Understanding GNN Computational Graph: A Coordinated Computation, IO, and Memory Perspective

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Abstract

Graph Neural Networks (GNNs) have been widely used in various domains, and GNNs with sophisticated computational graphs lead to higher latency and larger memory consumption. Optimizing the GNN computational graphs suffers from: (1) Redundant neural operator computation. The same data are propagated through the graph structure to perform the same neural operation multiple times in GNNs, leading to redundant computation which accounts for 92.4% of total operators. (2) Inconsistent thread mapping. Efficient thread mapping schemes for vertex-centric and edge-centric operators are different. This inconsistency prohibits operator fusion to reduce memory IO. (3) Excessive intermediate data. For GNN training which is usually performed concurrently with inference, intermediate data must be stored for the backward pass, consuming 91.9% of total memory requirement.

To tackle these challenges, we propose following designs to optimize the GNN computational graph from a novel coordinated computation, IO, and memory perspective: (1) Propagation-postponed operator reorganization. We reorganize operators to perform neural operations before the propagation, thus the redundant computation is eliminated. (2) Unified thread mapping for fusion. We propose a unified thread mapping scheme for both vertex- and edge-centric operators to enable fusion and reduce IO. (3) Intermediate data recomputation. Intermediate data are recomputed during the backward pass to reduce the total memory consumption. Extensive experimental results on three typical GNN models show that, we achieve up to $2.75 \times$ end-to-end speedup, $6.89 \times$ less memory IO, and $7.73 \times$ less memory consumption over state-of-the-art frameworks.

1 Introduction

Graph Neural Networks (GNNs) explore features of vertices and edges using neural operators and relationships through the graph structure. GNNs have shown great potentials in various domains, including Recommendation Systems (Ying et al., 2018; Wang et al., 2019a), Computer Vision (Yan et al., 2018; Qi et al., 2018), Natural Language Processing (Nguyen & Grishman, 2018; Yao et al., 2018), et al (Kipf & Welling, 2016; Hamilton et al., 2017).

With the fast development of GNNs, GNN models have evolved into more diversity and complexity in the computational graph, putting forward expensive requirements on both computation and memory resources. For example, training a GNN-based recommendation model consumes 16 GPUs (384 GB memory in total) using days of time (Ying et al., 2018). Improving the performance of GNNs with less resources suffers from: (1) From the computation perspective, GNN models perform neural operators through the graph structure, meaning that the same data of a vertex may be propagated to different edges. Thus, the same operation applied on these edges are executed multiple times for the same vertex data after propagation, leading to redundant computation in GNNs. We measure that such redundant computation account for 92.4% of total operators in an Edge-Conv model (Wang et al., 2019c), with the detailed setup in Section 7. (2) From the IO perspective, current systems involve writing/reading graph-sized feature data between two graph operators. Operators performed on vertices and edges are usually with inconsistent thread mapping schemes, which hinder applying fusion for these operators to reduce IO. (3) From the memory perspective, GNN models usually perform concurrent training and inference passes. Thus, excessive intermediate data produced during executing fused operators must still be stored for backward, leading to large memory space requirement. We measure in a Graph Attention Network (GAT) (Veličković et al., 2017) model that the intermediate data consume 91.9% of total memory.

To tackle these challenges and accelerate GNN computation with less memory consumption, we need a systematic GNN computational graph optimization framework which considers computation, IO, and memory. DGL (Wang et al., 2019b) provides two high-level operators, gSpMM and gS-DDMM, to express various GNN models, while such an ab-
We implement three popular GNN models with the techniques, propagation-postponed operator reorganization, which reduces an overview of our optimization recipe. Our three sections introduce preliminaries of GNNs. Section 3 introduces an overview of our optimization recipe. Our three techniques, propagation-postponed operator reorganization, unified thread mapping for fusion, and intermediate data re-computation are detailed in Section 4, 5, and 6, respectively. Section 7 presents evaluation results. Section 8 elaborates related work. Section 9 concludes the paper.

2 Preliminaries

2.1 GNN Operators

On a graph $G = (V, E)$ with the set of vertices $V$ and edges $E$, a GNN layer is composed of the following operators:

$$m_e = \text{Scatter}(h_v, h_u), (u, v, e) \in E,$$
$$m_e^{new} = \text{ApplyEdge}(m_e, m_e', \cdots),$$
$$h_v = \text{Gather}((m_e : (u, v, e) \in E)),$$
$$h_v^{new} = \text{ApplyVertex}(h_v, h_v', \cdots).$$

In the above equations, $v, u$ are vertex indices and $e$ is an edge index. $h_v$ refers to feature attached to vertex $v$, and $m_e$ attached to edge $e$.

Figure 1 visualizes the definitions of operators. Gather is a reduction operation that generates the feature of a vertex from features of edges connecting to it. Scatter generates the feature of an edge from features of vertices that the edge connects to. ApplyEdge and ApplyVertex are graph-irrelevant operators that transform the features of each edge and vertex, respectively. We further categorize Apply-operators based on their computation cost: element-wise operations are considered as lightweight Apply–, while computation-intensive operations like linear projection are considered expensive Apply–.

