key-value store specifically designed for DGL-KE. We rely on DGL to perform graph-related computation, such as sampling, and rely on existing deep learning frameworks, such as Pytorch [13] and MXNet [3], to perform tensor computation. DGL-KE is available at https://github.com/awslabs/dgl-ke.

We experimentally evaluate the performance of DGL-KE on different knowledge graphs and compare its performance against GraphVite and Pytorch-BigGraph. Our experiments show that DGL-KE is able to compute embeddings whose quality is comparable to that of competing approaches at a fraction of their time. In particular, on knowledge graph containing over 86M nodes and 338M edges DGL-KE can compute the embeddings in 100 minutes on a EC2 instance with 8 GPUs and 30 minutes on an EC2 instance with 4 machines with 48 cores/machine. These results represent a 5× and 2× speedup over the time required by GraphVite and Pytorch-BigGraph, respectively.

2 BACKGROUND

Definitions & Notation. A graph is composed of vertices and edges $G = (V, E)$, where V is the set of vertices and E is the set of edges. A knowledge graph (KG) is a special type of a graph whose vertices and edges have types. It is a flexible data structure that represents entities and their relations in a dataset. A vertex in a knowledge graph represents an entity and an edge represents a relation between two entities. The edges are usually in the form of triplets (h, r, t), each of which indicates that a pair of entities h (*head*) and t (*tail*) are coupled via a relation r.

Knowledge graph embeddings are low-dimensional representation of entities and relations. These embeddings carry the information of the entities and relations in the knowledge graph and are widely used in tasks, such as knowledge graph completion and recommendation. Throughput the paper, we denote the embedding vector of head entity, tail entity and relation with $\mathbf{h}$, $\mathbf{t}$ and $\mathbf{r}$, respectively; all embeddings have the same dimension size of d.

Knowledge Graph Embedding (KGE) Models. KGE models train entity embeddings and relation embeddings in a knowledge graph. They define a score function on the triplets and optimize the function to maximize the scores on triplets that exist in the knowledge graph and minimize the scores on triplets that do not exist.

Many score functions have been defined to train knowledge graph embeddings [17] and Table 1 lists the ones used by the KGE models in DGL-KE. TransE and TransR are two representative translational distance models, where we use L1 or L2 to define the distance. DistMult, ComplEx, and RESCAL are semantic matching models that exploit similarity-based scoring functions. Some of the models are much more computationally expensive than other models. For example, TransR is d times more computationally expensive than TransE because TransR has additional matrix multiplications on both head and tail entity embeddings, instead of just element-wise operations on embeddings in TransE.

Table 1: Knowledge graph models. M_r is a relation-specific projection matrix. TransE uses L1 or L2 norm in its score function.

Models	score function $f(\mathbf{h}, \mathbf{r}, \mathbf{t})$
TransE [2]	$-\|\|\mathbf{h} + \mathbf{r} - \mathbf{t}\|\|_{1/2}$
TransR [10]	$-\|\|M_r\mathbf{h} + \mathbf{r} - \mathbf{M_r t}\|\|_2^2$
DistMult [20]	$\mathbf{h}^\top \text{diag}(\mathbf{r})\mathbf{t}$
ComplEx [16]	$\text{Real}(\mathbf{h}^\top \text{diag}(\mathbf{r})\bar{\mathbf{t}})$
RESCAL [12]	$\mathbf{h}^\top \mathbf{M_r t}$
RotatE [15]	$-\|\|\mathbf{h} \circ \mathbf{r} - \mathbf{t}\|\|^2$

To train a KGE model, we define a loss function on a set of positive and negative samples from a knowledge graph. Two loss functions are commonly used. The first is the a logistic loss given by

$$\text{minimize} \sum_{\mathbf{h},\mathbf{r},\mathbf{t} \in \mathbb{D}^+ \cup \mathbb{D}^-} \log(1 + \exp(-y \times f(\mathbf{h}, \mathbf{r}, \mathbf{t}))),$$

where $\mathbb{D}^+$ and $\mathbb{D}^-$ are the positive and negative sets of triplets, respectively, and y is is the label of a triplet, $+1$ for positive and -1 for negative. The second is the pairwise ranking loss given by

$$\text{minimize} \sum_{\mathbf{h},\mathbf{r},\mathbf{t} \in \mathbb{D}^+} \sum_{\mathbf{h}',\mathbf{r}',\mathbf{t}' \in \mathbb{D}^-} \max(0, \gamma - f(\mathbf{h}, \mathbf{r}, \mathbf{t}) + f(\mathbf{h}', \mathbf{r}', \mathbf{t}')).$$

A common strategy of generating negative samples is to corrupt a triplet by replacing its head entity or tail entity with entities sampled from the graph with some heuristics to form a negative sample (h, r, t') or (h', r, t), where h' and t' denote randomly sampled entities. Potentially, we can corrupt the relation in a triplet. In this work, we only corrupt entities to generate negative samples.

Mini-batch training and Asynchronous updates. A KGE model is typically trained in a mini-batch fashion. We first sample a mini-batch of b triplets (h, r, t) that exist in a knowledge graph. The mini-batch training is sparse because a batch only involves in a small number of entity embeddings and relation embeddings. We can take advantage of the sparsity and train KGE models asynchronously with sparse gradient updates [14]. That is, we sample multiple mini-batches independently, perform asynchronous stochastic gradient descent (SGD) on these mini-batches in parallel and only update the embeddings involved in the mini-batches. This training strategy maximizes parallelization in mini-batch training but may lead to conflicts in updating gradients. When two mini-batches run simultaneously, they may use the same entity or relation embeddings. In this case, the gradient of the embeddings is computed based on

the stale information, which results in a slower convergence or not converging to the same local minimum.

