Marius++: Large-Scale Training of Graph Neural Networks on a Single Machine

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ABSTRACT

Graph Neural Networks (GNNs) have emerged as a powerful model for ML over graph-structured data. Yet, scalability remains a major challenge for using GNNs over billion-edge inputs. The creation of mini-batches used for training incurs computational and data movement costs that grow exponentially with the number of GNN layers as state-of-the-art models aggregate information from the multi-hop neighborhood of each input node. In this paper, we focus on scalable training of GNNs with emphasis on resource efficiency. We show that out-of-core pipelined mini-batch training in a single machine outperforms resource-hungry multi-GPU solutions. We introduce Marius++, a system for training GNNs over billion-scale graphs. Marius++ provides disk-optimized training for GNNs and introduces a series of data organization and algorithmic contributions that 1) minimize the memory-footprint and end-to-end time required for training and 2) ensure that models learned with disk-based training exhibit accuracy similar to those fully trained in mixed CPU/GPU settings. We evaluate Marius++ against PyTorch Geometric and Deep Graph Library using seven benchmark (model, data set) settings and find that Marius++ with one GPU can achieve the same level of model accuracy up to 8× faster than these systems when they are using up to eight GPUs. For these experiments, disk-based training allows Marius++ deployments to be up to 64× cheaper in monetary cost than those of the competing systems.

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1 INTRODUCTION

Graph Neural Networks (GNNs) have emerged as an important method for machine learning (ML) over graph-structured data [4] (referred to as graph learning). A diverse array of multi-layered [13, 39] and shallow [3, 44] models have been introduced to apply ML over chemical and protein structures [34], social networks [9], and knowledge graphs [31]. These models achieve state-of-the-art accuracy for two main predictive tasks: node classification and link prediction [21, 33, 47]. The accuracy improvements can be attributed to the ability of GNNs to encode data dependencies that arise due to the graph-structured nature of the data, thus, introducing a relational inductive bias into the model [2]. Yet, it is this exact property that makes GNNs hard to train over large-scale graphs.

Scalability of GNN training is highlighted as one of the major challenges in the literature [4]. The main challenge is that in GNNs the representation of a data point (i.e., graph node) depends on those of its neighbors in the input graph. For multi-layered GNNs, we need to combine information from a node’s multi-hop neighborhood to construct examples and form a mini-batch for training (e.g., Figure 1). This property leads to an exponential increase in the cost of computation and data movement required to form mini-batches as the number of GNN layers increase. To address this challenge, state-of-the-art GNN models are coupled with multi-hop sampling procedures to construct the necessary inputs for training [13, 45]. Consequently, current system solutions for scalable training of GNNs, such as Deep Graph Library (DGL) [41] and PyTorch Geometric (PyG) [11], propose using distributed solutions—across machines or with multiple GPUs—to minimize the time required for sampling, mini-batch creation, and training [49].

In this paper, we focus on the problem of scalable training of GNN models but with an emphasis on resource efficiency. Multi-GPU training across multiple machines introduces significant monetary costs that make large-scale GNN training inaccessible to practitioners and researchers that do not have access to industrial resources [49]. At the same time, distributed solutions introduce deployment and maintenance overheads [25]. Our recent work on the Marius system [29] demonstrated how to train shallow Graph Embedding models models over billion-scale graphs with a single GPU, while being faster than competing multi-GPU solutions, offering up to 7.5× reductions in deployment costs. Building upon these observations, we argue in favor of out-of-core pipelined mini-batch training of general GNNs on a single machine.

We introduce Marius++, a system that enables us to train general GNNs over billion-scale graphs in a single machine. A core design choice in Marius++ is to utilize the entire memory hierarchy—including the disk—to scale training. We show that while using a single GPU Marius++ can be 8× faster than the the best performing baseline that utilizes eight GPUs and can yield cost reductions of up to 64×. In addition, Marius++ offers a unified solution that
need for hyperparameter search and to simplify deployment, we develop an automated hyperparameter optimizer in Marius++. We first introduce a new metric that we refer to as Edge Permutation Bias which allows us to determine the bias that a certain partition replacement policy will introduce to the training procedure. We empirically show that the accuracy of a model is inversely correlated with the Edge Permutation Bias and describe how the number of physical and logical partitions affect the Edge Permutation Bias. Given this analysis, we introduce a methodology to automatically identify a near-optimal setting for the number of physical and logical partitions such that the trade-off between the accuracy of obtained models and training time is optimized. We experimentally demonstrate that our methodology yields hyperparameter settings which result in accuracy and training time matching the best configurations found through hyperparameter scans.

2 PRELIMINARIES

We review concepts on ML over graph data and approaches for training over large-scale graphs. We also summarize key ideas from Marius [29], such as the BETA replacement policy, that form background material for the techniques we develop in this work.

Machine Learning on Graphs ML over graphs can be grouped into two classes of learning problems, unsupervised and supervised tasks. The first aims at learning vector representations, also referred to as embeddings, of the nodes and edges that preserve the structure of an input graph. These embeddings can solve predictive tasks related to the geometry of the graph such as link prediction, i.e., the task of predicting the existence of an edge between two target nodes (e.g., predicting a gene/protein interaction in a biological network). The second family also uses vector representations of nodes but for specific downstream prediction tasks such as node classification where we seek to assign a label to a single target node (e.g., determine if a computer network node has malware or not).

Different neural architectures have been proposed to learn the aforementioned representations. These architectures can either be shallow models that rely on look-up tables or multi-layered GNNs that stack multiple neural network layers to learn the representations. Let $G = (V, E)$ be an input graph, with adjacency matrix $W \in \mathbb{R}^{V \times V}$ (or $W \in \mathbb{R}^{V \times V \times |T|}$ for graphs with edges of $|T|$ different types) and optional node features $X \in \mathbb{R}^{V \times d}$. Shallow models learn an embedding look-up $Z \in \mathbb{R}^{V \times d}$ and use the graph structure $W$ to form a reconstruction-based loss over the edges of $G$ using a fixed decoder function such as an inner product or cosine similarity [4]. Many state-of-the-art graph embedding models such as DistMult [44], TransE [3], and RotatE [36] follow this architecture. In GNNs, both the graph structure and node features are used to learn node representations. The node representations that form the base input to a GNN can be formed using the node features $X$, potentially concatenated with a learnable base-embedding $Z$: Given a node $v \in V$ let $h_v^{(0)} = f(X_v, Z_v)$ where $f$ is a combination function. Node representations in subsequent layers of a GNN are computed by aggregating over the representation of a target node and the representation of its one-hop neighbors: Given a node $v$ and its one-hop neighborhood $N_v$ we have that its representation at layer $k$ is given by $h_v^{(k)} = \text{AGG}(h_u^{(k-1)}, \{h_u^{(k-1)} : u \in N_v\})$ where $\text{AGG}$ is an aggregation function with learnable parameters such

Hyper-parameter Optimization for Disk-based Training The hyperparameters of the algorithms that control disk-based training in Marius++, i.e., the number of physical and logical partitions, can affect both the training time and the quality of the obtained model. For example, a large number of physical partitions can introduce opportunities for more randomization and better models but at the same time it leads to increased disk access costs. To alleviate the
as a weighted linear sum. GraphSage [13], Graph Attention Networks (GAT) [39], and Graph Convolution Networks (GCN) [21] are examples of GNN models which follow this design.