The four operators above are comprehensive enough to express any GNN model, but there are some widely-used combinations of operators, which current GNN systems also provide dedicated optimizations to. We name two most common combinations: Aggregate and ReduceScatter, as defined below. We add them to our operator abstraction operators for the convenience of expressing models.

$$h_v^{new} = \text{Aggregate}((h_u, m_e) : (u, e, v) \in E), h_v$$
$$= \text{Gather}(\{\text{ApplyEdge}(\text{Scatter}(h_v, h_u), m_e)\})$$
$$m_e^{new} = \text{ReduceScatter}((m_e' : (u \in N(v), e', v) \in E), h_v$$
$$= \text{ApplyEdge}(\text{Scatter}(\text{Gather}(\{m_e'\}), h_u), m_e),$$
$$(u, e, v) \in E$$

Aggregate generates a new vertex feature by reducing features from its neighbor vertices and edges. ReduceScatter generates a new edge feature by reducing and scattering among the groups of edges that connect to the same vertex, a typical example being the edge-softmax operation in the Graph Attention Network (GAT). Current GNN systems widely support fused Aggregate and ReduceScatter implementations when ApplyEdge is lightweight (Huang et al., 2020; Wang et al., 2019b).

Compared with related work, our operator abstraction...
2.2 Back-Propagation in GNN

The back-propagation algorithm is applied to train GNN models. One can prove that the backward pass of above set of operators still fall into this set. We list the key conclusions below, while the detailed proof is elaborated in Appendix.

- The backward pass of Gather (Scatter) is Scatter and ApplyVertex (Gather and ApplyEdge).
- The backward pass of ApplyEdge (ApplyVertex) is two ApplyEdge (ApplyVertex) operations.

The backward pass of Aggregate (ReduceScatter) can be analyzed by decomposing them into the four fine-grained operators. In summary, we can express both forward and backward pass of GNN using the same operator abstraction. A dataflow showing both passed and the four basic operators are in Figure 2. Figure 2 also show that the intermediate features are needed for computing gradients in the backward pass of the same layer. Therefore, all intermediate features need to be stashed in the memory for backward. During the forward pass, all intermediate features must be saved and later used to calculate parameter gradients in the backward pass. Take the GAT example again, Figure 3(a) marks all the feature tensors that are stashed and where they are used in the backward pass. State-of-the-art GNN systems follow the general strategy of saving outputs of all operators in the model, and only provide fused implementations for some common operator-combinations to avoid saving an $O(|E|)$ intermediate tensor (e.g., DGL’s built-in edge-softmax for GAT). A general approach for reducing memory consumption in training is lacked.

3 Design Overview

This paper proposes a systematic approach to optimize the GNN at inter-op level. In this section, we provide an overview of our designs by walking-through them on the model architecture of Graph Attention Network (GAT) (Veličković et al., 2017). Our proposed operator abstraction, in contrast, can construct whatever Aggregation-Combination constructs, and also Graph Attention Network (GAT) (Veličković et al., 2017), equivalent to our Aggregate and ApplyVertex, does not cover ApplyEdge. Therefore, the Aggregation-Combination can only express GNN models without applying neural networks to edge features, such as the vanilla GCN (Kipf & Welling, 2016) or GraphSAGE (Hamilton et al., 2017). Our proposed operator abstraction, in contrast, can construct whatever Aggregation-Combination constructs, and also Graph Attention Network (GAT) (Veličković et al., 2017), equivalent to our Aggregate and ApplyVertex, does not cover ApplyEdge. Therefore, the Aggregation-Combination can only express GNN models without applying neural networks to edge features, such as the vanilla GCN (Kipf & Welling, 2016) or GraphSAGE (Hamilton et al., 2017). As Figure 3(b) shows, a GAT layer is composed of Scatter, ApplyEdge, ReduceScatter, Aggregate, ended by an ApplyVertex. We tackle the aforementioned three design challenges with methods below:

Eliminating redundant computation through propagation postponed reorganization. Recall that the redundancy is caused by performing expensive Apply- (e.g. linear transformations) many times on the features propagated from the same source. We propose to reorder the operator sequence: to first apply expensive Apply- on the vertex features, and next propagate the result of the operation. For example, we show that in GAT (Veličković et al., 2017) models, the Scatter-ApplyEdge operator sequence can both be substituted by linear-projection on vertex features and Scatter- the result, as shown in Figure 3(b).

Reducing IO through completely fusing graph-related kernels. We propose to fuse a sequence of operators as long as they are graph-related kernels or lightweight Apply-. We choose not to fuse expensive Apply- like linear transformations because they can often be tackled with primitives in highly-optimized libraries, e.g. cuBLAS or cuDNN. The challenge here is that vertex-centric and edge-centric operators, i.e. operators that produce vertex- or edge-features, apply vertex-balanced and edge-balanced thread mapping in current GNN systems, respectively. The unmatched thread mapping schemes prohibit reusing intermediate data locally and force dumping data to the DRAM. With novel kernel designs, we show vertex- and edge-balanced thread map-
Avoiding saving intermediate data for backward pass after applying operator fusion with the unified thread mapping scheme, operators are fused while the intermediate features are still stored for the backward pass. After applying operator reorganization, the linear projection operator is preposed and applied on vertices to reduce computation. Vertex- or edge-features. This allows us to choose a unified single kernel and greatly reduces IO.

**4 Reducing Computation: Propagation-postponed Operator Reorganization**

**Motivation.** Many GNN models perform Scatter followed by a computation-intensive neural network (NN) as ApplyEdge. The same vertex feature is propagated to all its adjacent edges, and this duplication causes repeated NN computation in the ApplyEdge step.

**Challenge.** We describe above the intuition why propagation + NN operator causes redundant computation, but we lack a general formulation to identify and eliminate such redundancy. In particular, Scatter involves both redundant computation and per-edge unique computation: the redundant part is because multiple edges connected to the same vertex share identical vertex feature as input, and the unique part is because each edge combines features from a unique pair of two vertices. Separating the two parts and reducing the redundant part require a careful surgery on the original computational graph.