3 METHODS

A naive implementation of KGE training results in low computation-to-memory density for many KGE models, which prevents us from using computation resources efficiently. When performing computation on a batch, we need to move a set of entity and relation embeddings to computation resources (e.g., CPUs and GPUs) from local CPU memory or remote machines. For example, for a mini-batch with b positive triplets, k negative triplets, and d-dimensional embeddings, both the computational and data movement complexity of TransE is $O(bd(k+1))$, resulting in a computational density of $O(1)$. Given that computations are faster than memory accesses, reducing data movement is key to achieving efficient KGE training.

In addition, we need to take advantage of parallel computing resources. This includes multi-core CPUs, GPUs and a cluster of machines. Our training algorithm needs to allow massive parallelization while still minimizing conflicts when updating embeddings in parallel.

In this work, we implement DGL-KE on top of DGL [19], completely with Python. It relies on DGL for graph computation, such as sampling, and relies on deep learning frameworks, such as Pytorch and MXNet, for tensor operations.

3.1 Overview

DGL-KE provides a unified implementation for efficient KGE training on different hardware. It optimizes for three types of hardware configurations: (i) many-core CPU machines, (ii) multi-GPU machines, and (iii) a cluster of CPU/GPU machines. In each type of the hardware, DGL-KE parallelizes the training with multiprocessing to fully utilize the parallel computation power of the hardware.

For all hardware configurations, the training process starts with a preprocessing step to partition a knowledge graph and follows with mini-batch training. The partitioning step assigns a disjoint set of triplets in a knowledge graph to a process so that the process performs mini-batch training independently.

The specific steps performed during each mini-batch are:

(1) Sample triplets from the local partition that belongs to a process to form a mini-batch and constructs negative samples for the positive triplets.
(2) Fetch entity and relation embeddings involved in the mini-batch from the global entity and relation embedding tensors.
(3) Perform forward computation and back-propagation on the embeddings fetched in the previous step to compute the gradients of the embeddings.
(4) Apply the gradients to update the embeddings involved in the mini-batch. This step requires to apply an optimization algorithm to adjust the gradients and write the gradients back to the global entity and relation embedding tensors.

KGE training on a knowledge graph involves two types of data: the knowledge graph structure and the entity and relation embeddings. As illustrated in Figure 1, we deploy different data placement for different hardware configurations. In many-core CPU machines, DGL-KE keeps the knowledge graph structure as well as entity and relation embeddings in shared CPU memory accessible to all processes. A trainer process reads the entity and relation embeddings from the global embeddings directly through shared memory. In multi-GPU machines, DGL-KE keeps the knowledge graph structure and entity embeddings in shared CPU memory because entity embeddings are too large to fit in GPU memory. It may place relation embeddings in GPU memory to reduce data communication. As such, a trainer process reads entity embeddings from CPU memory and reads relation embeddings directly from GPU memory. In a cluster of machines, DGL-KE implements a C++-based distributed key-value store (KVStore) to store both entities and relation embeddings. The KVStore partitions the entity embeddings and relation embeddings automatically and strides them across all KVStore servers. A trainer process accesses embeddings from distributed KVStore with the pull and push API. We partition the knowledge graph structure and each trainer machine stores a partition of the graph. The graph structure of the partition is shared among all trainer processes in the machine.

The rest of this section describes various optimization techniques that we developed in DGL-KE: graph partitioning in the preprocessing step (Section 3.2), negative sampling (Section 3.3), data access to relation embeddings (Section 3.4), and finally applying gradients to the global embeddings (Section 3.5).

3.2 Graph partitioning

In distributed training, we partition the graph structure and embeddings and store them across machines. Thus, a machine may need to read entity and relation embeddings from other machines to construct mini-batches. The key of optimizing distributed training is to reduce communication required to retrieve and update entity and relation embeddings.

To reduce the communication caused by entity embeddings in a batch, we deploy METIS partitioning [6] on the knowledge graph in the preprocessing step. For a cluster of P machines, we split the graph into P partitions so that we assign a METIS partition (all entities and triplets incident to the entities) to a machine as shown in Figure 2. With METIS partitioning, the majority of the triplets are in the diagonal blocks. We co-locate the embeddings of the entities with the triplets in the diagonal block by specifying a proper data partitioning in the distributed KVStore. When a trainer process samples triplets in the local partition, most of the entity embeddings accessed by the batch fall in the local partition and, thus, there is little network communication for accessing entity embeddings.

3.3 Negative sampling

KGE training samples triplets to form a mini-batch and constructs a large number of negative samples for each triplet. For all hardware, DGL-KE performs sampling on CPUs and offloads the sampling computation to DGL for efficiency. If we construct negative samples independently for each triplet, a mini-batch will contain many entity embeddings, which results in accessing many embeddings.

We deploy joint negative sampling to reduce the number of entities in a mini-batch (PBG uses a similar strategy). In this approach, instead of independently corrupting every triplet k times, we group