**Scaling GNN Training** To compute $h_i^{(k)}$, a k-layer GNN requires sampling a target node’s k-hop neighborhood. For small graphs, the full neighborhood may be returned, but this is not feasible for large graphs. Sampling a fixed number of neighbors at each hop is a common strategy to limit neighborhood sizes [13]. We discuss how sampling at scale bottlenecks existing systems.

Training GNNs over graphs requires efficient access to graph edges and node information. When neither fit in GPU memory, both are stored in CPU memory and sampled to produce batches which are then transferred to the GPU for computation (known as mini-batch GNN training). Batch preparation requires: 1) sampling a set of target nodes, 2) sampling the k-hop neighborhood of each of the target nodes (Figure 1), and 3) loading node embeddings and/or features for all nodes (target and neighbors) in the batch. Sampling of target nodes is dependent on the learning task. For node classification, target nodes are sampled in batches uniformly at random from the training nodes. For link prediction, edges are sampled uniformly at random from the training edges, and the unique nodes in the sampled set of edges are taken as the target nodes. Construction of batches can become the bottleneck in training. For instance, a 3-layer GraphSage node classification model on Papers100m takes PyG 1200ms to sample neighbors while the forward and backward pass only takes 170ms (Table 3). Pipelining and asynchronous preparation of batches are typical solutions to this problem [11], but fall short on machines with limited CPU resources and underutilize the GPU [20]. In order to unblock graph learning pipelines, more efficient graph sampling is required (Section 4).

Representations of large graphs can exceed CPU memory and either require distribution to multiple machines [12, 19, 37, 40, 49] or storing graph data on disk [22, 29]. In disk-based training the node representations are divided into partitions that are swapped in-and-out of CPU memory. Marius [29] introduced disk-based training for shallow link prediction models with the guarantee that all graph edges are processed during each epoch of training and introduced the BETA partition-replacement algorithm:

**Properties of the BETA Algorithm** [29] BETA guarantees that all graph edges are processed during each epoch of training while IO is minimized. It does so by swapping one partition at each round such that the new partition brought to memory maximizes the number of new edges available for training. This property of BETA allowed Marius to learn shallow models for link prediction of comparably accuracy with those obtained by distributed systems but 4.2x faster and 6.7x cheaper by using a single machine. This work builds upon the aforementioned property and extends BETA to training of GNNs for both link prediction and node classification.

### 3 SYSTEM OVERVIEW

Marius++ consists of two main components (Figure 2): 1) a processing layer for mixed CPU-GPU training and 2) a storage layer responsible for transferring data between disk and CPU memory.

**Processing Layer** Using Figure 2 as a guide, we describe the lifetime of a mini-batch in Marius++. Mini-batch construction is performed on the CPU and begins when a set of nodes (or edges) are sampled. Utilizing efficient sampling algorithms and the DENSE data structure the k-hop neighborhood of the target nodes is then sampled from the in-memory subgraph (Section 4). Next, the representations for all nodes (target and neighbors) are loaded from the partition buffer into the mini-batch before it is transferred to the GPU. If applicable, representations of edge types are kept in GPU memory as in our prior work [29]. Once on the GPU, the target nodes of the mini-batch are encoded by unrolling the DENSE data structure and the final representations of the target nodes are decoded to calculate the loss. Following that, the gradients of the model parameters are computed and the GNN parameters are updated on the GPU. Node embedding gradients (if applicable) are transferred back to the CPU where they are applied to the partition buffer. This training procedure allows us to support both link prediction and node classification for shallow models and GNNs.

To execute the above training procedure in a pipelined manner, operations are grouped together into pipeline stages with bounded queues between stages, as in prior work [29]. By pipelining in this way, we perform all data movement asynchronously and independently from the computation, allowing us to fully utilize the GPU. Because of asynchronous reads and writes of embedding parameters, our pipeline introduces the possibility of stale embeddings arriving on the GPU. From our previous work [29], we use bounded staleness to mitigate this issue. Overall, the pipelined training architecture allows Marius++ to efficiently utilize the GPU through asynchronous sampling and data movement.

**Storage Layer** In order to scale beyond CPU memory, Marius++ uses a partition buffer manager to iterate over node partitions and edges which reside on disk. In the CPU memory buffer, we store a subset of the node partitions and all edges between nodes which reside in the subset. During training we must iterate over all training edges (link prediction) or nodes (node classification), requiring data on disk to be swapped into the buffer, introducing IO overheads. At the same time, the CPU-GPU pipeline samples from the subset of data residing in memory, which limits randomness in samples and model quality. In order to minimize IO while maximizing randomness, we use a set of two-level replacement policies: Two-Level BETA, Dispersed, and Sequential. These policies are considered two-level in that they utilize logical partitions in CPU memory and physical partitions on disk. We describe the partitioning scheme and replacement policies in more detail in Section 5 and provide rules for best configuring the partitioning scheme in Section 6.

### 4 EFFICIENT MINI-BATCH TRAINING

We next present the Delta Encoding of Neighborhood SampEls (DENSE) data structure to minimize the memory footprint and time required for k-hop neighborhood sampling by reusing samples across layers and utilizing optimized parallel algorithms. We start by defining the components of DENSE, then discuss how it is constructed, and finally how it is used for a GNN forward pass.

#### 4.1 DENSE Data Structure

In Marius++, we store the output of multi-hop sampling in the DENSE data structure consisting of five arrays: 1) node_ids containing all node IDs involved in the sampled subgraph, 2) nbrs containing the sampled single-hop edges for nodes in node_ids, 3)
**Algorithm 1: Multi-hop Neighborhood Sampling**

**Input:** target_nodes: unique node IDs to perform sampling;

fan_outs: list of the max neighbors to sample per hop

1. \( \text{node}_\text{id}_\text{offsets} = [0] \); \( \text{node}_\text{ids} = \text{target}_\text{nodes} \)
2. \( \text{nbr}_\text{offsets} = [] \); \( \text{nbrs} = [] \); \( \Delta = \text{target}_\text{nodes} \)
3. for \( i \) in range(len(fan_outs)) do
4. \( \Delta_\text{nbrs}, \Delta_\text{offsets} = \text{singleHopSampling}(\Delta, \text{fan}_\text{outs}[i]) \)
5. \( \text{nbr}_\text{offsets} = \text{concat}(\Delta_\text{offsets}, \text{nbr}_\text{offsets} + \text{len}(\Delta_\text{nbrs})) \)
6. \( \text{nbrs} = \text{concat}(\Delta_\text{nbrs}, \text{nbrs}) \)
7. \( \Delta = \text{computeNextDelta}(\Delta_\text{nbrs}, \text{node}_\text{ids}) \)
8. \( \text{node}_\text{id}_\text{offsets} = \text{concat}([0], \text{node}_\text{id}_\text{offsets} + \text{len}(\Delta)) \)
9. \( \text{node}_\text{ids} = \text{concat}(\Delta, \text{node}_\text{ids}) \)
10. return \( \text{DENSE(node}_\text{id}_\text{offsets, node}_\text{ids, nbr}_\text{offsets, nbrs)} \)

**DENSE Data Structure Creation**

Given a set of target node IDs to encode with a \( k \)-layer GNN, Marius++ samples a \( k \)-hop neighborhood for each target node and creates DENSE according to Algorithm 1. We define the target nodes to be \( \Delta_k \) (Line 2). Assuming \( k > 0 \), the first iteration samples single-hop neighbors for node IDs in \( \Delta_k \) (Line 4). The output of single-hop sampling is a list of neighboring edges \( \Delta_k_\text{nbrs} \) with the neighbors for each node in \( \Delta_k \) sequentially beginning at the offset given by \( \Delta_k_\text{offsets} \). We discuss more details of single-hop sampling in Section 4.2. If \( k > 1 \), the next step is to sample two-hop neighbors of \( \Delta_k \). This amounts to sampling single-hop neighbors for the unique nodes in \( \Delta_k_\text{nbrs} \). However, Marius++ makes the following optimization to reuse previous samples: For the second-hop, we sample neighbors for the unique nodes in \( \Delta_k_\text{nbrs} \) which do not appear in \( \Delta_k \). We define these nodes to be \( \Delta_{k-1} \) (Line 7) \( \Delta_{i-1} = \text{unique}_\text{ids}(\Delta_i_\text{nbrs}) \setminus \bigcup_{j=2}^{k-1} \Delta_j \).