**Insight.** Our key insight is that the root of this possible computation redundancy is performing repeated neural computation on features scattered from the same source. Take figure 4(a) as an example. Figure 4(a) shows the computation and data flow for a part of one EdgeConv layer with one Scatter operator followed by an ApplyEdge operator. Features on vertices are first scattered to edges with func-
Following our insight phase, we find a sufficient condition to identify redundancy and mutative law. Although concatenate and the non-linear neural operation do not follow the commutative and distributive law, we find that the LP and concatenate can be seen as two LP followed by an add: $\tilde{a}^T \tilde{h}_u + a_r^T \tilde{h}_v$. Therefore, there is redundancy in computation if we don’t perform operator reorganization, and we postpone Scatter and change the execution order from Scatter-ApplyEdge into ApplyVertex-Scatter. As shown in Figure 3(b), we first apply LP to features on vertices, then scatter them to edges and perform add, followed by a LeakyReLU, which still need to be applied on edges. The total computation cost is reduced to $4|\mathcal{V}|f + 2|\mathcal{E}|$.

**5 Reducing IO: Unified Thread Mapping for Fusion**

**Motivation.** GNN systems suffer from excessive global memory writing/reading between production-consumption operators. Take the GAT model in Figure 3 as an example: the edge features produced by the ApplyEdge step needs to be written-out to the global memory, and read-in again by the next ReduceScatter operator. The output of ReduceScatter step is again stored and loaded by the succeeding Aggregate kernel. Both procedures involve writing/reading a $O(|\mathcal{E}|)$-sized feature tensor. Kernel fusion is widely exploited to reduce the data movement. In fact, the edge-softmax in current systems are commonly implemented by a hand-optimized fused kernel to reduce IO.

Our target is to apply kernel fusion to further eliminate the aforementioned two edge feature store/load, and completely fuse all graph-related operators (Scatter, ApplyEdge, ReduceScatter, Aggregate).

**Challenge.** The challenge in applying fusion to graph-related operators is the diverged thread-mapping schemes between edge-centric and vertex-centric operators. By edge-centric, we mean the operator whose output is edge features, and by vertex-centric the ones producing vertex fea-
each worker is assigned to loop over the incoming-edge set of a vertex and compute features for these edges. We can increase the number of threads in the same group to exploit parallelism, since features for each edge can be calculated in parallel. The example in Figure 5(c) reveals a potential issue of imbalanced workload, but the issue is minor as long as we have enough parallelism to fully occupy the GPU, and worth taking if it enables kernel fusion and saves excessive IO. On the other hand, when applying edge-balanced mapping to vertex-centric operator, we need to handle the cross-thread reduction shown in Figure 5(d). Cross-thread reduction can be implemented on GPU via atomic arithmetic. Observe that edge-balanced mapping improves workload balancing, but atomic arithmetic can introduce overhead, which we need to compare against the benefit of kernel fusion.

**Approach.** Following our insight that both edge-balanced and vertex-balanced schemes can be applied to all operators, we propose to eagerly fuse all graph-related operators with unified thread mapping. By the phrase graph-related, we refer to all operators except the expensive `Apply-` ones such as linear projection. In the GAT example, the sequence of Scatter, ReduceScatter, Aggregate all fall into this definition, and we are able to fuse them into one single kernel by applying same thread-mapping. In general, we can select between vertex-balanced or edge-balanced mapping based on performance profiling. A special case is when `ReduceScatter` is involved: since an intermediate vertex-feature needs to be reused between two operators, we can only apply the vertex-centric mapping and buffer the vertex-feature in the GPU shared-memory.

**Example.** In GAT, there are three graph-related operator that have a potential to fuse: Scatter, ReduceScatter and Aggregate. As `ReduceScatter` requests vertex-centric mapping, we apply unified vertex-balanced mapping to fuse these three operators into one kernel, which saves excessive IO. Assuming one GAT layer has `h` heads and a feature length of `f`, before operator fusion, the IO of these graph-related operators is

\[
4|\mathcal{E}|h + 3|\mathcal{E}| f + 7|\mathcal{V}| hf + |\mathcal{E}| hf + |\mathcal{V}| hf + |\mathcal{E}| hf + 2|\mathcal{E}| hf.
\]

With intermediate data reused, the IO is reduced to

\[
|\mathcal{V}| hf + 5|\mathcal{E}| h + 2|\mathcal{E}| hf.
\]

### 6 Reducing Memory: Intermediate Data Recomputation for Training

**Motivation.** GNN systems suffer from excessive memory consumption, because all the intermediate feature tensors are saved for the backward pass. Section 5 described our techniques to fuse all graph-related operators in the forward pass. Fusion saves not only IO but also memory since no intermediate tensors need to be written-out and read-in. We intend to extend operator fusion for the back-propagation based training scenario to reduce memory consumption.
Figure 6. Diagram of the intermediate data recomputation. (a) Edge features are stored for the backward propagation. (b) Edge features are recomputed without storing in the off-chip memory.

**Challenge.** The challenge of avoiding saving intermediate data is two folds: (1) it passes the values on the forward computational graph; (2) it passes the intermediate features in the forward pass to the backward computational graph for gradients computing. We can fuse operators both in forward and backward pass, which solves (1). But this is not enough for training, as intermediate data are still needed for backward.

Take Figure 6(a) as an example, which shows a toy example composed of one Scatter step and one Gather step, with operator fusion technique already applied. For the forward pass, we’ve successfully eliminated the $O(|E|)$ intermediate data produced by Scatter with operator fusion technique by fusing the Scatter-Gather procedure into one operator, in which the values of the intermediate data are temporarily stored in on-chip memory instead of the off-chip memory. But as we still need this intermediate data for backward propagation, we have to stash the intermediate data in off-chip memory.

