Accelerating GCN Inference on Small Graphs

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Outline

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Graph Neural Network (GNN)

Many applications [Zhang, 2019, Khemani et al., 2024]

- A huge graph: social networks, knowledge representations.
- A large number of (small) graphs: molecular graphs in bioinformatics.

Many variants

- Graph convolutional network (GCN)and [Kipf and Welling, 2017]
- Graph sample and aggregate network (GraphSAGE) [Hamilton et al., 2017]
- Graph attention network (GAT) [Velivcković et al., 2018]

Graph Convolutional Network (GCN)

$$\mathbf{H}^{(\ell+1)} = \sigma\left(\widetilde{\mathbf{D}}^{-\frac{1}{2}}\widetilde{\mathbf{A}}\widetilde{\mathbf{D}}^{-\frac{1}{2}}\mathbf{H}^{(\ell)}\mathbf{W}^{(\ell)} + \mathbf{b}^{(\ell)}\right), \quad \ell = 0, 1, \cdots, L-1, \tag{1}$$

Related work

Related work on accelerating GNN/GCN inference

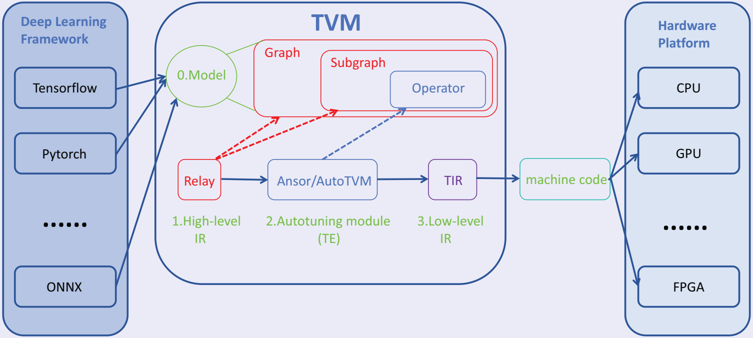
- Survey papers: [Liu et al., 2022, Abadal et al., 2022].
- Algorithm:
  - Reducing the feature dimension [Yik et al., 2022].
  - Sampling multi-hop neighbours [Zhang et al., 2023a].
  - Model reduction [Tan et al., 2023].
- Implementation:
  - Software implementation: DGL, PyG, DGI [Yin et al., 2023].
  - Hardware implementation: [Zhang et al., 2023b].

Related work on accelerating batched matrix multiplication

- Dimensions are the same in a batch: batch_matmul in TVM.
- Variable dimensions in a batch: MAGMA, Intel MKL.
- Our previous work on accelerating batched matrix multiplication for variable small sizes based on TVM [Dai and Chen, 2024].

Deep Learning Compiler: TVM [Chen et al., 2018]

Work flow of TVM



Supports in TVM for accelerating GCN

- TVM has introduced sparse tensors to support the inference of GCN.
- Internally, sparse tensors will be converted into dense ones.
- Currently TVM only supports inference on a single graph.

Outline

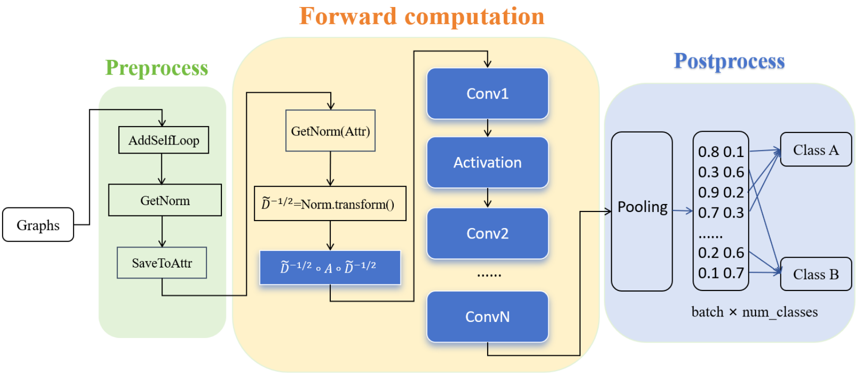
Main contribution and the optimizations deployed

- We replace (single large) sparse-dense matrix multiplication with (batched small) ones in GCN.
- We rearrange the order of basic operators in the forward computation of GCN to avoid redundant computation.
- We implement these optimizations in TVM to provide efficient GCN inference for batched graphs.