**Algorithm 2: Multi-layer GNN Computation**

**Input:** DENSE, node_vectors: base node representations for \( \text{node}_\text{ids} \) in DENSE; layers: a list of GNN layers

1. for \( i \) in range(len(layers)) do
2. \( \text{node}_\text{vector} = \text{layers}[i].\text{forward(node}_\text{vector}, \text{DENSE}) \)
3. \( \text{DENSE} = \text{truncate(DENSE)} \)
4. return node_vectors

For example, in Figure 3, target node A, a sampled one-hop neighbor of target node B, is excluded from \( \Delta_1 \). In this way, Marius++ samples single-hop neighbors for a given node \( n \) at most once, but these edges can be reused to encode \( n \) at multiple GNN layers. We discuss methods for computing \( \Delta \) below.

The final DENSE data structure output from multi-hop sampling is constructed by combining individual \( \Delta \)s and their neighbors into single arrays (Lines 5, 6, 8, 9), taking care to update offsets as necessary. For example, \( \text{node}_\text{ids} = \text{concat}_{i=0,...,k} \Delta_i \) and \( \text{nbrs} = \text{concat}_{i=3,...,k} \Delta_i_\text{nbrs} \) (neighbors are not needed for \( \Delta_0 \)). The \( \text{node}_\text{id}_\text{offsets} \) array stores the boundaries between \( \Delta \)s in \( \text{node}_\text{ids} \). Such a structure provides the following property: \( \Delta_k \) contains the target nodes, \( \{\Delta_{k-1}, \Delta_k\} \) contain all sampled nodes in the one-hop neighborhood of the target nodes, \( \{\Delta_{k-2}, \Delta_{k-1}, \Delta_k\} \) contain all sampled nodes in the two-hop neighborhood of the target nodes, etc. After constructing the \( \text{node}_\text{id}_\text{offsets, node}_\text{ids, nbr}_\text{offsets, and nbrs arrays, Marius++ transfers them to the GPU for computation. We also transfer a node\_representations array which stores the base vector representation for each node ID in node\_ids. Once on the GPU, the final repr_map array is computed which maps each neighbor in the nbrs array to the index of its representation in node\_representations.**

**Using the DENSE Data Structure**

After sampling a \( k \)-hop neighborhood and transferring it to the GPU we utilize DENSE to perform a \( k \)-layer GNN forward pass as described in Algorithm 2. The contents of DENSE allow Marius++ to standardize the input to each GNN layer and to use optimized dense GPU kernels for computation. In particular, the stacked structure translates to the following property: the unique input nodes for the \( i \)-th GNN layer (first layer index zero) are \( \text{concat}_{i=1,...,k} \Delta_i \), the unique output nodes are \( \text{concat}_{i=(i+1)...k} \Delta_i \), and the neighbors to use for aggregation are \( \text{concat}_{i=(i+1)...k} \Delta_i_\text{nbrs} \). These are sequential subsets.
of node_ids and nbrs in DENSE (e.g. Figure 3). Marius++ automatically removes Δs and their Δ_nbrs as they are no longer needed (Line 3). Thus, the input nodes for each layer are always node_ids and the nodes which should be encoded are always the node_ids after node_id_offsets[1]. The full nbrs array is used for aggregation at each layer. To show how to use DENSE for common GNN layers, we provide an example implementation of neighborhood aggregation in Algorithm 4, discussed in the following section.

Continuing the running example in Figure 3, the two-layer GNN first uses {Δ₀, Δ₁, Δ₂} and {Δ₁_nbrs, Δ₂_nbrs} to encode {Δ₁, Δ₂} after one GNN layer. It then truncates Δ₀ and Δ₁_nbrs and uses the encoded {Δ₁, Δ₂} together with {Δ₂_nbrs} to encode {Δ₂} after two layers as desired. The sampled edges in Δ₂_nbrs are reused for encoding in both GNN layers.

4.2 Algorithms for Individual Components

We now describe efficient implementations of the single-hop sampling and delta computation methods used to create DENSE in Algorithm 1 and of an example GNN layer forward pass.

**Single Hop Sampling** Single-hop sampling can bottleneck DENSE creation because it must load millions of neighboring graph edges. To minimize sampling time, Marius++ introduces a parallel algorithm which distributes the workload across available CPU threads. Given a set of node IDs \( I \) and a requested number of neighbors \( k \), single-hop sampling should return up to \( k \) neighbors for each node \( i \in I \) as an edge list with the neighbors for node \( i \) sequential.

To support single-hop sampling, when a graph is loaded into CPU memory, Marius++ constructs two sorted versions of the edge list: 1) one sorted by source node ID and 2) one sorted by destination node ID. In each edge list the neighbors of a node are contiguous (Line 5) and using precomputed offsets to read and write sequential chunks of memory (Line 8, 11), Marius++ is able to efficiently sample single-hop neighbors for a batch of nodes.

**Delta Computation** As described above, for constructing DENSE, Marius++ computes a set of nodes we call \( \Delta \) after each hop of sampling. Specifically, given a set of unique node IDs \( I \) and a list of newly sampled neighbor IDs \( N \), \( \Delta \) is the set of unique nodes in \( N \) but not in \( I \). To parallelize the computation across \( N \) and \( I \) Marius++ introduces an optimized bit map algorithm described below.

To compute \( \Delta \), Marius++ utilizes a bit vector of size equal to the number of nodes in memory with each entry initialized to zero. Then, in parallel, for every node ID \( n \in N \) we write a one to the bit vector for all node IDs \( i \in I \), again in parallel. Once this is completed, the remaining indices in the bit vector which are set, are the node IDs of \( \Delta \). However, we still need to find these indices. We use a similar technique to the one described above for single-hop sampling. Given \( T \) threads, each thread \( t \in [0, T − 1] \) is assigned an equal chunk \( B_t \) of the bit vector and all threads count in parallel \( c_t \): the number of ones in their chunk. The sum of these individual counts is the size of \( \Delta \). With this knowledge, we can pre-allocate the output array and write to it in parallel. As for single-hop sampling (Algorithm 3, Line 3), we also calculate a local offset \( L_t \) which stores the starting index for where thread \( t \) should begin writing in the output array. We update \( L_t = \sum_{j < t} c_j \). Each thread then performs the following in parallel: Scan \( B_t \) and for each index \( i \) which is one, write \( i \) to \( \Delta \) at index \( L_t \), then increment \( L_t \). The strength of this implementation is that the entire calculation is done in parallel.