**Insight.** Our key insight is that we can trade memory with computation: if the intermediate data is memory consuming but lightweight to compute, we can recompute those needed intermediate data during backward. Based on this, we propose a recomputing technique to deal with the intermediate data in the backward pass, which solves (2).

**Approach.** Following our insight that memory can be traded with computation, we propose an empirical criterion $\frac{\text{ComputationCost}}{\text{MemoryCost}}$ to identify the recomputing opportunity of an operator. If $\frac{\text{ComputationCost}}{\text{MemoryCost}}$ is no more than $O(1)$, which means we can save one element’s memory with no more than one computation, we just recompute the value during the backward pass, because we can save memory with little damage to the runtime latency. Otherwise, we stash the intermediate data as the performance improvement is limited. In the toy example in figure 6(b), we recompute the $O(|E|)$ intermediate data instead of stashing it because the computation cost of Scatter is small. By recomputing, we save $O(|E|)$ memory consumption with $O(|E|)$ computation. We will show later by experiments that this overhead is usually no more than 10% in GNN.

**Recomputation with fusion.** Our recomputing technique usually works for graph-related operators and lightweight operators, which take up much memory space but lightweight to compute. Occasionally, our proposed fusion technique is also applied to graph-related operators and lightweight operators. If we perform fusion without recomputation, we have to stash those needed intermediate data, which still costs a lot of memory space. By fusion-recomputation combo, we eliminate those intermediate data in the whole training process.

**Example.** In GAT, three operators are fused: one Scatter, one ReduceScatter (edge-softmax), and one Aggregate. So there are two intermediate data we have to handle: output of Scatter and output of ReduceScatter, both of which are $O(|E|)$. As the $\frac{\text{ComputationCost}}{\text{MemoryCost}}$ of this Scatter is only $O(1)$, we can just recompute it during backward propagation. The ReduceScatter operator edge-softmax first perform reduction to compute the maximums and the sum of all the exponential as denominator, which is a Gather, followed by a $O(1)$ division to compute the final edge value (Scatter and ApplyEdge). The recomputing score $\frac{\text{ComputationCost}}{\text{MemoryCost}}$ is $O(|\log|V||)$ for Gather and $O(1)$ for Scatter and ApplyEdge. According to our standard for recomputing, we store all the maximums and denominators during forward, which only takes $O(|V|)$, and recompute the other results within $O(1)$ time. By our proposed recomputation technique, two $O(|E|)$ intermediate data are eliminated with $O(1)$ overhead in latency.

7 EXPERIMENT

In this section, we implement our proposed techniques and evaluate them on multiple GNN models and datasets. We (1) demonstrate the overall performance improvements; (2) conduct ablation studies to provide detailed analysis on the benefits brought by each technique; (3) evaluate our implementations on devices with smaller DRAM which couldn’t fit in without our optimization.

7.1 Experimental Setup

7.1.1 Benchmarks

- **Graph Attention Network (GAT)** (Veličković et al., 2017) is one of the most classic GNN models, which adopts attention mechanisms to learn the relative weights between connected vertices instead of the identical or predetermined weights. It first Scatter features to edges and compute attention scores with learnable parameters, then perform ApplyEdge followed by Aggregate.
- **Edge Convolution (EdgeConv)** (Wang et al., 2019c) transforms the point clouds into a k-nearest neighbor graph to represent the topological information, in which points are viewed as vertices and their relative position...
is modeled as edges. It first Scatter vertex features to edges to compute their relative position, then Apply neural operations on edges and performs Gather to generate vertex embeddings.

- **Mixture Model Network (MoNet)** (Monti et al., 2016) introduces pseudo-coordinates to determine the relative position among vertices to learn the weight function adaptively. It first performs ApplyEdge to compute gaussian kernel, followed by Aggregate.

We choose these models because they represent the trend that GNN models will evolve into more diversity and complexity, from static edge value without gradient (Kipf & Welling, 2016; Hamilton et al., 2017) to gradient computation on edge feature (Veličković et al., 2017; Monti et al., 2016; Wang et al., 2019c).

### 7.1.2 Baselines

- **Deep Graph Library (DGL)** (Wang et al., 2019b) is one of the mainstream GNN framework on GPUs, which adapts to existing deep learning software such as PyTorch. It outweights PyG (Fey & Lenssen, 2019) in various GNN models. (Chen et al., 2020)
- **FuseGNN** (Chen et al., 2020) is a system for GNN training on GPUs with efficient CUDA kernel implementations and applies operator fusion technique. As fuseGNN does not implement EdgeConv and MoNet, we only compare with it on GAT.

### 7.1.3 Datasets

For GAT and MoNet, we use four commonly-used GNN datasets for evaluation, including Cora, Citeseer, Pubmed, and Reddit (Kipf & Welling, 2016; Hamilton et al., 2017). For EdgeConv, we use ModelNet40 classification task with 12,311 meshed CAD models from 40 categories, consisting in predicting the category of a previously unseen shape (Wu et al., 2015; Wang et al., 2019c).

### 7.1.4 Platforms & Metrics

We implement our proposed technique with a C++ and CUDA backend and a Pytorch-based front-end. Our main evaluation platform is a server with a 10-core 20-thread Intel Xeon Silver 4210 CPU running @ 2.2GHz and an NVIDIA RTX 3090 GPU with CUDA 11. Besides, we use an NVIDIA RTX 2080 GPU to demonstrate our design can achieve comparable performance against RTX 3090.