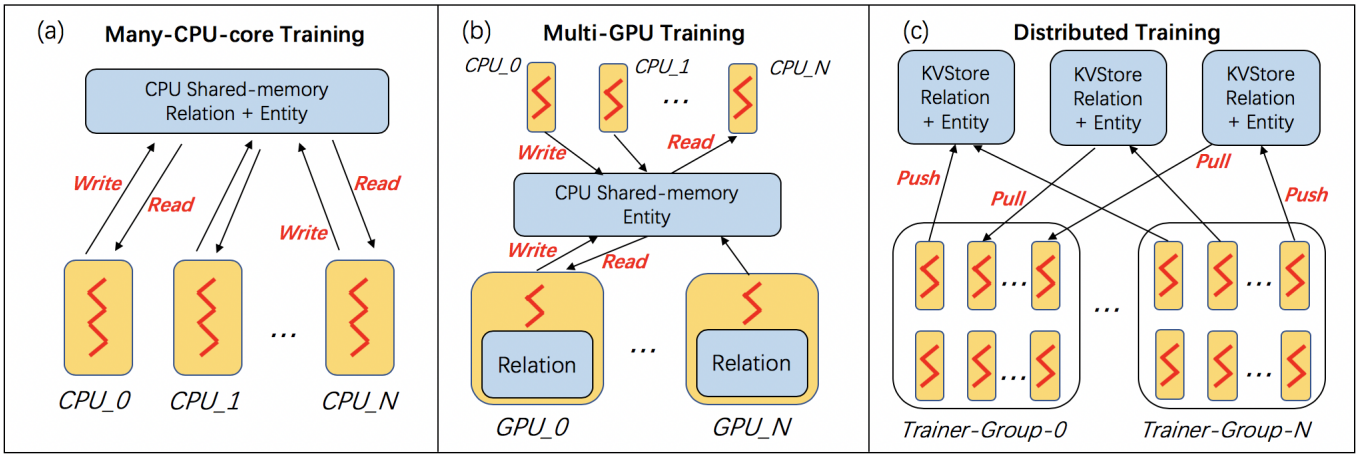


Figure 1: The optimized data placement of DGL-KE in three different parallel hardware.

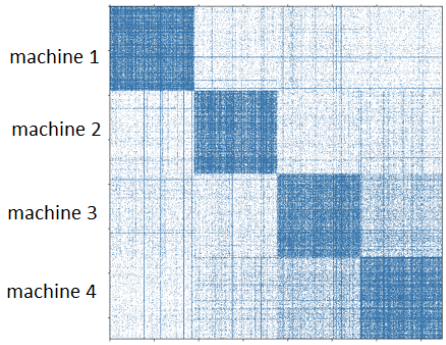


Figure 2: Adjacent matrix of FB15k [2] after applying METIS partitioning, indexed by machine partition. Note that majority of the edges fall within a partition. As a result, the adjacency matrix has majority of non-zeros lying on the diagonal blocks.

the triplets into sets of size g and corrupt them together. For example, when corrupting the tail entities of a set, we uniformly sample k entities to replace the tail entities of that set. We corrupt the head entities in a similar fashion. This negative sampling strategy introduces two benefits. First, it reduces the number of entities in a mini-batch, resulting in smaller data access. For a d-dimensional embedding, each mini-batch of size b now only needs to access $O(bd + bkd/g)$ instead of $O(bd(k + 1))$ words of memory. When g grows as large as b, the amount of data accessed by this negative sampling is about b times smaller (b is usually in the order of 1000). This benefit is more significant in multi-GPU training because we store entity embeddings in CPU memory and send the entity embeddings to the GPUs in every mini-batch. Second, it allows us to replace the original computation with more efficient tensor operations. Inside a group of negative samples, head entities and tail entities are densely connected. We now divide the computation of a score function on a negative sample into two parts. For example, the score function of TransE_l2, $-||\mathbf{h} + \mathbf{r} - \mathbf{t}||_2$, is divided into $\mathbf{o} = \mathbf{h}+\mathbf{r}$ and $-||\mathbf{o}-\mathbf{t}'||_2$. The vector $\mathbf{o}$ is computed as before because there are only b pairs of $\mathbf{h}$ and $\mathbf{r}$. The computation of $-||\mathbf{o} - \mathbf{t}'||_2$ is converted into a generalized matrix multiplication, which can be performed using highly optimized math libraries.

We also deploy non-uniform negative sampling with a probability proportional to the degree of each entity (PBG uses a similar strategy). On a large knowledge graph, uniform negative sampling results in easy negative samples [8]. One way of constructing *harder* negative samples is to corrupt a triplet with entities sampled proportional to the entity degree. In order to do this efficiently, instead of sampling entities from the entire graph, we construct negative samples with the entities that are already in the mini-batch. This is done by uniformly sampling some of the mini-batch's triplets and connecting the sampled head (tail) entities with the tail (head) entities of the mini-batch's triplets to construct the negative samples. Note that this uniform triplet sampling approach leads to an entity sampling approach that is proportional to the entity degree in the mini-batch. In practice, we combine these negative samples with uniformly negative samples to form the full set of negative samples for a mini-batch.

In the distributed training, we sample entities from the local METIS partition to corrupt triplets in a mini-batch to minimize the communication caused by negative samples. This ensures that negative samples do not increase network communication. It in general results in harder negative samples. The corrupted head/tail entities sampled from the local METIS partition are topologically closer to the tail/head entities of the triplets in the batch.

3.4 Relation partitioning

Both GraphVite and PBG treat relation embeddings as dense model weights. As a result, for each mini-batch they incur the cost of retrieving them and updating them. If the number of relations in the knowledge graph is small, this is close to optimal and does not impact the performance. However, when the knowledge graph has a large number of relations (greater than the mini-batch size; $\approx$ 1000),

the number of distinct relations in each mini-batch will be a subset of them and as such, treating them as dense model weights will result in unnecessary data access/transfer overheads. To address this limitation, DGL-KE performs sparse relation embedding reads and sparse gradient updates on relation embeddings. This significantly reduces the amount of data transferred in multi-processing, multi-GPU, and distributed training.