A series of optimization techniques deployed

- Replacing sparse operators with dense ones in both DGL and TVM.
- Reordering basic operators to avoid redundant computations in both DGL and TVM.
- Applying associative law to reduce number of arithmetic operations in TVM.
- Providing batched dense matrix multiplications targeting for small matrices in both DGL and TVM.
- Utilizing TVM complier optimization (mainly constant folding).

The different stages of GCN inference



- The preprocessing part includes loading input graph data and preparing adjacency matrix.
- The computing part includes normalization of adjacency matrix, convolution and activation.
- After getting output of the last layer, we apply postprocessing to obtain embedding or classification result of node, edge or graph.

Replacing sparse-dense matrix multiplication by dense ones

The intuition

- Cons: This optimization increases the number of arithmetic operations.
- Pros: Fully leverages GEMM optimizations, such as cache reuse and vectorization.
- For small matrices, overhead can be compensated by benefits.

Implementation details

- For DGL, we propose DGL*-Dense by uniformly adopting numpy.dot to replace torch.sparse.mm.
- For TVM, we propose TVM*-Dense for employing relay.nn.dense instead of relay.nn.sparse_dense.

Hadamard product

Defined for matrices of the same size

- $H = A \odot B$, defined as $H_{ij} = A_{ij} * B_{i,j}$.

Accelerating product of a diagonal matrix with a dense one

- $D_{m\times m}$ is a diagonal matrix with $D_{ii} = d_i$.
- We want to compute $D \cdot A$ efficiently.
- Let $e = [1, ..., 1]^t$ and $d = [d_1, \ldots, d_m]^t$.
- $D \cdot A$ can be computed as: $(D \cdot e \cdot e^t) \odot A$.
- $D \cdot e \cdot e^t = [d, \ldots, d]$.
- By $D \circ A$, we mean compute $D \cdot A$ in a Hadamard product way.
- Similarly, we have
  - $A \cdot D$ can be computed as: $A \odot (e \cdot e^t \cdot D)$.
  - By $A \circ D$, we mean compute $A \cdot D$ in a Hadamard product way.

Reordering basic operators (I): Basic idea

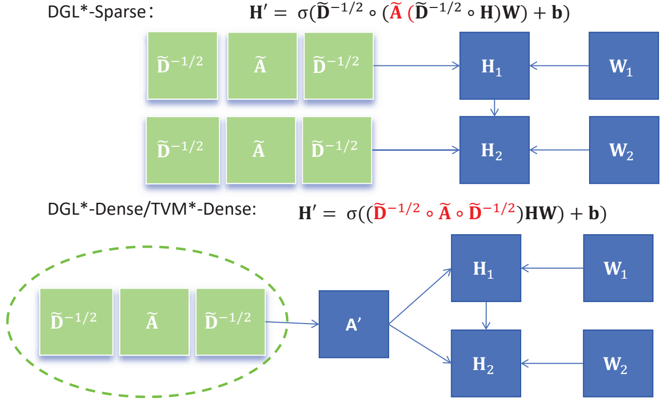


Figure: Basic operators reordering in a two-Layer GCN

- Pros: Efficiently compute product of diagonal degree matrix $\widetilde{\mathbf{D}}^{-\frac{1}{2}}$ by another dense matrix by utilizing Hadamard product operation.
- Cons: Redundant computation of $\widetilde{\mathbf{D}}^{-\frac{1}{2}}\widetilde{\mathbf{A}}\widetilde{\mathbf{D}}^{-\frac{1}{2}}$ when $\#conv > 1$.