### 7.2 End-to-End Performance

**GAT**. As fuseGNN doesn’t support multi-head attention, we use the setting: 2 layers with 128 hidden dimensions for evaluation and the end-to-end training results are shown in Figure 7. Compared with DGL, we achieve an average of 2.07× (up to 2.75×) speedup and save an average of 1.48× (up to 3.53×) memory consumption. Compared with fuseGNN, we achieve an average of 1.85× (up to 3.41×) speedup and save an average of 1.29× (up to 2.55×) less memory consumption. The average IO is increased by 1.3% due to recomputation. On Cora, Citeseer and PubMed, we achieve great speedup mainly because we perform unified vertex-balanced fusion, which is friendly for these datasets. The memory consumption is not greatly saved because what we eliminate is the $O(|E|)$ intermediate data and the number of edges is small in these datasets. But on Reddit with 233K vertices and 115M edges, we save great memory consumption (3.88GB) compared with DGL (13.7GB) and fuseGNN (9.89GB) mainly because our proposed fusion-recomputation combo eliminates the $O(|E|)$ intermediate data during training. The memory saving will be more significant if applying multi-head mechanism as in the original paper (Veličković et al., 2017).

**EdgeConv**. We use the same setting as the original paper (Wang et al., 2019c): EdgeConv layers=4 with hidden dimensions={64, 64, 128, 256}, the number of nearest neighbors k=20/40, and the batch size=32/64, with a total of four different settings, and the end-to-end training results are shown in Figure 7. Compared with DGL, we achieve an average 1.52× (up to 1.69×) speedup and save an average of 4.58× (up to 7.73×) peak memory usage and 5.32× (up to 6.89×) IO. We apply operator organization and operator fusion technique in EdgeConv. As the Gather function is max, only an $O(|V|)$ array is needed for back propagation, and recomputation is not applied to further reduce memory consumption. Due to the overhead of transforming a point cloud into graph, the end-to-end speedup is not
as significant as it should be. However, the memory is largely saved because we optimize the graph-related operators which cause large memory consumption. Note that our memory consumption remains unchanged when k changes, for k is the average number of edges for each vertices. By implementing fusion-recomputation combo, we eliminate all the \( O(|E|) \) intermediate data.

**MoNet.** We use the setting: 2 layers with 16 hidden dimensions, \( k=3 \ r=2 \) for Cora, \( k=3 \ r=3 \) for Pubmed and Citeseer, \( k=2 \ r=1 \) for Reddit, where \( k \) is the gaussian kernel size and \( r \) is the dimension for pseudo coordinates in gaussian mixture model. As shown in Figure 7, compared with DGL, we achieve an average of 1.69\( \times \) (up to 2.00\( \times \)) speedup and save an average of 1.47\( \times \) (up to 3.93\( \times \)) peak memory usage and 1.30\( \times \) (up to 2.01\( \times \)) IO. Different from GAT, MoNet doesn’t have Scatter in the beginning, therefore operator reorganization is not needed.

### 7.3 Ablation Studies

Without special declaration, we use the setting as follows. (1) GAT: head=4 with feature dimension=64, on Reddit. (2) EdgeConv: \( k=40 \) batch size=64, layer=4 with hidden dimensions=\{64, 64, 128, 256\} for training, layer=1 with feature dimensions=64 if only forward. (3) MoNet: \( k=2 \ r=1 \) with feature dimension=16, on Reddit.

**Reorganization.** Figure 8 illustrates the benefits of operator reorganization for reducing computation, IO, and memory consumption in GAT and EdgeConv. MoNet has no Scatter and therefore no need for operator reorganization. Due to memory limitation of our device, we evaluate GAT with Pubmed. The baseline is implemented with Scatter before ApplyEdge, and the implementation with operator reorganization postpone Scatter and perform ApplyVertex first. To clearly show the impacts brought by operator reorganization, We use forward pass for comparison. The experiment results are consistent with theoretical analysis: as redundant computation is eliminated, latency is reduced and redundant IO caused by redundant computation is also eliminated; as we perform ApplyVertex before Scatter, one \( O(|V|) \) and one \( O(|E|) \) intermediate data are generated, but if we perform Scatter first followed by ApplyEdge, two \( O(|E|) \) intermediate data are generated. For the forward pass, operator reorganization improves latency by 1.68\( \times \), IO by 3.06\( \times \), and peak memory usage by 1.30\( \times \) on average.

**Fusion.** Figure 9 illustrates the benefits brought by operator fusion. We fuse all the graph-related operators with our proposed unified thread mapping scheme, and our proposed fusion technique can be applied to all of these three models. More details about our implementation can be found in appendix. We use For GAT, fusion has a little negative impact on latency, slightly reduces IO and greatly reduces memory consumption. As we use shared memory to perform operator fusion, which introduces extra overhead and Reddit is a very unbalanced graph, the latency is still largely determined by the unbalanced workload after performing fusion. The neural operators consumes the major part of IO, the relative IO reduction is not significant. The absolute value of IO reduction and memory reduction are about same level. For EdgeConv, IO and memory consumption are greatly reduced, and latency is slightly improved, mainly because of saving write-in and read-out for intermediate data. As the absolute value of IO in EdgeConv is much smaller that GAT, the relative IO reduction is much more significant. For MoNet, latency, IO, and memory are all significantly saved, mainly because of the largely improved data locality and saving for broadcast. For the forward pass, the operator fusion technique improves latency by 1.68\( \times \), IO by 1.16\( \times \), and peak memory usage by 4.92\( \times \) on average.