To further reduce data access to relation embeddings in a mini-batch, DGL-KE decomposes computations among computing units by introducing a novel relation partitioning approach. This partitioning tries (i) to equally distribute triplets and relations among partitions and (ii) to minimize the number of distinct relations assigned to each partition as a result of (i). The first goal ensures that the computational and memory requirements are balanced across the computing units, whereas the second goal ensures to minimize the relation data that needs to be transferred. In order to derive such a relation partitioning, we use the following fast greedy algorithm. We sort the relations based on their frequency in a decreasing order. We iterate over the sorted relations and greedily assign a relation to the partition with the smallest number of triplets so far. This strategy usually results in balanced partitioning while ensuring that each relation belongs to only one partition. However, the above algorithm will fail to produce a balance partitioning when the knowledge graph contains very frequent relations. In such cases, the number of triplets for those relations may exceed the partition size. To avoid load imbalance, we equally split the most frequent relations across all partitions. After relation partitioning, we assign a relation partition to a computing unit. This ensures that the majority of relation embeddings are updated by only one process at a time. This optimization applies to many-CPU-core training and multi-GPU training.

A potential drawback of relation partitioning is that it restricts the relations that may appear inside a mini-batch. This reduces the randomization of stochastic gradient descent, which can impact the quality of the embeddings. To tackle this problem, we introduce randomization in the partitioning algorithm and at the start of each epoch we compute a somewhat different relation partitioning.

When we use relation partitioning in multi-GPU training, we store all relation embeddings on GPUs and update relation embeddings in GPUs locally. This is particularly important for KGE models with large model weights on relations, such as TransR and RESCAL. Take TransR for an example. It has an entity projection matrix on each relation, which is much larger than a relation embedding. Moving them to CPU is the bottleneck of the entire computation. If we keep all of these projection matrices in GPUs, the communication overhead drops from $O(bd^2)$ to $O(bd)$, which is significantly smaller than the naive solution, usually in the order of 100 times smaller.

3.5 Overlap gradient update with batch processing

In multi-GPU training, some of the steps in a mini-batch computation run on CPUs while the others run on GPUs. When we run them in serial, the GPU remains idle when the CPU writes the gradients. To avoid GPU idling, we overlap entity embedding update with the batch computation in the next mini-batch. This allows us to overlap the computation in CPUs and GPUs. Note that even though this approach can potentially increase the staleness of the embeddings used in a mini-batch, the likelihood of that happening is small for knowledge graphs with a sufficiently large number of entities relative to the number of training processes.

To perform this optimization, we split the gradient updates into two parts: one involving relation embeddings, which are updated by the trainer process, and the other involving the entity embeddings, which are off-loaded to a dedicated gradient update process for each trainer process. Once the trainer process finishes writing the relation gradients, it proceeds to the next mini-batch, without having to wait for the writing of the entity gradients to finish. Our experiments show that overlapping gradient updates provide 40% speedup for most of the KGE models on Freebase.

3.6 Other optimizations

Periodic synchronization among processes. When training KGE models with multiprocessing completely independently, different processes may run at a different rate, which results in inconsistent model accuracy. We observe that the trained embeddings sometimes have much worse accuracy at some runs. As such, we add a synchronization barrier among all training processes after a certain number of batches to ensure that all processes train roughly at the same rate. Our observation is that the model can be trained stably if processes synchronize after every few thousand batches.

Distributed Key-Value store. In DGL-KE, we implement a KVStore for model synchronization with efficient C++ back-end. It uses three optimizations specifically for distributed KGE training. First, because relations in knowledge graphs may have a long-tail distribution, it reshuffles relation embeddings to avoid single hot-point of KVStore. Second, DGL-KE uses shared-memory access instead of network communication if the worker processes and KVStore processes are on the same machine. This optimization significantly reduces networking overhead especially with METIS partitioning. Third, it launches multiple KVStore servers in a single machine to parallelize the computation in KVStore. All KVStore servers inside a machine access embeddings via shared-memory. Finally, we overlap gradient communication and local gradient computation in KVStore.

4 RELATED WORK

A few packages have been developed to compute embeddings of knowledge graphs efficiently and scale to large knowledge graphs.

OpenKE [5] is one of the first packages for training knowledge graph embeddings and provides a large list of models. However, it is implemented entirely in Python and cannot scale to large graphs.

Pytorch-BigGraph (PBG) [9] is developed with an emphasis on scalability and distributed training on a cluster of machines. The package does not support GPU training. Although PBG and DGL-KE share similar negative sampling strategies, PBG 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 embeddings. It treats entity embeddings as sparse model weights and relation embeddings as dense model weights. The random 2D partitioning along with the use of dense model weights for relation

Table 2: Evaluation hardware configuration.

EC2 Type	Hardware Config	Eval Section
r5dn.24xlarge	2x24 cores, 700GB RAM, 100Gbps network	sec 6.2, 6.3
p3.16xlarge	2x16 cores, 500GB RAM, 8 V100 GPUs	sec 6.1

Table 3: Knowledge graph datasets.

Dataset	# Vertices	# Edges	#Relations	Systems
FB15k [2]	14,951	592,213	1345	DGL-KE, GraphVite
WN18 [2]	40,943	151,442	18	DGL-KE, GraphVite
Freebase [1]	86,054,151	338,586,276	14,824	DGL-KE, PBG

embeddings results in a large amount of communication, especially for knowledge graphs with many relations.

GraphVite [21] focuses on multi-GPU training and does not support distributed training. When it trains a large knowledge graph, it keeps embeddings on CPU memory. It constructs a subgraph, moves all data in the subgraph to GPU memory and performs many mini-batch training steps on the subgraph. This method reduces data movement between CPUs and GPUs at the cost of increasing the staleness of the embeddings, which results in slower convergence.

5 EXPERIMENTAL METHODOLOGY

DGL-KE is implemented in Python and relies on PyTorch for tensor operations, as is the case in PBG, whereas GraphVite is done mostly in C++ with a Python wrapper. We report DGL-KE performance in two broad sections: (i) on multi-GPU in section 6.1, many-core CPU in section 6.2 and distributed training in Section 6.3, (ii) against GraphVite [21] and PBG [9] in Section 6.4 on identical hardware.

