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Reducing Communication in Graph Neural Network Training

Berkeley
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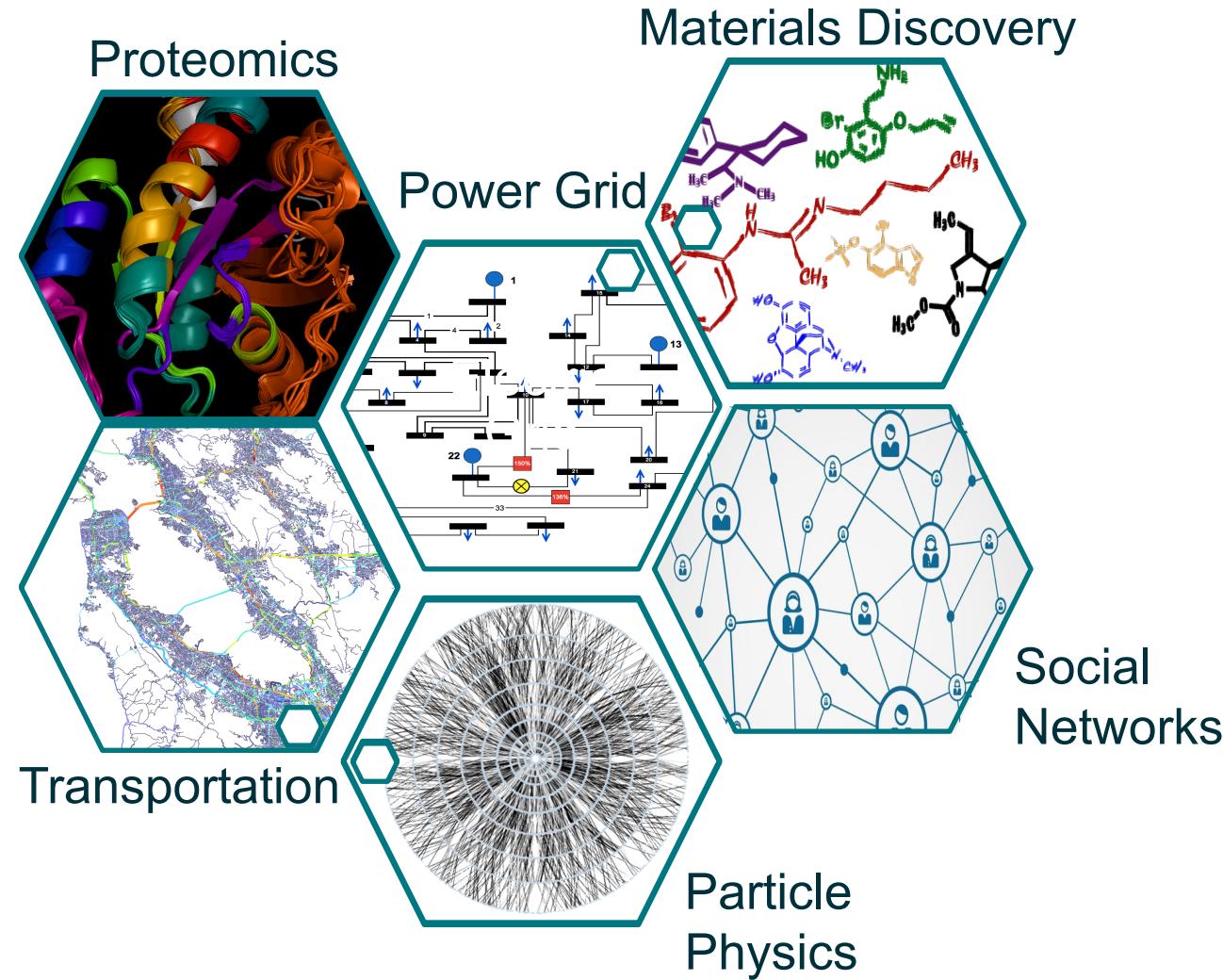
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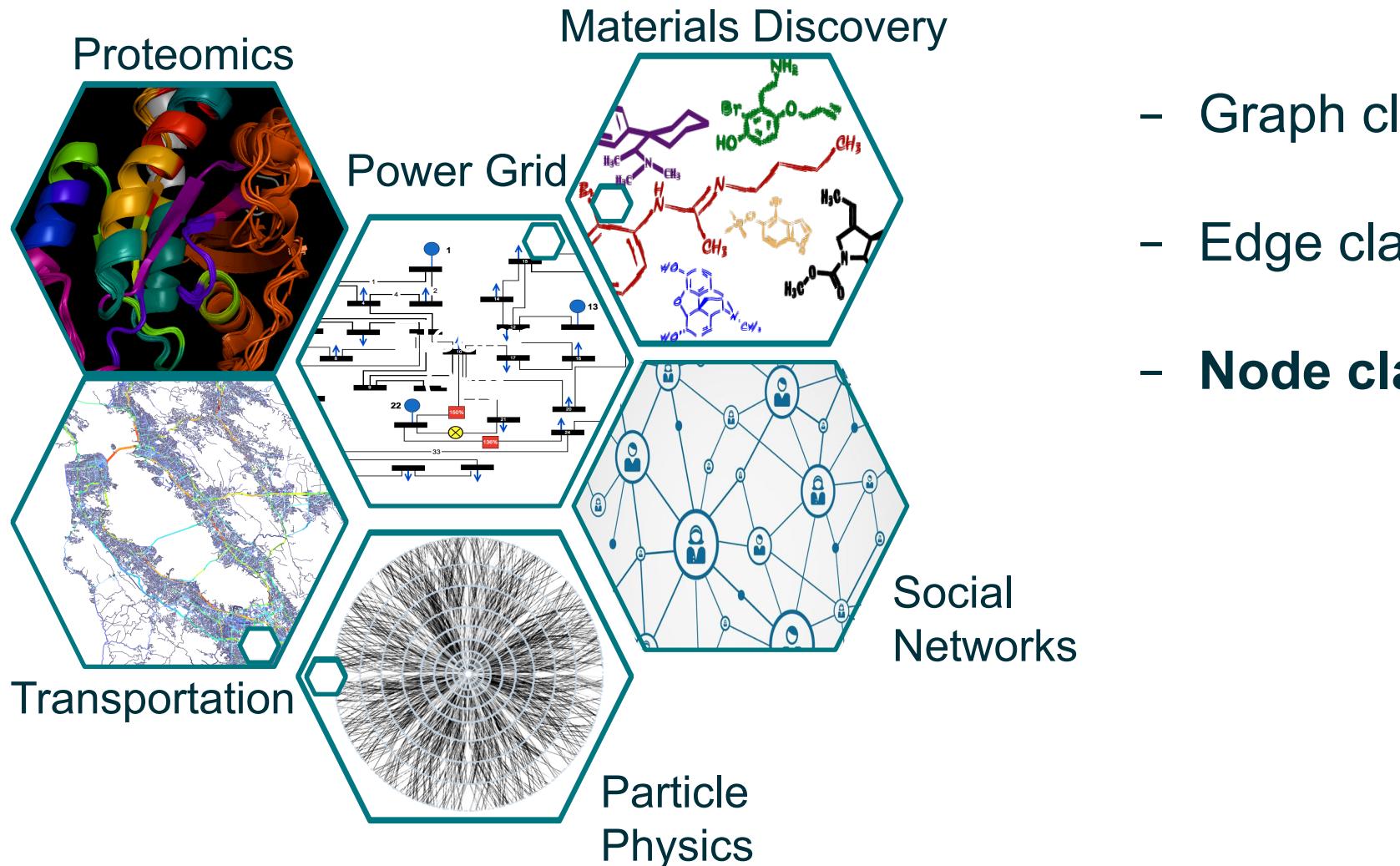
November 18th, 2020