**Recomputation.** Figure 10 illustrates the benefits brought by intermediate recomputation on GAT and MoNet. As the Gather function in EdgeConv is max, only the indices of the maximum have to be stashed (which is \( O(|V|) \)) and there is no need for recomputation. We use three implementations for comparison: (1) without our unified thread mapping operator fusion technique; (2) with the fusion technique without recomputation technique, which means intermediate data have to be stashed; (3) with both our proposed fusion technique and recomputation technique. For GNN training, only fusion cannot reduce memory consumption, as even if we eliminate some intermediate data during the forward pass with operator fusion, we still need to stash them to perform back propagation. However, with our proposed recomputation technique, we can also eliminate those intermediate data during backward propagation at a small cost of computation. In GAT, recomputation saves 2.21\( \times \) memory at the cost of slowing down by 7.1\%. In MoNet, recomputation saves 1.55\( \times \) memory and accelerates by 5.9\%.
Section 7.4 Evaluation on Different GPUs

With our proposed three techniques, we are able to perform the same training task on devices with much smaller memory capacity. We evaluate our models with the same setting as Section 7.3 on RTX 2080, all of which cannot be done without our proposed techniques due to memory capacity limits. Figure 11 show that our implementation on RTX 2080 can even achieve 1.17× end-to-end speedup over DGL on RTX 3090 with 7.73× less memory for EdgeConv.

8 RELATED WORK

8.1 GNN Systems

NeuGraph (Ma et al., 2019) first introduces SAGA (Scatter, ApplyEdge, Gather and ApplyVertex) abstraction to describe GNNs. It is the first system that bridges the gap between graph processing systems and DNN systems. After that, GNN systems can be categorized as following types:

**GNN computation graph optimization** includes operator reorganization, operator fusion, data flow optimization, etc., and many efforts have been made to solve the challenges in optimizing GNN computation graph: (1) **Redundant neural operator computation**. Prior work attempts to tackle the computation redundancy via manually modifying the operator combinations to a functionally-equivalent but efficient version. For example, DGL (Wang et al., 2019b) provides a GAT implementation in its GNN-module library, where the ApplyEdge (the linear projection) is separated into two functions applied to vertex-features ahead of propagation. However, a theory inside this practice needs to be extracted for optimizing similar scenarios, as we do in this paper. (2) **Inconsistent thread mapping**. Fusion is widely used in conventional Deep Neural Networks (DNNs) (Niu et al., 2021). FuseGNN (Chen et al., 2020) manages to fuse any two edge-centric operators, but lacks the technique to fuse a vertex-centric operator with an edge-centric one, which we address in this paper via unified thread mapping. (3) **Excessive intermediate data**. Huang et al., (Huang et al., 2021) reduces intermediate data during forward but cannot handle back propagation because the intermediate data are missed. FuseGNN (Chen et al., 2020) stashes the intermediate data during forward, but lacks the recomputation technique, which still consumes great memory space.

**GNN runtime optimization** includes neighbor grouping, graph reordering etc., which introduces a preprocessing procedure to schedule the workload assignment and memory layout. GNNAdvisor (Wang et al., 2021) and Huang et al., (Huang et al., 2021) both utilize neighbor grouping to balance the workloads among GPU threads and blocks and exploit memory locality. GNNAdvisor further use Rabbit Reordering (Arai et al., 2016) to maximize the graph modularity by clustering. By neighbor grouping and graph reordering, the runtime workload balance and memory locality are improved by introducing some preprocessing overhead.

8.2 DNN Systems

TASO (Jia et al., 2019) proposes a novel computation graph optimizer for DNNs that can automatically generate graph substitutions. DNNFusion (Niu et al., 2021) proposes a set of fusion methodologies to work in conjunction with computation graph rewriting for DNN inference. Chen et al., (Chen et al., 2016) introduces the recomputation technique to DNN training to trade computation with memory. Our proposed operator reorganization technique is more of eliminating computing redundancy, while DNN computation graph substitution is more of finding a better substitution. Our unified thread mapping operator fusion technique is also different from operator fusion in DNNs, as GNN introduces graph-related operator, which brings about the divergent thread mapping between edge-centric and vertex-centric operators. And unlike DNN recomputation, which incurs roughly 30% of additional latency (Chen et al., 2016), overhead by our proposed recomputation technique is <10% as we utilize the characteristics of GNN training.

9 CONCLUSION

In this paper, we present a thorough study of GNN computational graph optimization. We point out GNN systems suffer from redundant neural operator computation, inconsistent thread mapping, and excessive intermediate data. We propose a systematic framework with propagation-postponed
operator reorganization, unified thread mapping for fusion, and intermediate data recomputation. We achieve up to $2.75 \times$ end-to-end speedup, $6.89 \times$ less memory IO, and $7.73 \times$ less memory consumption over state-of-the-art frameworks. We even enable running large-scale GNN models with an NVIDIA RTX 2080 GPU, which require the newest NVIDIA RTX 3090 GPU, with a comparable latency. More specifically, we provide an optimization-friendly perspective to understand GNN computational graph, which can be extended to other hardware platforms.

**REFERENCES**


A GNN Operators

This section formally describes our taxonomy of GNN operators, briefly introduced in Section 2.1 as 4 basic operators: Scatter, Gather, ApplyEdge, and ApplyVertex, and 2 high-level operators: ReduceScatter and Aggregate. We further illustrate how to construct popular GNN models from this set of operators.