5.1 Hardware platform

We conduct our evaluation on EC2 CPU and GPU instances; see Table 2 for machine configurations.

5.2 Datasets

We use three datasets to evaluate and compare the performance of DGL-KE against that of GraphVite and PBG. Table 3 shows various statistics for these datasets. FB15k and Freebase were derived from the Freebased Knowledge Graph [1], whereas WN18 was derived from WordNet [11]. The FB15k and WN18 datasets are standard benchmarks for evaluating KGE methods. The Freebase dataset corresponds to complete Freebase Knowledge Graph. All datasets are downloaded from [7].

5.3 Evaluation methodology

We evaluate the performance of the different KGE models using a link (relation)-prediction task. We split each dataset into training, validation, and test subsets. For FB15k and WN18, we used the same splits used in previous evaluations [15] (available in [7]). Freebase is split with 5% of the triplets for validation, 5% for test, and the remaining 90% for training.

We perform the link-prediction task using two different protocols. The first, used for FB15k and WN18, works as follows. For each triplet (h, r, t) in the validation/test set, referred to as *positive triplet*, we generate all possible triplets of the form (h', r, t) and (h, r, t') by corrupting the head and tail entities, and then remove any triplets that already exist in the dataset. The remaining triplets form the *negative triplets*. The second protocol, used for Freebase, is similar to the first one with the following two differences: (i) we use only 2000 negative triplets; 1000 sampled uniformly from the entire set of negative samples and 1000 sampled proportionally to the degree of the corrupted entities; and (ii) we do not remove from the 2000 negative triplets any triplets that are in the dataset. The reason for the second protocol is due to the size of Freebase, which makes the first protocol computationally expensive.

We assess the performance by using the standard metrics [9] of Hit@k (for $k \in \{1, 3, 10\}$), Mean Rank (MR), and Mean Reciprocal Rank (MRR). All these metrics are derived by comparing how the score of a positive triplet relates to the scores of its associated negative triplets. For a positive triplet i, let S_i be the list of triplets containing i and its associated negative triplets ordered in a decreasing score order, and let $rank_i$ be the position of i in S_i. Hit@k is the average number of times positive triplets are among the k highest ranked triplets; MR is the average rank of the positive triplets, whereas MRR is the average reciprocal rank of the positive triplets. Mathematically, they are defined as

$$\text{Hit@}k = \frac{1}{Q}\sum_{i=1}^{Q} \mathbb{1}_{rank_i \leq k},$$

$$\text{MR} = \frac{1}{Q}\sum_{i=1}^{Q} rank_i,$$

and

$$\text{MRR} = \frac{1}{Q}\sum_{i=1}^{Q} \frac{1}{rank_i},$$

where Q is the total number of positive triplets and $\mathbb{1}_{rank_i \leq k}$ is 1 if $rank_i \leq k$, otherwise it is 0. Note that Hit@k and MRR are between 0 and 1, whereas MR ranges from 1 to the $\sum_i^Q |S_i|$.

5.4 Software environment

We run Ubuntu 18.04 on all EC2 instances, where the Python version is 3.6.8 and Pytorch version is 1.3.1. On GPU instances, the CUDA version is 10.0. When comparing the performance of DGL-KE against that of GraphVite and PBG, we use GraphVite v0.2.1 downloaded from Github on November 12 2019 and PBG downloaded from their Github repository on October 15 2019. All frameworks use the same Pytorch version.

5.5 Hyperparameters

For the FB15k and WN18 and all methods (DGL-KE and GraphVite) we perform an extensive hyper-parameter search [1] and report the results that achieve the best performance in terms of MRR, as we believe it is a good measure to assess the overall performance of the methods. Due to the size of Freebase, we only report results for a single set of hyper-parameter values that perform the best on FB15k.

[1]The hyperparameters used for different settings can be found here to reproduce the results: https://github.com/awslabs/dgl-ke/tree/master/examples

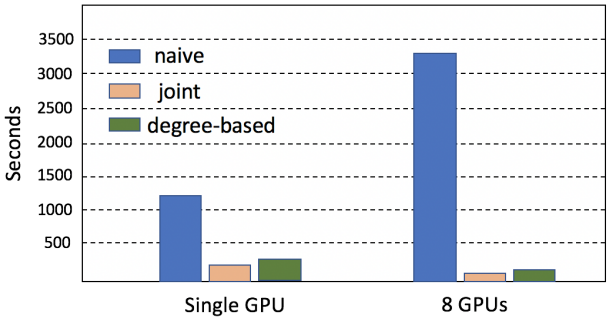


Figure 3: The effect of negative sampling in GPU training on FB15k.

Table 4: The performance of KGE models on Freebase with and without degree-based negative sampling with eight GPUs.

	TransE		ComplEx		DistMult	
	with	w/o	with	w/o	with	w/o
Hit@10	0.834	0.783	0.777	0.638	0.742	0.731
Hit@3	0.773	0.675	0.741	0.564	0.698	0.697
Hit@1	0.689	0.527	0.677	0.485	0.639	0.652
MR	41.16	43.99	108.43	162.74	123.10	128.91
MRR	0.743	0.619	0.716	0.539	0.678	0.682

To ensure that the accuracy results are comparable, all methods use exactly the same test set and evaluation protocols described in the previous section.

6 RESULTS

6.1 Multi-GPU training

A multi-GPU machine has massive computation power but relatively low communication bandwidth between CPU memory, which makes the various optimizations described in Sections 3.3–3.6 relevant. A detailed evaluation of these optimizations follows.