Why focus on graphs?

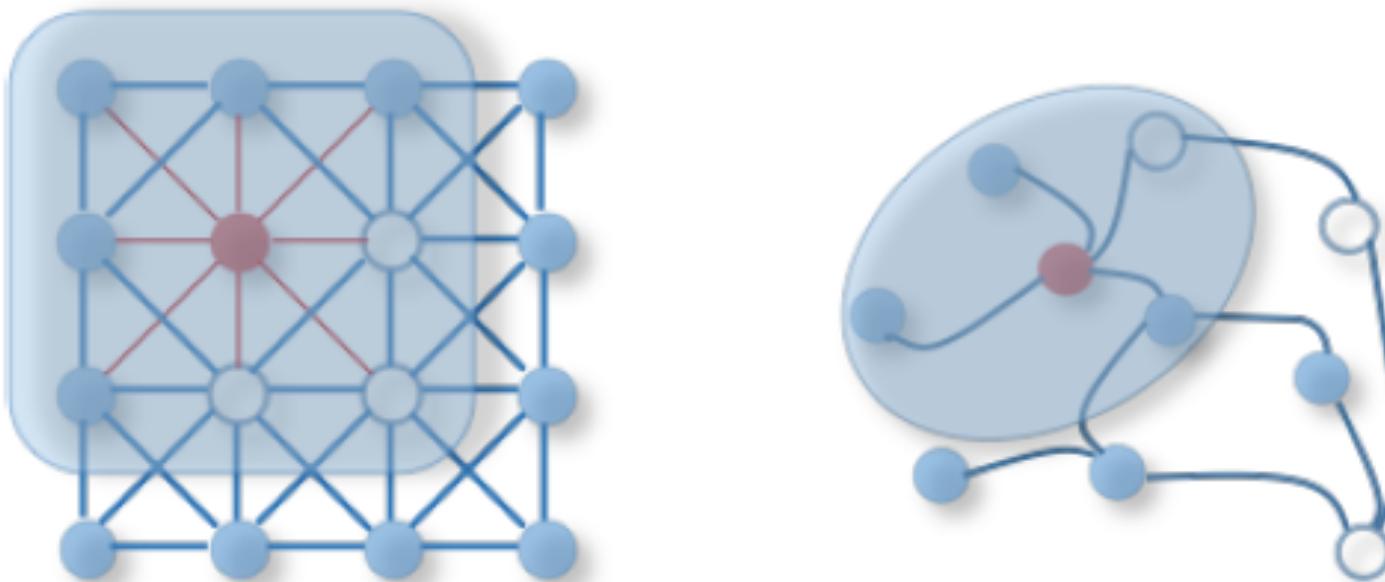


Learning problems on graphs



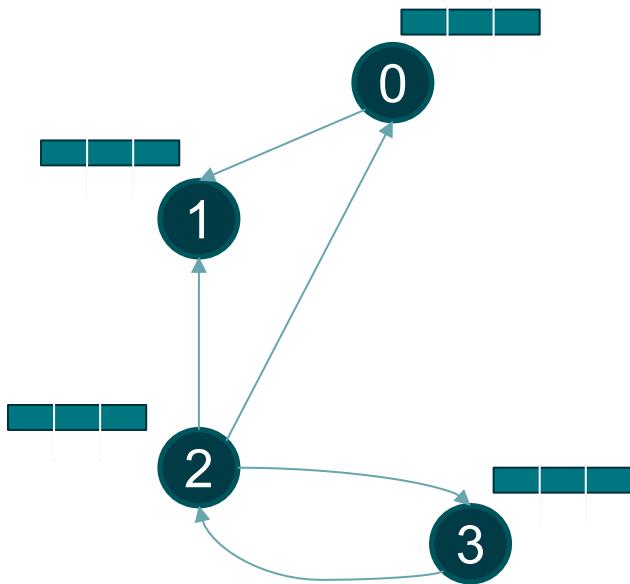
- Graph classification
- Edge classification
- Node classification

Why not use CNNs?