A.1 Operator Definition

Let a graph be \( G = (V, E) \), where \( V \) represents the set of vertices, and \( E \) represents the set of edges. The elements in \( E \) is tuples of \((u, e, v)\), where \( u, v \in V \) and \( e \) is a unique id. The tuple \((u, e, v)\) indicates there is an edge indexed by \( e \) pointing from \( u \) to \( v \). We define four basic operators as follows:

- **Scatter**: \( m_e = \phi(h_u, h_v), (u, e, v) \in E \). For every edge, perform a binary operation (function \( \phi(\cdot, \cdot) \)) on the features attached to the two vertices that the edge connects to.
- **Gather**: \( h_v = \psi\{m_e : (u, e, v) \in E\} \). For every vertex, perform a reduction operation to the features attached to all edges that connects to it.
- **ApplyEdge**: \( m_e^{\text{new}} = f_e(m_e, m_e'), (u, e, v) \in E \). For every edge, perform the same function \( f_e \) that transforms its current feature (and any history features). This operator is graph-irrelevant, meaning that its outcome does not change if the graph structure (connections) changes.
- **ApplyVertex**: \( h_u^{\text{new}} = f_v(h_v, h_v), v \in V \). For every vertex, perform the same function \( f_v \) that transforms its current feature (and any history features). This operator is also graph-irrelevant like ApplyVertex.

Through composing the above four operators, we also propose two high-level operators that are widely seen in GNN models:

- **Aggregate**: \( h_u^{\text{new}} = \psi\{f_e(\phi(h_u, h_v), m_e)\}, (u, e, v) \in E \). It is a sequence of three basic operators: Scatter to generate edge features, ApplyEdge to transform the edge feature or combine it with any history features, and finally Gather to reduce edge features and generate new vertex features. A typical example is the neighborhood feature-reduction in vanilla GCN, where each vertex takes the sum of all its neighbor-vertices’ features, essentially \( h_u^{\text{new}} = \text{sum}\{w_e : h_e : (u, e, v) \in E\} \). This step can be expressed by Aggregate by binding \( \phi \) as copying source-vertex’s feature, \( f_e \) as multiplying the edge weight \( w_e \), and \( \psi \) as summation.
- **ReduceScatter**: \( m_e^{\text{new}} = f_e(\psi\{m_e\}, h_u, m_e'), (u, e, v) \in E \). It is a sequence of three basic operators: Gather to reduce edge features into vertex features based on the vertex’s adjacent edge group, and Scatter to broadcast the reduction results to all edges, and finally ApplyEdge to combine the broadcast values and any history features into new edge features. This operation can be used when the edge features are normalized within a neighborhood set, as happens in the edge-softmax. Edge-softmax performs \[ m_e^{\text{new}} = \text{softmax}(\{m_e' : (u \in N(v), e', v) \} | e) \], where
\[
\text{softmax}(x_1, \ldots, x_n)[i] = \frac{e^{x_i - \text{max}_i(x_k)}}{\sum_{j=1}^{n} e^{x_j - \text{max}_i(x_k)}}
\]. This step can be expressed by the following code snippet:

\[
\begin{align*}
\text{RS1: } & \psi \leftarrow \text{max}, \phi \leftarrow \text{copy}, f_e \leftarrow \text{subtraction}, \\
\text{RS2: } & \psi \leftarrow \text{sum}, \phi \leftarrow \text{copy}, f_e \leftarrow \text{division}.
\end{align*}
\]

A.2 Construct GNN Models

**GCN**

Vanilla GCN is defined as:
\[
h_v^{(l+1)} = \sigma \left( b^{(l)} + \sum_{u \in N(v)} e_{uv} h_u^{(l)} W^{(l)} \right)
\]
where \( \sigma \) is an activation function, \( b \) is a bias, and \( W \) is weight to learn. With four basic operators, we first perform ApplyVertex, then copy source vertex’s feature to edges (Scatter) and multiply the edge weights (ApplyEdge) to obtain \( e_{uv} h_u^{(l)} W^{(l)} \), followed by a gather with summation (Gather) and an activation (ApplyVertex), as shown in figure 12(a). Figure 12(b) shows how to describe the same procedure with an high-level operator Aggregate.

**GAT**

GAT is defined as:
\[
h_v^{(l+1)} = \sum_{u \in N(v)} e_{uv} W^{(l)} h_u^{(l)}
\]
\[
e_{ij}^{l} = \text{edge-softmax} \left( \text{LeakyReLU} \left( \alpha^T \left[ W h_i || W h_j \right] \right) \right)
\]
where \( W \) and \( \alpha \) are learnable parameters. Figure 12(c) shows one way to compute this. Assume the input node feature vectors are concatenated into a feature matrix \( H^{(l)} \in \mathbb{R}^{n \times f^{(l)}} \), and operator reorganization technique is already applied. We first perform a dense matrix multiplication to transform this feature matrix into \( H^{(l)} = H^{(l)} \times W^{(l)} \in \mathbb{R}^{n \times f^{(l+1)}} \) with torch.nn.linear. We decompose the weight vector \( a \in \mathbb{R}^{2 \times f^{(l+1)}} \) into \( [a_l || a_r] \).
and compute attention scores \( A_i = \tilde{H}^{(i)} \times a_i \in \mathbb{R}^{n \times 1} \) and
\( A_r = \tilde{H}^{(i)} \times a_r \in \mathbb{R}^{n \times 1} \).