6.1.1 Negative sampling. Joint negative sampling shown in Section 3.3 has two effects: (i) enable more efficient tensor operators and (ii) reduce data movement in multi-GPU training. Figure 3 shows the result. To illustrate the speedup of using more efficient tensor operators, we run the TransE model on FB15k with all data in a single GPU. Joint negative sampling gives about 4× speedup. To illustrate the speedup of reducing data movement, we run the TransE model on FB15k in 8 GPUs, where entity embeddings are stored in CPU memory. Join negative sampling gets much larger speedup, e.g., about 40×, because naive sampling requires swapping many more entity embeddings between CPU and GPU than joint negative sampling and data communication is the bottleneck.

6.1.2 Degree-based negatvie sampling. Although degree-based negative sampling does not speed up training, it improves the model accuracy (Table 4) on Freebase. This suggests that non-uniform negative sampling to generate "hard" negative samples is effective, especially on large knowledge graphs.

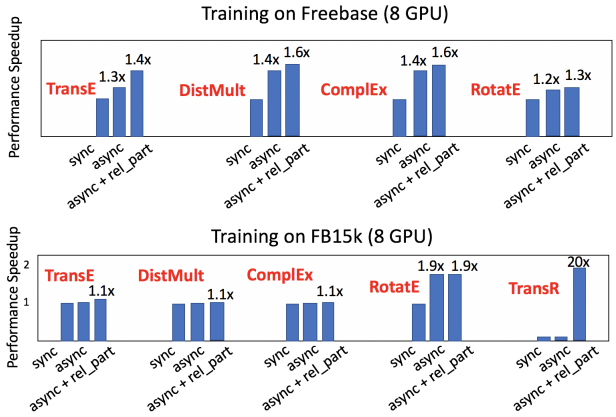


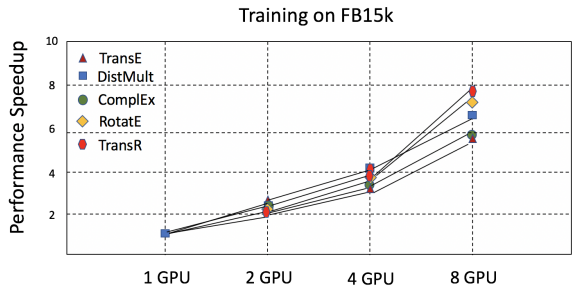
Figure 4: Speedup of different optimizations on multi-GPU.

6.1.3 Overlap gradient update with batch computation. This technique overlaps the computation of GPUs and CPUs to speed up the training. Figure 4 shows the speedup of using this technique (comparing **sync** and **async**) on FB15k and Freebase. It has limited speedup on small knowledge graphs for some models, but it has roughly 40% speedup on Freebase for almost all models. The effectiveness of this optimization depends on the computation time in CPUs and GPUs. Large knowledge graphs, such as Freebase, require hundreds of GBytes to store entity embeddings and suffers from slow random memory access in entity embedding update. In this case, overlapping the CPU/GPU computation has significant benefit.

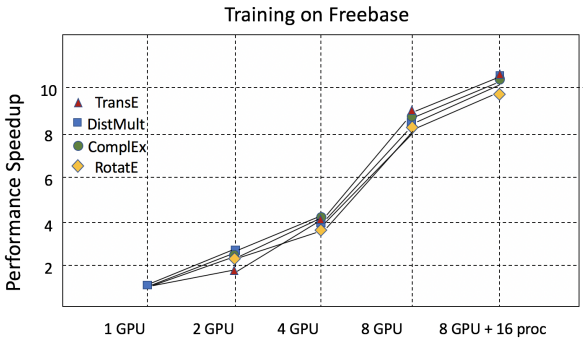
6.1.4 Relation partitioning. After relation partitioning, we pin relation embeddings (and projection matrices) in each partition inside a GPU, which reduces data movement between CPUs and GPUs. The speedup is highly related to the model size and the number of relations in the dataset. Figure 4 shows the speedup of using relation partitioning in multi-GPU training (comparing **async** and **async + rel_part** bar) on FB15k and Freebase. Relation partitioning has significant speedup on TransR because the relation-specific projection matrices result in a large amount of data communication between CPU and GPU. Even for models with only relation embeddings, relation partitioning in general gets over 10% speedup.

6.1.5 Overall speed and accuracy. After deploying all of the optimizations, we measure the speedup of DGL-KE with multiple GPUs on both FB15k and Freebase. Figure 5 shows that DGL-KE accelerates training almost linearly with multiple GPUs. On Freebase, DGL-KE further speeds up by running 16 processes on 8 GPUs. By running two processes on each GPU, we better utilize the computation in GPUs and PCIe buses by overlapping computation and data communication between CPUs and GPUs.

With all these techniques, we train KGE models efficiently. For small knowledge graphs, such as FB15k, DGL-KE trains most of KGE models, even as complex as RotatE and TransR, within a few minutes. For large knowledge graphs, such as Freebase, DGL-KE trains many of KGE models around one or two hours and trains



(a) Training on FB15k



(b) Training on Freebase

Figure 5: Speedup of multi-GPU training.

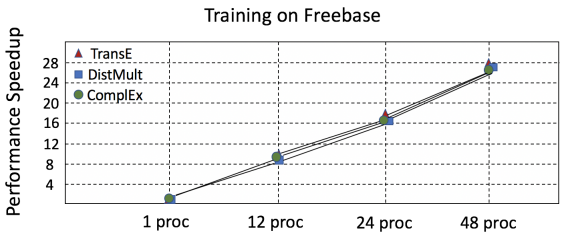


Figure 6: Speedup of many-core training.

more complex models within a reasonable time. For example, we train TransR in about 8 hours using 8 GPUs.