**Single GNN Layer Computation** In Algorithm 4, we describe how to use the Marius++ DENSE data structure to perform neighborhood aggregation, a common component of GNN layers like...
Algorithm 4: GNN Additive Aggregation Using DENSE

Input: DENSE: inputs: node representations for DENSE node_ids
1. nrb_data = inputs.index_select(DENSE.repr_map)
2. nrb_aggr = segment_sum(nrb_data, DENSE.nbr_offsets)
3. self_data = inputs[DENSE.node_id_offset[1]:]
4. outputs = nrb_aggr + self_data
5. return outputs

GraphSage [13] (see Section 2). We assume a simplified GNN which computes: \( h_i^{(l+1)} = h_i^{(l)} + \sum_{j \in \text{Nbrs}_i} h_j^{(l)} \). This can be done by using the repr_map array to select the node representation for each neighbor (Line 1). Neighborhood aggregation can then be performed using a dense segment sum according to the nrb_offsets—recall that the neighbors for each node are contiguous chunks (Line 2). The segment sum operation is well suited for the GPU hardware. Finally, we can combine the neighbor aggregations for each node with their own features (Lines 3-4). As detailed above, by construction, all node_ids and their corresponding representations are needed as input for the GNN layer, and the node_ids after node_idOffsets[1] are the nodes which should be encoded.

5 DISK BASED GNN TRAINING

In this section, we focus on scaling GNN training on a single machine beyond CPU memory and develop algorithms for disk-based learning. We start by introducing the general setup then shift to link prediction and introduce Two-Level BETA. Finally, we introduce the Dispersed and Sequential algorithms for node classification.

5.1 Disk-Based Training Setup

Data Layout Disk-based training requires that we partition the graph on disk and load these partitions into memory for training. In particular, graph nodes are randomly partitioned into \( p \) non-overlapping physical partitions. The vector representations for each node partition are stored sequentially on disk (Figure 2). Each partition is of equal size. Based on the node partitions, the graph edge list is grouped into \( p^2 \) edge buckets, where edge bucket \((i, j)\) contains all edges with source node in partition \( i \) and destination node in partition \( j \). The edge triplets in each edge bucket are also stored sequentially on disk. To support training, there is a CPU memory partition buffer which can store \( c \) partitions. When a specific set of \( c \) partitions are placed in the buffer, all \( c^2 \) pairwise edge buckets are also loaded into memory. Together these partitions and edges make up an induced subgraph which we call the in memory subgraph.

One Training Epoch Given the above, we wish to iterate over all training examples stored on disk exactly once per epoch. There are two main questions: 1) Which node partitions (and corresponding edge buckets) should be loaded into memory and in what order? 2) For a specific in memory subgraph, which examples should be used for training before the subgraph is updated? We call the solution to the former the replacement policy and the solution to the latter the training example selection policy (needed because a specific training example may appear in memory many times each epoch).

The replacement policy creates a sequence of partition sets each with cardinality \( c \) which are loaded consecutively into the CPU buffer to complete the epoch. Every time the contents of the partition buffer change a new in memory subgraph \( S_i \) is induced. Thus, any replacement policy introduces a sequence of in memory subgraphs \( S = \{S_1 \ldots S_k\} \). Between each \( S_i \), one or more physical partitions and their corresponding edge buckets are replaced with new ones residing on disk. For each \( S_i \), the training example selection policy creates a set of training examples \( E_i \) which should be processed before moving to \( S_{i+1} \). Before training can proceed on \( E_i \), we need to first pay the cost of creating the data structures for single-hop neighborhood sampling (Section 4.2). Thus, one epoch proceeds by loading the partitions and edges for \( S_1 \), preparing data structures for \( S_1 \), generating mini-batches from \( E_1 \), loading \( S_2 \), etc.

5.2 Link Prediction

Using the above framework, we first discuss how naive replacement and training example selection policies introduce bias in training. Then we introduce Two-Level BETA and how it addresses this bias.

Bias in Disk-based Training A naive combination of a replacement policy and a training example selection policy can lead to correlated training examples which focus on the same set of nodes for many consecutive gradient updates. This can lead to biased models and is of particular concern for GNNs which contain shared parameters that are updated during each gradient step.

Our prior solution for disk-based link prediction which utilizes the BETA replacement policy (Section 2) and a greedy training example selection policy suffers from the above problem. To see why, note that each successive in memory subgraph \( S_{i-1} \) and \( S_i \) generated by BETA differ by one replaced node partition and that the greedy policy assigns all edges in each edge bucket \( eb \) for training in the first subgraph which contains \( eb \). The combination of these policies means that all the edges in each \( E_i \) for \( i > 1 \) have their source or destination node in the same partition: assume \( p \) is the partition which is in \( S_i \) but not in \( S_{i-1} \). Then all edge buckets (and therefore edges) assigned to \( E_i \) will contain \( p \). Edge buckets containing other partitions in \( S_i \) will have been previously assigned to \( S_{i-1} \) or earlier according to the greedy policy. This combined policy results in reduced randomness in the order edges are processed each epoch—concat(\( shuffle(E_i) \)). This reduction in randomness results in accuracy degradation compared to training with the full graph in memory where edges are processed according to a random permutation. Using vanilla BETA, for a GraphSage GNN [13] on FB15k-237 [38], a standard benchmark for link prediction, accuracy is reduced by 16% with disk-based training compared to in-memory.

Maximize Randomness and Minimize IO In Marius++ we have three goals for disk-based link prediction: 1) maximize the randomness in the order training examples (edges) are processed each epoch, 2) minimize the total IO between disk and CPU, and 3) ensure reads/writes to disk are efficient. To achieve the first goal, we need a combined policy which is more flexible than the BETA/greedy approach. One way to increase randomness is to use smaller partition sizes by using more physical partitions \( p \). Smaller partitions allow for the training example selection policy to assign examples to subgraphs at a finer granularity and fixes fewer nodes together in a partition for the whole training process. However, the BETA replacement policy is not well suited for small partitions as the number of subgraphs per epoch \( |S| \) generated by BETA grows linearly.
with $p$. This introduces more overhead to prepare each subgraph $S_i$ for training. Nevertheless, the BETA replacement policy does satisfy our second goal—it ensures that all training examples (edges) appear in at least one in memory subgraph each epoch with near minimal disk-to-CPU IO. As such, our goals for maximizing randomness and minimizing IO are coupled together and we need an improved replacement policy for disk-based link prediction.

Two-Level BETA We now introduce Two-Level BETA for disk-based link prediction. In Two-Level BETA, the disk is still organized according to $p$ physical partitions, $c$ of which can fit in the CPU buffer. However rather than applying the BETA replacement policy over physical partitions, we randomly group them into logical partitions each epoch (Figure 2). Grouping is done without data movement, only a mapping is maintained on the CPU. We then utilize the BETA replacement policy to generate a sequence of subgraphs $S^I = \{S^I_1 \ldots S^I_n\}$ operating on the logical partitions. Each subgraph $S^I_i$ contains $c_j$ logical partitions in memory with $p/c = 1/c_j$. $S^I_1$ and $S^I_{i+1}$ differ by one replaced logical partition. Marius++ then automatically maps logical subgraphs to their physical subgraphs $S = \{S_1 \ldots S_n\}$. Training can then proceed using $S$. By utilizing logical partitions, Two-Level BETA decouples the number of subgraphs per-epoch from the number of physical partitions. This allows Marius++ to improve randomness by utilizing smaller partitions without increasing the overhead of subgraph preparation.