Reordering basic operators (II): Some extra details

Complexity analysis

- Size of the adjacency matrix **A**: $m * m$.
- Size of the feature matrix **H**: $m * p_i$.
- Size of the weight matrix **W**: $p_i * q_i$.
- The saved number of floating-point operations is $m \sum_{i=1}^{n} (p_i + q_i) - 2m^2$.

Implementation of *Conv* layer from TVM

$$\mathbf{H}^{(\ell+1)} = \sigma\left(\widetilde{\mathbf{D}}^{-\frac{1}{2}} \circ \left(\mathbf{W}^{(\ell)^T}\left(\widetilde{\mathbf{D}}^{-\frac{1}{2}} \circ \mathbf{H}^{(\ell)}\right)^T \widetilde{\mathbf{A}}^T\right)^T + \mathbf{b}^{(\ell)}\right) \tag{2}$$

This is because implementation of matrix multiplication in Relay layer of TVM only accommodates $C = \mathbf{A}\mathbf{B}^T$ through operator relay.nn.dense.

Exploiting the associative law of matrix multiplication

Recall the core computation of GCN

$$\mathbf{A}_{m\times m} * \mathbf{H}_{m\times p} * \mathbf{W}_{p\times q} \tag{3}$$

Simple complexity analysis

- Order $(\mathbf{A} * \mathbf{H}) * \mathbf{W}$ incurs $2(m^2p + mpq)$ FLOPS.
- Order $\mathbf{A} * (\mathbf{H} * \mathbf{W})$ incurs $2(m^2q + mpq)$ FLOPS.

Implementation details

- Depending on values of p and q, one can choose computing order incurring the smallest number of FLOPS.
- DGL utilizes this feature.
- Our implementation DGL* and TVM* also utilizes this feature.

The other two optimizations utilizing TVM

Batched matrix multiplication for TVM

- Treat sparse matrices as dense ones.
- Utilize batch_matmul in TVM for batched dense matrix multiplication of the same size.
- TVM*-B groups matrices of the same size into one group.
- TVM*-M firstly sorts matrices by their dimensions and performs zero-padding on adjacency matrices to match the maximum dimension of adjacency matrices in the batch (default size: 32).

TVM compiler level optimization with constant folding

- Constant folding: identifies a constant expression and replace it with a constant value at compile time.
- The adjacency matrices, degree vectors, and weight matrices in GCN are stored in the relay layer of TVM as constant expressions.

Outline

Information of selected datasets and experimental environment

Table: Information of selected datasets.

Name	#Graphs	$\#\text{Nodes}_{\max}$	#Classes	Application	Accuracy
AIDS	2000	95	2	small molecules	98.35%
BZR	405	57	2	small molecules	80.99%
COX2	467	56	2	small molecules	78.16%
DHFR	756	71	2	small molecules	71.29%
Cuneiform	267	36	30	computer vision	70.41%
Letter-low	2250	8	15	computer vision	84.13%
Synthie	400	99	4	Synthetic	93.00%

- Seven datasets from TUDataset Morris et al. [2020] are selected for performance evaluation.
- GCNs are pretrained to obtain reasonable accuracies (training/testing=4/1).
- Intel i7-9700F @ 3.0 GHz, 16 GB DDR4-2666.
- LLVM 13.0.0, g++ 9.4.0, TVM 0.12.0 and DGL 2.1.

Different implementations to compare

- DGL: Current implementation of GCN inference in DGL.
- DGL*-reimplementSparse: A re-implementation of DGL, featuring a rewritten convolution implementation in the PyTorch platform.
- DGL*-Sparse: essentially DGL*-reimplementSparse but only timing the most compute-intensive four parts for fair comparision.
- DGL*-DirectDense: A direct translation of DGL-sparse with sparse matrix multiplications replaced by dense ones.
- DGL*-Dense: Re-arranging the order of dense operations.
- TVM: Current implementation of TVM on GCN inference for single graph.
- TVM*-Dense: Replacing the sparse tensor operations by dense ones and re-arranging the order of dense operations.
- TVM*-B: Support batch processing on TVM through combining matrices in same dimension, which is not affected by batch size.
- TVM*-M: Support batch processing on TVM through padding to the maximum dimension in a batch.