With a maximum speedup of 11× against single-GPU training, we sacrifice little on accuracy. Table 5 and Table 6 shows the accuracy of DGL-KE with 1 and 8 GPUs on FB15k and Freebase. The *1GPU* columns shows the baseline accuracy and the *Fastest* shows the accuracy with the fastest configuration on 8 GPUs, which is one process per GPU for FB15k and two processes per GPU for Freebase. In all experiments, the number of epochs is the same for both settings. Here, we only show TransR with 8 GPUs on Freebase because training TransR on one GPU takes a very long time.

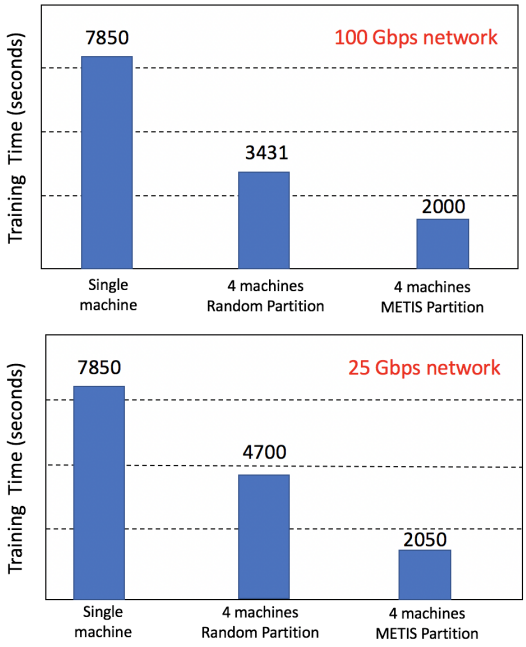


Figure 7: The runtime of DGL-KE distributed training for TransE on Freebase.

6.2 Many-core training

Many of the techniques illustrated in multi-GPU training can also be applied to multi-core training. Figure 6 shows that DGL-KE speeds up well on an r5dn instance with 48 CPU cores. The training accuracy of TransE and DistMult with 48 CPU cores is shown in Table 7 (column labeled "Single").

6.3 Distributed training

In distributed training, we use 4 r5dn.24xlarge EC2 instances as our cluster environment. In this section, we compare the single-machine training with distributed training for TransE using both random partitioning and METIS partitioning on Freebase.

METIS partitioning on distributed training gets nearly 3.5× speedup compared with the single-machine baseline (Figure 7) without sacrificing any model accuracy (Table 7). The training speed of using METIS partitioning gets about 20% speedup over random partitioning because METIS partitioning leads to much lower overhead than random partitioning.

6.4 Overall performance

We evaluate DGL-KE on the datasets in Table 3 and compare with two existing packages: GraphVite and PBG on both CPUs and GPUs. Because GraphVite and PBG only provide a subset of the models in DGL-KE, we only compare with them with the models available in these two packages.

6.4.1 Comparison with GraphVite. DGL-KE is consistently faster than GraphVite on both FB15k and WN18 (Figure 9 and Figure 10) when training all KGE models to reach similar accuracy. Due to the space limit, we only show the accuracy comparison on FB15k

Table 5: The overall performance of DGL-KE after various optimizations with 8 GPUs on FB15k.

	TransE_l1		DistMult		ComplEx		RotatE		TransR	
	1GPU	Fastest	1GPU	Fastest	1GPU	Fastest	1GPU	Fastest	1GPU	Fastest
Hit@10	0.860	0.857	0.884	0.879	0.892	0.884	0.885	0.874	0.820	0.815
Hit@3	0.775	0.765	0.806	0.796	0.838	0.823	0.819	0.804	0.742	0.738
Hit@1	0.553	0.536	0.636	0.614	0.724	0.698	0.665	0.647	0.596	0.593
MR	44.58	45.83	60.61	63.32	60.55	66.19	39.78	41.69	60.48	65.48
MRR	0.676	0.664	0.732	0.716	0.789	0.769	0.752	0.736	0.682	0.679

Table 6: The overall performance of DGL-KE after various optimizations with 8 GPUs on Freebase.

	TransE_l2		DistMult		ComplEx		RotatE		TransR	
	1GPU	Fastest	1GPU	Fastest	1GPU	Fastest	1GPU	Fastest	1GPU	Fastest
Hit@10	0.865	0.822	0.839	0.837	0.837	0.830	0.750	0.730	N/A	0.765
Hit@3	0.823	0.759	0.813	0.810	0.812	0.803	0.718	0.697	N/A	0.723
Hit@1	0.771	0.669	0.785	0.780	0.785	0.773	0.668	0.653	N/A	0.545
MR	31.64	38.44	44.93	48.58	47.79	51.40	187.7	197.51	N/A	103.06
MRR	0.806	0.726	0.805	0.801	0.804	0.794	0.699	0.682	N/A	0.642

Table 7: The accuracy of random partitioning and METIS partitioning for distributed training on Freebase.

	TransE			DistMult		
	Single	Random	METIS	Single	Random	METIS
Hit@10	0.796	0.790	0.790	0.751	0.739	0.731
Hit@3	0.734	0.735	0.726	0.712	0.709	0.700
Hit@1	0.634	0.689	0.634	0.696	0.619	0.612
MR	54.51	64.05	34.59	123.1	128.23	136.19
MRR	0.696	0.726	0.692	0.68	0.692	0.691

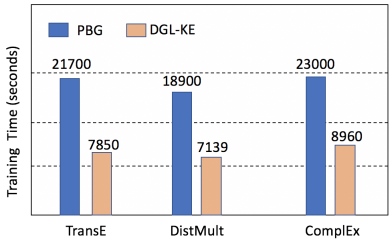


Figure 8: The runtime of PBG and DGL-KE on Freebase with multi-CPU training on a single machine. Both run nine epochs.