To generate training examples the Two-Level BETA algorithm utilizes a randomized training example selection policy: Given the sequence of in memory subgraphs $S = \{S_1 \ldots S_n\}$, for each edge bucket $eb$. Marius++ identifies the set of subgraphs $S_{eb}$ which contain $eb$. We then pick one $S_i$ at random from $S_{eb}$ and assign $eb$ to $E_i$ for training. Random edge bucket assignment spreads out the processing of edges which have endpoints in a specific partition across the epoch, helping to break the poor structure of our previous approach described above. Note that one may attempt to perform random assignment at the granularity of a single edge, but this is prohibitively expensive for large graphs with billions of edges. The randomized training example selection policy also leads to a balanced workload across subgraphs. When prefetching is used to mask the IO latency required to create $S_{i+1}$ during computation on $S_i$, balanced workloads enable more overlapping of IO and compute.

5.3 Node Classification

We now focus on algorithms for disk-based training of node classification models and introduce the Dispersed and Sequential algorithms. The setup remains as described in Section 5.1, but now the training examples are labeled graph nodes rather than edges.

Dispersed Training Algorithm To iterate over all training examples during an epoch we require that all labelled vertices in the partition buffer at some point during each epoch. Given the above requirement, the Dispersed training algorithm for disk-based node classification generates the sequence of subgraphs $S$ for training according to the replacement policy in Algorithm 5. Each partition is brought into the buffer one by one in a random order. As before, the replacement policy operates on logical partitions and Marius++ maps the resulting subgraphs to their corresponding physical partitions. For the goal of bringing each partition into memory, this replacement policy is guaranteed to have minimal disk-to-CPU IO as partitions are read from disk exactly once. To assign labeled train nodes to the per-epoch in-memory subgraphs, the Dispersed training algorithm utilizes a randomized training example selection policy. 

Sequential Training Algorithm Instead of ensuring that all train nodes appear in CPU memory the Dispersed algorithm ensures that all nodes in the graph appear in CPU memory. We find that in large-scale graphs [16, 17], it is often the case that the set of nodes labeled for training is only one to ten percent of all graph vertices. In fact, the base representations for the train nodes can generally fit in CPU memory, even when the full graph is many times larger. Thus, the Dispersed training algorithm can result in more IO than is necessary to process all train nodes each epoch. The problem is that the labeled vertices for training are spread across all node partitions, forcing each of them to be transferred from disk to CPU.

We introduce Sequential disk-based training to alleviate this issue by changing the organization of the data on disk. Rather than randomly partitioning the graph, all train nodes are assigned sequentially to the first $k$ partitions. If we have $p$ total partitions for a graph with $|V|$ nodes and $T$ train nodes, $k = \lceil T/\lceil V/P \rceil \rceil$. Non-train nodes are assigned to partitions randomly as before. It is still the case that all partitions are the same size. The Sequential algorithm assumes that $k$ is less than the buffer capacity $c$, i.e. all partitions with train nodes can fit in CPU memory at once. If this assumption does not hold, Dispersed training should be used.

For Sequential disk-based node classification we generate only one subgraph for training each epoch $S = \{S_0\}$. $S_0$ contains the $k$ train node partitions together with $c - k$ other randomly chosen partitions and their corresponding edge buckets. By construction, all train nodes are processed during $S_0$. With only a single in-memory subgraph per epoch, the Sequential training setup leads to zero intra-epoch IO cause by updating subgraphs $S_i$ to $S_{i+1}$.

6 HYPERPARAMETERS FOR DISK TRAINING

In the previous section we described methods for training with graph data stored on disk. We now ask how to set the hyperparameters involved in these algorithms—the number of physical partitions $p$, the buffer capacity $c$, and number of logical partitions $I$—to minimize training time and maximize model accuracy. We focus on the Two-Level BETA algorithm for link prediction but extend our discussion to the Dispersed and Sequential algorithms for node classification at the end of this Section. Note that maximizing the

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Algorithm 5: Dispersed Replacement Policy

| Input: | parts: list of logical partitions $[0 \ldots I - 1]$; $c_j$: number of logical partitions which can fit in memory |
|---|---|
| 1 | $S^I_0 = \text{rand\_perm(parts)}[0 : c_j]$; disk = parts $\setminus S^I_0$; $i = 1$ |
| 2 | while $\text{on\_disk\_size()} > 0$ do |
| 3 | $i = i + 1$; $S^I_i = \text{copy}(S^I_{i-1})$; $r_i = \text{rand\_int}(c_j)$ |
| 4 | $r_2 = \text{rand\_int}(\text{disk\_size}())$; $S^I_{i+1} = \text{disk}[r_2]$; disk.pop($r_2$) |
| 5 | return $\{S^I_1 \ldots S^I_I\}$ |
buffer capacity \( c \) best approximates training with the full graph in memory and thus leads to better runtime and accuracy. As such, we focus our discussion on \( p \) and \( l \) but, at the end of this Section, we give a concrete rule for setting \( c \). We start by connecting \( p \) and \( l \) to model accuracy, then focus on their effect on runtime, and conclude by using this information to present hyperparameter rules.

**Effect of \( p \) and \( l \) on Accuracy** To study the effect \( p \) and \( l \) have on model accuracy, we introduce a proxy metric which we term the *Edge Permutation Bias* \( B \). Recall from Section 5.2, that model quality can degrade if training consecutively iterates over correlated examples. This problem is general to ML workloads \([7, 14, 15]\). We design the Edge Permutation Bias to capture the extent to which the sequence of training examples generated by Two-Level BETA exhibits the aforementioned phenomenon. Figure 4a illustrates the dependency between \( B \) and model accuracy. The depicted results correspond to empirical measurements over a benchmark model (GraphSage \([13]\)) and data set (FB15k-237 \([38]\)). We find the same behavior to hold across settings.

We now define \( B \). Let \( E = \{E_1, \ldots, E_n\} \) be the sequence of edge bucket sets \( E_i \) assigned as training examples for each in memory subgraph \( S_i \) (Section 5.2). If an \( E_i \) contains edges which focus on a small subset of graph nodes, then we have the undesired correlation described above. We empirically measure this occurrence as follows: Let \( V \) be the set of nodes in the graph. For each node \( v \in V \) we keep a tally \( t_v^0 \) as we iterate over \( E \) which measures how many edges we expect to have seen containing this node after each \( E_i \). The tallies are cumulative and we assume a uniform degree distribution. We normalize such that \( t_v^0 = 1 \). This implies \( t_v^0 \in [0, 1] \). After each \( E_i \) we calculate \( d_i = \max_{x,y \in V} (t_x^2 - t_y^2) \). Given this, the Edge Permutation Bias \( B = \max_i d_i \in [0, 1] \).

Intuitively, we are interested in how evenly the tallies are incremented during the training epoch. Biased assignments will lead to processing many edges for a subset of nodes at once while ignoring the remaining graph vertices. This leads to high variance in model gradients across the epoch. With this in mind, an edge permutation bias of \( x \) means that \( x + a \) percent of the edges containing a certain node have been processed before \( a \) percent of the edges of another node have been processed (for some \( a \in [0, 1-x] \)).