The common computations of all implementations

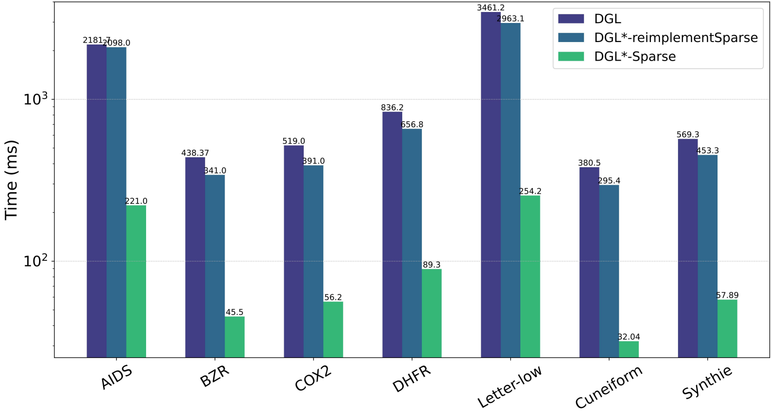
The four parts

- Hadamard product (H-product): $A^* = \widetilde{\mathbf{D}}^{-\frac{1}{2}} \circ \widetilde{\mathbf{A}} \circ \widetilde{\mathbf{D}}^{-\frac{1}{2}}$.
- Conv: $A^*\mathbf{H}^{(\ell)}\mathbf{W}^{(\ell)} + \mathbf{b}^{(\ell)}$.

Method	H-product (ms)	Conv1 (ms)	ReLu (ms)	Conv2 (ms)
DGL*-Sparse	42.9	93.4	**11.3**	73.5
DGL*-DirectDense	42.1	70.0	12.2	48.0
DGL*-Dense	**18.0**	**60.7**	12.3	**40.1**

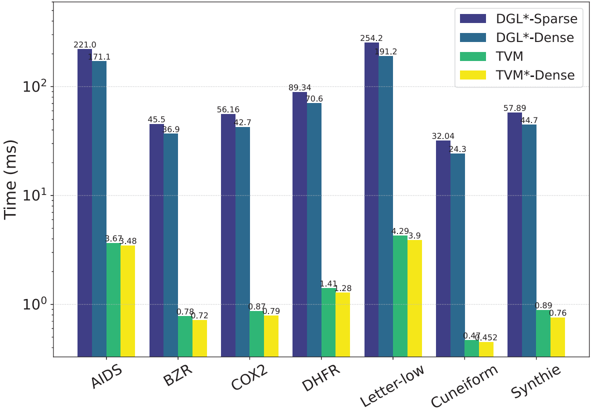
- The table reports the timings of three implementations in DGL on AIDS dataset.
- Replacing the sparse operators by dense ones brings speedup.
- Re-ordering the computation also brings speedup.

End-to-end evaluation



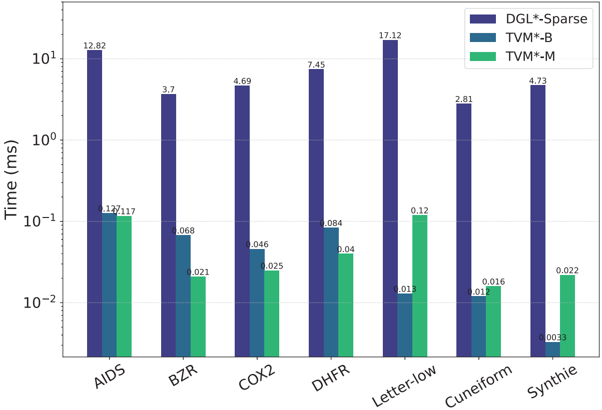
- DGL*-reimplementSparse has similar performance with original DGL.
- The difference with DGL*-Sparse shows the overhead of preprocessing and postprocessing part are high.