After that, \( M_0 \in \mathbb{R}^n \) are generated by
\[ M_0 = u \_ \text{add}_v(A_l, A_r) \]

An ApplyEdge operator is then applied to generate
\[ M_1 = \text{LeakyReLU}(M_0) \in \mathbb{R}^n \]

followed by a ReduceScatter operator to generate
\[ M_2 = \text{edge}\_softmax(M_1) \in \mathbb{R}^n \]

An Aggregate operator is performed to generate
\[ \tilde{H}^{(i+1)} = \text{reduce}_\text{sum}(M_2, \tilde{H}^{(i)}) \in \mathbb{R}^{n \times f^{(i+1)}} \]

In our implementation, we fuse the computation of \( M_0, M_1, M_2, \tilde{H}^{(i+1)} \) into one operator, as shown in figure 12(d).

**EdgeConv**

Figure 12(e) shows one way to compute EdgeConv. The mathematical definition of one EdgeConv layer is
\[ h_v^{(i+1)} = \max_{u \in \mathcal{N}(v)} \left( \Theta \cdot (h_u^{(i)} - h_v^{(i)}) + \Phi \cdot h_v^{(i)} \right) \]

where \( \mathcal{N}(v) \) is the neighbor of \( v \), \( \Theta \) and \( \Phi \) are linear layers. In SOTA gnn framework DGL, one edgeconv layer is computed as shown in figure 12(e). Define the input node feature matrices as \( H^{(i)} \in \mathbb{R}^{n \times f} \). The \( (h_u^{(i)} - h_v^{(i)}) \) is computed by
\[ E^{(i)} = u \_\text{sub}_v(H^{(i)}) \in \mathbb{R}^{e \times f^{(i)}} \]

followed by one linear ApplyEdge
\[ E^{(i)}_{\Theta} = \Theta \cdot E^{(i)} \in \mathbb{R}^{e \times f^{(i+1)}} \]

An linear ApplyVertex is performed to compute \( \Phi \cdot h_v^{(i)} \):
\[ N^{(i)}_{\Phi} = \Phi \cdot H^{(i)} \in \mathbb{R}^{n \times f^{(i+1)}} \]

followed by
\[ E_{\Theta + \Phi}^{(i)} = e \_\text{add}_v(E_{\Theta}^{(i)}, N_{\Phi}^{(i)}) \in \mathbb{R}^{e \times f^{(i+1)}} \]

In the end, a reduce function is called to update the node features
\[ H^{(i+1)} = \text{reduce}_\text{max}(E_{\Theta + \Phi}^{(i)}) \in \mathbb{R}^{n \times f^{(i+1)}} \]

**GMMConv**

GMMConv is defined as:
\[ m_{uv} = f(x_u, x_v), x_u \in \mathcal{N}(v) \]
\[ w_k(m) = \exp\left(-\frac{1}{2}(m - \mu_k)^T \Sigma_k^{-1}(m - \mu_k)\right) \]

If here is a linear projection, \( \Sigma_k \) is a covariance matrix of the gaussian kernel, \( \mu_k \) is the mean of the gaussian kernel. By setting covariance matrix and mean as parameters with gradient, GMMConv could learn weight \( w_k \) in training process (ApplyEdge).

\[ h_v^{(i+1)} = \frac{1}{K} \sum_{u \in \mathcal{N}(v)} \sum_{k} w_k(m_{uv})h_{u_k}^{(i)} \]

To get node feature, GMMConv multiplies node embedding with gaussian weight, followed by gathering the sum of multi-kernels of embeddings (Gather).

**B Back-propagation of GNN Operators**

In this subsection, we derive the backward pass of the four GNN operators, and show that they can still be constructed by the four basic operators. Here \( \circ \) represents composition of operators where the latter operator gets applied first.

**Gather**; The backward pass of Gather is a Scatter followed by an ApplyEdge.

\[ \text{Forward: } h_v = \psi(m_e : (u, e, v) \in \mathcal{E}), \]
\[ \text{Backward: } \text{grad} m_e = \text{grad} h_e \times \frac{\partial \psi}{\partial m_e} \]
\[ = \text{ApplyEdge}_{f_e \leftarrow (\times \text{grad} m_e)} \]
\[ \circ \text{Scatter}_{\Phi \leftarrow \text{copy}_v} \]

**Scatter**; The backward pass of Scatter is a Gather followed by an ApplyVertex.

\[ \text{Forward: } m_e = \phi(h_u, h_v), (u, e, v) \in \mathcal{E}, \]
\[ \text{Backward: } \text{grad} h_v = \sum_{(v, e, u) \in \mathcal{E}} \text{grad} m_e \times \frac{\partial \phi}{\partial h_v} \]
\[ + \sum_{(v, e', u) \in \mathcal{E}} \text{grad} m_{e'} \times \frac{\partial \phi}{\partial h_u} \]
\[ = \text{ApplyEdge}_{f_e \leftarrow (\times) [\frac{\partial \phi}{\partial m_e} \circ \frac{\partial \phi}{\partial m_{e'}}]'} \]
\[ \circ \text{Gather}_{\Phi \leftarrow [\sum \text{grad} m_e, \sum \text{grad} m_{e'}]} \]

**Apply-**; The backward pass of graph-irrelevant Apply- is also graph-irrelevant, and can be derived in the same way.
Figure 12. Construct GNN models with GNN operators.
as operators in neural networks.

**Forward:** \( y = f(x, w) \)

**Backward:**

\[
\text{grad} w = \text{grad} y \times \frac{\partial f}{\partial w} \\
\text{grad} x = \text{grad} y \times \frac{\partial f}{\partial x}
\]

Hence the backward of \text{Apply-} is two \text{Apply-}, one calculating the gradient of input and one for the gradient of weight parameters.

Figure 13 visualizes the forward-backward dataflow of each GNN operator.