We empirically show in Figure 4c that \( B \) decreases with increasing physical partitions. The observed trends can be characterized by the equation \( B = O(p^{-\alpha_1}) \) for some constant \( \alpha_1 > 1 \). In Figure 4b we show the effect of the number of logical partitions on \( B \). Decreasing the number of logical partitions decreases the Edge Permutation Bias roughly according to \( B = O(l^{-\alpha_2}) \) for \( 0 < \alpha_2 < 1 \). While, we do not provide a closed-form characterization of \( B \) as a function of \( p \) and \( l \) we find that the aforementioned trends hold across data sets. Moreover, describing the limiting behavior of \( B \) with respect to \( p \) and \( l \) suffices to obtain a concrete methodology for optimizing these hyperparameters (described below).

**Effect of \( p \) and \( l \) on Training Time** We now focus on how \( p \) and \( l \) effect the per-epoch runtime \( T \). To do so, we analyze three metrics which influence training time: 1) the total IO in terms of bytes transferred from disk to CPU memory (\( I/O \)), 2) the number of in-memory subgraphs generated per epoch (\( |S| \) ), and 3) the smallest size of disk reads (\( R \)) in bytes. As Quantities 1 and 2 increase, the total training time increases—recall that preparing each subgraph for training requires creating single-hop sampling data structures—while a decrease in Quantity 3 leads to an increased runtime.

By construction in Two-Level BETA, the number of logical partitions affects Quantities 1 and 2. In Figure 4b we show that as \( l \) increase the total IO decreases and the number of subgraphs per-epoch increases. The limiting behavior of \( I/O \) and \( |S| \) with respect to \( l \) is: \( I/O = O(\ell^{-\alpha_1}) \) for \( \alpha_1 > 1 \) and \( |S| = O(1) \). For the purposes of this work, we assume that the training time is dominated by the number of subgraphs per-epoch instead of the total IO for two reasons: First, the relative difference between the best and worst IO is usually only between 5-25 percent and second, prefetching can overlap IO with compute. Thus, we take the training time \( T = O(I/O) \).

The training time \( T \) is also affected by the number of physical partitions \( p \) through Quantity 3. As \( p \) increases, the size of each partition on disk decreases linearly and the size of each edge bucket decreases quadratically—the smaller of these quantities is the smallest disk read size \( R \). As a result, disk access transitions from large sequential reads/writes to small random reads/writes with increasing \( p \). Given the hardware constraints of block storage, the latter can become a performance bottleneck. In particular, read sizes \( R \) less than the disk block size \( D \) hurt performance. Thus, we model the effect of \( p \) on training time \( T \) according to \( T = O(1) \) for \( p \leq \alpha_4 \) and \( O(p) \) for \( p > \alpha_4 \), with \( \alpha_4 \) representing the number of partitions which cause the smallest disk reads to equal the block size \( D \).

**Methodology for Setting Hyperparameters** Given the effect of \( p \) and \( l \) on the model accuracy and training time described above, together with the desire to maximize the buffer capacity \( c \), we now present rules for setting the Two-Level BETA hyperparameters. We assume a graph \( G = (V, E) \), that the vector representation of each node is of dimension \( d \), that CPU memory is of capacity \( CPU \) bytes, and that the disk block size is \( D \). First we calculate the total overhead of storing all node representations as \( NO = |V| \cdot d = 4 \) bytes (using floating point numbers). Likewise the edge overhead \( EO \) can be calculated from \( |E| \) and the number of bytes used to represent each edge. Then, the overhead of each node partition is \( PO = NO/p \) and the expected size of each edge bucket is \( EBO = EO/p^2 \).

With the above definitions, the number of physical partitions affects the Edge Permutation Bias \( B \) and training time \( T \) as follows: \( B = O(p^{-\alpha_1}) \) for some constant \( \alpha_1 > 1 \) and \( T = O(1) \) for \( p \leq \alpha_4 \) and \( O(p) \) for \( p > \alpha_4 \) with \( \alpha_4 = \min(\text{NO}/D, \sqrt{EO/D}) \). Thus, to minimize the \( B \) without increasing training time, we set \( p = \alpha_4 \). We then maximize \( c \) such that \( c \cdot PO + 2 \cdot c^2 \cdot EBO + F \leq CPU \). The edge term is multiplied by two because Marius++ utilizes two sorted versions of the edge list (Section 4.2) and we leave some extra CPU space for working memory (fudge factor \( F \)). Finally, the Edge Permutation Bias and training time are affected by the number of logical partitions according to \( B = O(l^{-\alpha_2}) \) for \( 0 < \alpha_2 < 1 \) and \( T = O(l) \). As such, we minimize both by minimizing \( l \). Two-Level BETA imposes the constraint that the number of logical partitions in the buffer \( c_1 \geq 2 \) and that \( p/c = l/c_1 \). Therefore \( l = 2 \cdot p/c \).

While we have focused our analysis on Two-Level BETA, note that the Dispersed algorithm for node classification shares the same three hyperparameters. We set \( p \) and \( c \) for Dispersed training as described for link prediction. Unlike the above, however, for node classification the logical buffer capacity \( c_1 \) is constrained only to be larger than one (rather than two). Thus we set \( l = p/c \). Finally, the
We discuss the setup used throughout the experiments.

Datasets, Models and Evaluation
We use the two largest OGB node classification graphs—Mag240M and Papers100M—and the largest OGB link prediction graph WikiKG90Mv2 (Wiki) [16, 17]. As a second graph for large-scale link prediction we use Freebase86m (FB) [48]. A summary of the data set properties is shown in Table 1. For Mag240M we use only the paper nodes and citation edges, we denote this graph as MAG240M-C. We do this because 768-dimensional features are only provided for the paper nodes. We evaluate the quality of link prediction models using the commonly reported MRR metric [22, 29, 48]. For node classification, we report multi-class classification accuracy. We use a GraphSage (GS) [13] GNN for node classification. For link prediction we three models on Freebase86m: a shallow DistMult model (DM), GraphSage, and a GAT [39] GNN. On WikiKG90Mv2 we use only the first two. Model choices are common [20, 49].

Baselines We compare against DGL 0.7 and PyG 2.0.3. Both systems provide an API which contains a dataloader and GNN layer implementations. Both systems provide limited support for training link prediction at scale: PyG does not provide a negative sampler. We implemented negative sampling based on the negative sampling used in Marius++. DGL provides a negative sampler but the implementation limits the amount of negative samples that can be used to train in a reasonable amount of time. Further details for baselines are provided for each experiment.

Implementation
Marius++ is implemented in about 16,000 lines of C++ and 5000 lines of Python. We use the C++ API of PyTorch [23], as the underlying tensor and autograd engine, and OpenMP [30] for CPU parallelization. For the GAT forward pass implementation we make use of a segment-max kernel from PyTorch-Sparse [10].

Hardware setup
All comparisons are performed using AWS P3 instances (Table 1). Each machine is attached with an EBS volume with 1GBps of bandwidth and 10000 IOPS to serve as disk storage. Baseline systems do not support training if graph data does not fit in CPU memory. For each data set, we compare Marius++ to existing systems using the smallest P3 instance which has enough CPU memory to train. We allow baseline systems to use multiple GPUs for training if available. Marius++ uses only one GPU. For Marius++ disk-based training, a single P3.2xLarge is used. To reduce costs, we also utilize our own internal machines for microbenchmarks.