Performance of relevant implementations on handling graphs one by one



- DGL*-Dense achieves $1.3\times$ on average over DGL*-Sparse.
- TVM*-Dense achieves an average speedup of $1.1\times$ over TVM.
- TVM achieves on average $20\times$ speedup over DGL*-Dense.

Performance of relevant implementations on handling graphs in batch



- Batch size: 32.
- TVM*-B achieves an average speedup of $475.6\times$ over batched DGL*-Sparse.
- TVM*-M achieves an average speedup of $170.4\times$ over batched DGL*-Sparse.

Why do the performance of TVM*-B and TVM*-M vary with data?

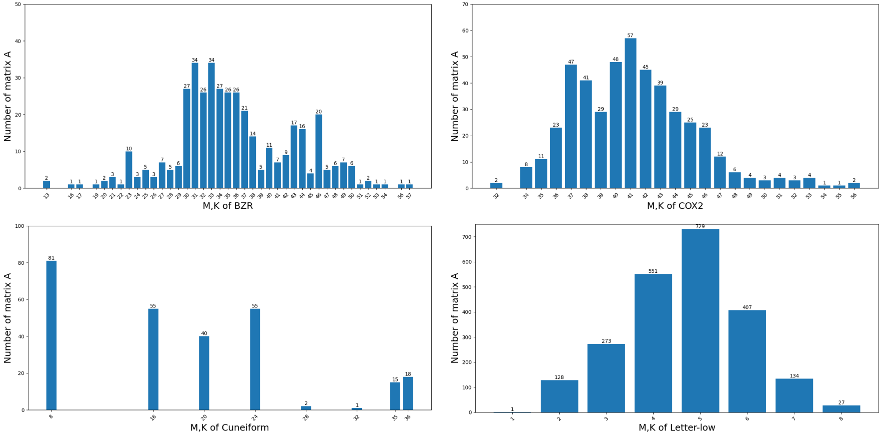
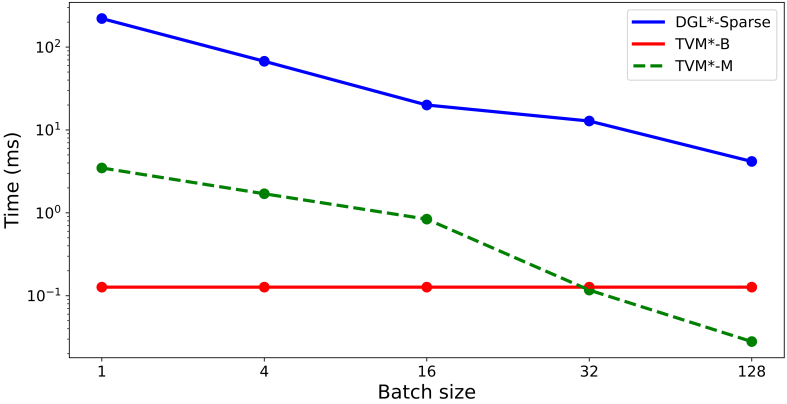


Figure: Comparison of matrix size distribution on different datasets.

- The dimensions have a wide range for the datasets BZR and COX2.
- The dimensions are highly centralized for Cuneiform and Letter-low.

Performance of batch processing on AIDS as the batch size increases



- TVM*-B ignores the given batch size and merges matrices of the same dimensions into a batch.

Outline

Conclusion and future work

- Targeting on small size graphs, we propose implementing GCN inference fully relying on dense operators.
- Several optimization strategies were proposed, such as replacing single sparse matrix multiplication by efficient batched dense matrix multiplication with TVM support and rearranging the order of basic operators.
- Experiments show that our method outperforms DGL and TVM on small graph datasets from real applications.

Future work

- Reducing the overhead of components other than the "most compute-intensive operations".
- Migrate the acceleration techniques to GNNs other than GCNs.

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