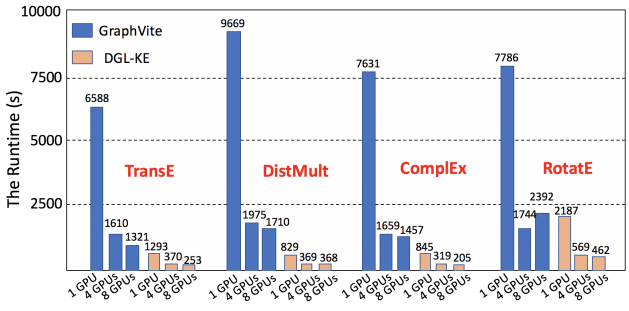


Figure 9: The runtime of GraphVate and DGL-KE on FB15k.

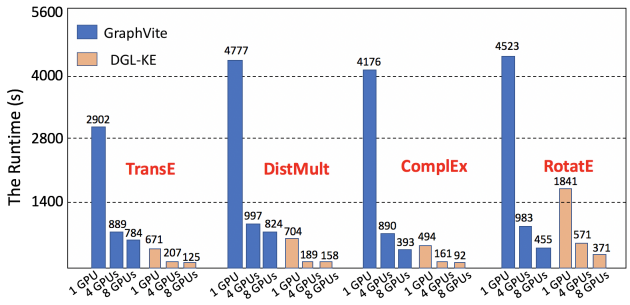


Figure 10: The runtime of GraphVate and DGL-KE on WN18.

(Table 8) [2]. We conduct this experiment on a p3.16xlarge instance. For most of the models, DGL-KE is 5× faster than GraphVite. This is mainly due to DGL-KE converges faster than GraphVite. In all cases, DGL-KE only needs less than 100 epochs to converge but GraphVite needs thousands of epochs. When evaluating GraphVite, we use the recommended configuration by the package for each algorithm when running on 1 GPU and 4 GPUs, while having some hyperparameter tuning for 8 GPUs to get compatible results with 1 GPU runs. When evaluating DGL-KE, we use the same dimension size of entity and relation embedding as GraphVite, but tune hyper-parameters such as learning rate, negative sample size and batch size, for better accuracy.

6.4.2 Comparison with PBG. We compare DGL-KE with PBG on an r5dn.24xlarge EC2 instance. In this experiment, we run nine epochs on both PBG and DGL-KE and compare the total training time (seconds). As we can see, DGL-KE runs 2.5x-2.7x times faster than PBG when training KGE models on Freebase (Figure 8) with multi-CPU training on a single machine. There are many factors that contribute to the slower training speed in PBG. One of the major factors is that PBG handles relation embeddings as dense model weights. As such, the computation in a batch involves in

[2] More complete results are shown in our arxiv version: https://arxiv.org/abs/2004.08532

Table 8: The accurancy of DGL-KE and GraphVite on FB15k with 1, 4 and 8 GPUs.

TransE						
	DGL-KE			GraphVite		
	1 GPU	4 GPU	8 GPU	1 GPU	4 GPU	8 GPU
Hit@10	0.873	0.866	0.863	0.869	0.873	0.872
Hit@3	0.801	0.791	0.789	0.793	0.791	0.781
Hit@1	0.612	0.613	0.611	0.606	0.586	0.373
MR	40.84	44.52	45.12	37.81	38.89	40.63
MRR	0.717	0.713	0.711	0.711	0.700	0.588

DistMult						
	DGL-KE			GraphVite		
	1 GPU	4 GPU	8 GPU	1 GPU	4 GPU	8 GPU
Hit@10	0.895	0.890	0.882	0.892	0.876	0.873
Hit@3	0.835	0.825	0.806	0.834	0.814	0.800
Hit@1	0.702	0.680	0.645	0.715	0.697	0.646
MR	44.50	51.79	56.54	40.51	69.15	60.11
MRR	0.777	0.762	0.736	0.783	0.765	0.733

ComplEx						
	DGL-KE			GraphVite		
	1 GPU	4 GPU	8 GPU	1 GPU	4 GPU	8 GPU
Hit@10	0.892	0.881	0.879	0.867	0.830	0.810
Hit@3	0.839	0.824	0.816	0.788	0.742	0.718
Hit@1	0.735	0.705	0.694	0.643	0.591	0.572
MR	50.47	68.17	70.13	58.68	153.4	145.6
MRR	0.795	0.773	0.764	0.727	0.679	0.660

RotatE						
	DGL-KE			GraphVite		
	1 GPU	4 GPU	8 GPU	1 GPU	4 GPU	8 GPU
Hit@10	0.888	0.883	0.881	0.875	0.892	0.887
Hit@3	0.820	0.813	0.812	0.814	0.830	0.823
Hit@1	0.647	0.640	0.648	0.691	0.688	0.646
MR	34.38	35.47	35.71	41.75	35.87	43.26
MRR	0.744	0.737	0.740	0.762	0.768	0.743

all relation embeddings in the graph, which is 10 times more than necessary on Freebase. In contrast, DGL-KE reduces the number of relation embeddings involved in a batch and significantly reduces the amount of computation and data movement.

7 CONCLUSIONS

We develop an efficient package called DGL-KE to train knowledge graph embeddings at a large scale. It implements a number of optimization techniques to improve locality, reduce data communication, while harnessing parallel computing capacity. As a result, DGL-KE significantly outperforms the state-of-the-art packages for knowledge graph embeddings on a variety of hardware, including many-core CPU, multi-GPU as well as cluster of machines. Our experiments show that DGL-KE scales well with machine resources almost linearly while achieving very high model accuracy. DGL-KE is available at https://github.com/awslabs/dgl-ke.

8 ACKNOWLEDGMENTS

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