Hyperparameters
To ensure a fair comparison between systems, we use the same values for model and training parameters. We make sure to request the same number of neighbors per layer for each system but differences in mini-batches across systems are expected due to the use of different sampling algorithms. For throughput based parameters (e.g. data loader worker threads) we tune each system and use the best configuration. Marius++ disk-based training hyperparameters are set as discussed in Section 6 unless otherwise mentioned. In general, we choose hyperparameters to be those used for each data set by OGB or prior works [13, 16, 17, 39]. We train for ten epochs except on Freebase86m where we train for five.

Sequential training algorithm contains the hyperparameters $p$ and $c$. We set them as described above for Two-Level BETA.

### 7 EVALUATION

We evaluate Marius++ on four large-scale benchmark data sets, two from the OGB large-scale challenge [16], and compare against the popular SoTA systems DGL and PyG. We show that:

1. Marius++ reaches the same level of accuracy 2-8x faster and 6-64x cheaper than DGL and PyG on all evaluated datasets (Table 2) for both node classification and link prediction.
2. The DENSE data structure used by Marius++ reduces minibatch preparation and GNN compute times by up to 26x and 8x respectively for mixed CPU-GPU training.
3. Marius++ can scale training with disk storage utilizing two-level replacement policies. Two-level BETA outperforms our prior BETA algorithm with both respect to runtime and accuracy. Disk-based training support allows Marius++ to train on the Mag240M-C data set with 383GB of storage overhead using just an AWS P3.2xLarge machine containing 61GB of RAM.
4. The hyperparameter optimization in Marius++ yields configurations that achieve the highest throughput and model quality, lowering the deployment burden for large-scale training.

#### 7.1 Experimental Setup

We discuss the setup used throughout the experiments.

(a) Model Accuracy vs. Bias $B$
(b) Effect of logical partitions
(c) Effect of physical partitions

Figure 4: Empirical measurements on the effect of Two-Level BETA parameters using GraphSage on FB15k-237.

![GraphSage FB15k-237](image)

Table 1: Setup. CPU Mem & graph storage overhead ($\text{GB}$) in GB. NC: Node Classification, LP: Link Prediction

| Machine       | CPU Mem | GPU (k/hr) |
|---------------|---------|------------|
| P2.2xlarge    | 3       | 61, 1      | 356e |
| P4xlarge      | 32      | 24, 4      | 12.24|
| P3.8xlarge    | 64      | 48, 8      | 24.48|
| Internal      | 64      | 250        | 1    |

Hyperparameters
- $p$ and $c$: Set as described above for Two-Level BETA.
- $l$: Number of Logical Partitions
- $p$: Number of Physical Partitions
- $B$: Edge Permutation Bias
- $\delta$: Number of Subgraphs
- $\text{Normalized Total IO}$

 Sequential training algorithm contains the hyperparameters $p$ and $c$. We set them as described above for Two-Level BETA.
For DGL, we use five times fewer negative samples per training edge compared to Marius++ to prevent GPU out-of-memory issues. We train all systems using a single GPU for fairness reasons; multi-GPU link prediction training leads to accuracy loss due to asynchronous updates to CPU embeddings and DGL’s multi-GPU training ran out of CPU memory. We report the MRR for a single run due to cost considerations, but report runtime averaged across all training epochs. Both data sets fit in CPU memory on an AWS P3.4xLarge machine.

### Results

Marius++ trains shallow models (DistMult) 6× and 7× faster than the best baseline on Freebase86m and WikiKG90Mv2 respectively. With GraphSage, Marius++ is 6× and 7× faster than PyG on the two data sets. Interestingly, DGL and PyG report similar runtimes for GraphSage and the more computationally expensive GAT on Freebase86m. This is because these systems are not bottlenecked by compute, but rather by CPU sampling operations. While PyG and Marius++ reach comparable model quality, DGL is consistently lower due to its use of fewer negative samples. On WikiKG90Mv2, DGL does not complete the ten training epochs within two days. As such we only report the runtime and cost of one epoch. Notice that efficient support for link prediction GNNs can lead to significantly improved model quality on some data sets—GraphSage on WikiKG90Mv2 improves MRR from .4184 to .4683.

Marius++ can also perform disk-based training for link prediction. We train the above models on Freebase86m and WikiKG90Mv2 using Two-Level BETA on a P3.2xLarge machine. We utilize a partition buffer which stores 1/2 and 1/4 of the two graphs in memory. Marius++ is able to reach similar model quality to the in memory setting using a 3× cheaper machine. In general epoch times are slower for two reasons: 1) Two-Level BETA requires performing disk IO during every epoch and 2) the P3.2xLarge machine has 4× fewer CPU resources available for mini-batch preparation leading to longer sampling times. Yet, epoch runtimes remain 1.1×-4.5× faster than baseline systems with the full graph in memory.

### 7.4 Evaluating DENSE

We have shown that Marius++ is faster than existing systems. The key reason for this result is the efficient mini-batch sampling and forward pass computation using the DENSE data structure. To demonstrate the benefits of our approach, we measure CPU sampling time and GPU compute time for Marius++, DGL, and PyG.
We include FB15k-237 (14541 nodes, 272115 edges) and vary AWS GPUs with 16GB. Deeper GNNs could be of interest on models which achieve the best model quality. We also include the runtime and model quality for disk-based link prediction. We enable prefetching to overlap IO with computation. Two-Level BETA hyperparameters are set as described in Section 6. For BETA, we use manually tuned hyperparameters.

Results are shown in Table 4. We report the model MRR achieved when training with the full graph in CPU memory as an upper bound on the best possible disk-based model quality. Two-Level BETA consistently allows for faster training and higher model quality compared to BETA. Epoch time is reduced for IO bottlenecked configurations (shallow models) — Two-Level BETA is 1.28× faster than BETA for DistMult on Freebase86m. The reason for this is that Two-Level BETA more evenly distributes computation across the per-epoch subgraphs, allowing for more IO to be overlapped with training. We also observe that Two-Level BETA results in better model quality compared to BETA. This is evident for GNN models which have shared parameters but is applicable to shallow models as well. The gap between in memory MRR and disk MRR is reduced by 80 and 40 percent for GraphSage on FB15k-237 and Freebase86m respectively. Yet completely recovering the in memory MRR for disk-based link prediction remains a challenge and area of interest for future work. Some model and data set combinations lose significant model quality, e.g., GAT on FB15k-237 or GS on Wiki. With Two-Level BETA, we have taken a first step to considering both runtime and model quality for disk-based link prediction. We utilize a buffer capacity that can store 1/4 of all partitions in memory. This provides a challenging setting for disk-based link prediction. We enable prefetching to overlap IO with computation. Two-Level BETA hyperparameters are set as described in Section 6. For BETA, we use manually tuned hyperparameters.

### 7.5 Disk Based Training

In Sections 7.2 and 7.3, we showed that Marius++ disk-based training allows for cheaper training on massive graphs. We now evaluate disk-based training in more detail.

#### Link Prediction: Two-Level BETA versus BETA

We compare Two-Level BETA with vanilla BETA. We use DistMult, GraphSage, and GAT on the knowledge graphs FB15k-237, Freebase86m, and WikiKG90Mv2. We include FB15k-237 (14541 nodes, 272115 edges) to measure the bias present in disk-based training algorithms while utilizing all neighbors for GNNs and all negatives for evaluation.

| Graph | Model | Epoch Time | Disk MRR |
|-------|-------|------------|----------|
|       |       | TL-BETA | BETA | TL-BETA | BETA |
| 237   | DM    | .178     | 1.95   | .2659 | .2431 |
| 237   | GS    | .07      | 1.32   | .2736 | .2696 |
| 237   | GAT   | .351     | 3.90   | .2341 | .2076 |
| FB    | DM    | .753     | 17.51  | .7220 | .7189 |
| FB    | GS    | .7342    | 5.08   | .7123 | .6976 |
| FB    | GAT   | .7418    | 46.02  | .7053 | .6860 |
| Wiki  | DM    | .3941    | 22.54  | .4071 | .3951 |
| Wiki  | GS    | .4658    | 76.16  | .4078 | .4080 |

We utilize a buffer capacity that can store 1/4 of all partitions in memory. This provides a challenging setting for disk-based link prediction. We enable prefetching to overlap IO with computation. Two-Level BETA hyperparameters are set as described in Section 6. For BETA, we use manually tuned hyperparameters.

We report the model MRR achieved when training with the full graph in CPU memory as an upper bound on the best possible disk-based model quality. Two-Level BETA consistently allows for faster training and higher model quality compared to BETA. Epoch time is reduced for IO bottlenecked configurations (shallow models) — Two-Level BETA is 1.28× faster than BETA for DistMult on Freebase86m. The reason for this is that Two-Level BETA more evenly distributes computation across the per-epoch subgraphs, allowing for more IO to be overlapped with training. We also observe that Two-Level BETA results in better model quality compared to BETA. This is evident for GNN models which have shared parameters but is applicable to shallow models as well. The gap between in memory MRR and disk MRR is reduced by 80 and 40 percent for GraphSage on FB15k-237 and Freebase86m respectively. Yet completely recovering the in memory MRR for disk-based link prediction remains a challenge and area of interest for future work. Some model and data set combinations lose significant model quality, e.g., GAT on FB15k-237 or GS on Wiki. With Two-Level BETA, we have taken a first step to considering both runtime and model quality for disk-based link prediction.

#### Two-Level BETA Hyperparameters

We evaluate the runtime and model quality (MRR) of Two-Level BETA trained with hyperparameters set using Marius++ hyperparameter optimization against the best performing configurations found by hyperparameter scans. We report the best runtime and MRR independently, i.e. the scanned configuration which achieves the best runtime may not be the one which achieves the best model quality. We also include the runtime and MRR for the worst performing set of hyperparameters.
We utilize two different models—DistMult as a more IO bottlenecked configuration and GraphSage as a more compute bound model—and train on two data sets (FB15k-237 and Freebase86m). Results are shown in Table 5. For all settings, the hyperparameters rules introduced in Section 6 result in configurations which achieve nearly optimal runtime and MRR simultaneously. The consequences of poor hyperparameter configurations are also evident: On Freebase86m, the worst configuration is ~2.75x slower than optimal for DistMult and 10% lower in MRR for GraphSage.

Node Classification: Dispersed and Sequential Finally, we compare the performance of Dispersed and Sequential. We use the Papers100M data set and GraphSage model with varying CPU memory buffer capacities. Hyperparameters use Marius++ optimization. For comparison, we include the results of the best performing configurations from a hyperparameter scan for Dispersed training. Results are shown in Table 6. Numbers are averaged over three runs and we include standard deviations to show statistical significance as many models achieve similar accuracy. Both Sequential and Dispersed training produce final models with near in-memory accuracy, even with only 1/4 of the graph in CPU memory at a time. In general, we find the accuracy degradation for node classification models trained on disk is gradual with decreasing CPU memory capacity, a property which is not necessarily true for link prediction. In terms of runtime, Sequential is always faster than Dispersed due to the elimination of intra-epoch IO. As a result, Sequential disk-based node classification is our method of choice in the case where the labeled training nodes and their features can fit in CPU memory.

8 RELATED WORK

Many recent works focus on ML over graphs [43]:

Systems for GNNs and Graph Embeddings Many systems propose using mixed CPU/GPU training of GNNs [8, 12, 19, 20, 24, 50]. Two such popular systems are DGL [41] and PyTorch Geometric [11] [17]. When the GPU does not have sufficient memory to store all data required for training, both systems follow a mixed CPU/GPU sampling-based mini-batch approach. Complementary to these systems, many works focus on scaling different dimensions of GNN training: To reduce the overhead of mixed CPU-GPU training, some works highlight the importance of GPU oriented data communication or caching [8, 20, 24, 26, 27]. Additional works focus on speeding up GNNs with optimized GPU kernels [42]. In general, these works focus on orthogonal challenges of GNN training than those discussed here and these ideas can be incorporated into Marius++ to further improve performance. Finally, there are works that focus on scaling the training of graph embeddings with shallow models [1, 22, 29, 48]. DGL-KE [48] for instance, supports mixed CPU-GPU and distributed CPU training of graph embeddings. Finally, our prior work Marius [29] utilizes a pipelined training architecture to achieve state-of-the-art throughput.

Large-Scale Training To scale GNN training to graphs which exceed the CPU memory capacity of a single box, many works opt for a distributed multi-machine approach [12, 19, 49]. In particular, recent work introduces DistDGLv2 as a distributed version of DGL [49]. DistDGLv2 utilizes METIS partitioning, co-location of data with mini-batch computation, and asynchronous mini-batch preparation to scale training. Other works distribute training in a serverless manner [37]. In Marius++, we utilize a disk-based approach to scaling beyond CPU memory, as we believe it is a more resource efficient training paradigm. Our disk-based training on the Papers100m data set is 6.7x cheaper than DistDGLv2 training on the same graph (based on the cost to 66% accuracy reported for each system). A few other works have previously supported disk-based training, primarily for link prediction with graph embeddings [22, 29]. However, with Marius++ we extend this support to the node classification learning task and GNNs. Finally, all works that scale training beyond CPU memory utilize some form of graph partitioning [22]. Sun et al. [35] utilize partition recombination to improve shallow model quality in comparison to static partitions used by PyTorch BigGraph. This method is similar to our two-level partition abstraction; however, we extend support to GNNs and analyze the effect of two-level policies on training time and accuracy.

Neighborhood Sampling Many works focus on reducing the overhead of the neighborhood aggregation required for GNNs. Initial approaches used unbiased neighborhood sampling [13] whereby a fixed number of neighbors are sampled per node. Follow up works attempted to address scalability issues by sampling a fixed number of neighbors per layer rather than per node [5, 51]. Other works decouple the sampling frequency from the mini-batch frequency [32]. Marius++ focuses on unbiased sampling. Furthermore there are works which focus on making mini-batch training more efficient by increasing the density of edges between nodes in a mini-batch [6, 46]. These contributions can be incorporated in Marius++ and are orthogonal to our study. Finally, recent works utilize GPUs to speed up sampling [8, 18], Marius++ supports on-device sampling for graphs which fit in GPU memory, but focuses on CPU-based sampling to scale training to large graphs.

9 CONCLUSION

This paper introduced Marius++ a system for pipelined mini-batch training of GNNs in a single machine. We empirically showed that Marius++ with one GPU can achieve the same level of model accuracy up to 8x faster than popular competing systems using eight GPUs. These results highlight the need for optimizing single GPU implementations of ML systems before resorting to multi-GPU approaches. To achieve these results, we introduced a series of contributions such as the Delta Encoding of Neighborhood SampleEx (DENSE) data structure to minimize the memory footprint of sampling and the two-level data replacement policies for disk-based training. Finally, we present a mathematical model of biases introduced due to data movement in disk-based training which we believe to be of interest for future work on general ML systems.
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