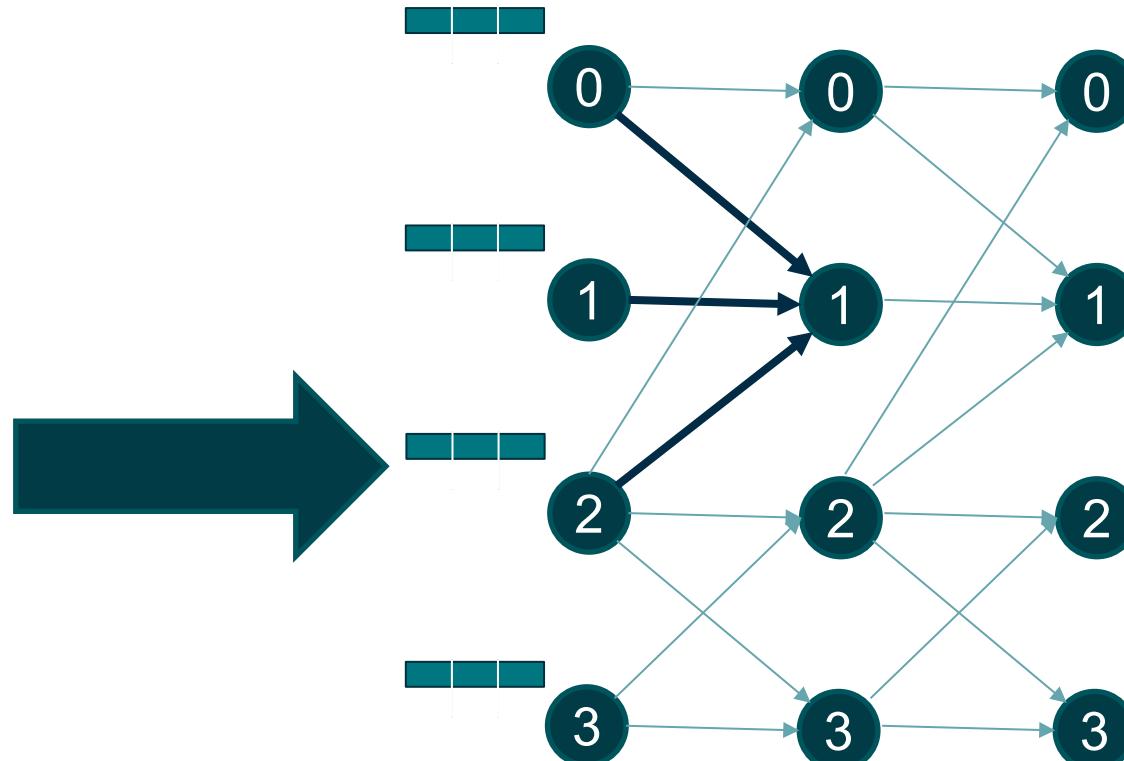


- Must generalize convolution

GNN basics

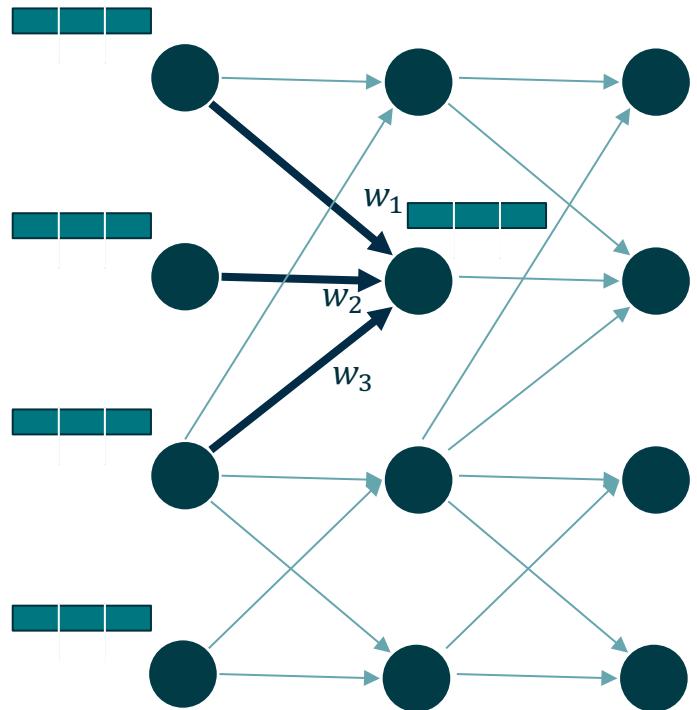


Input Graph



GNN of Input Graph

GNN training basics



1. Initialize feature vectors in layer 0
2. Sum neighbors' vectors for each node
3. Apply weight to vector sums

GNN issues

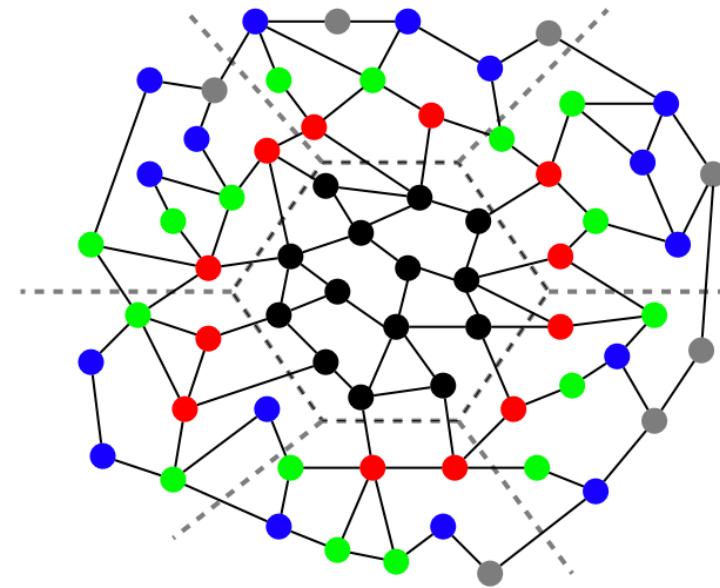
- GNN models are huge: $O(nfL)$
 - » n : number of vertices
 - » f : length of feature vector
 - » L : number of layers
- Need to distribute GNN training + inference

Why not use mini-batch SGD?



No dependencies

sample



Layered dependencies

- Layered dependencies → space issue persists
- Focus on full gradient descent

How do we distribute GNN training?

1. Formulate GNN training with sparse-dense matrix multiplication operations
 - » Both forward and back propagation
2. Distribute with distributed sparse-dense matrix multiplication algorithms
 - Focus on node classification, but methods are general



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GNN Training with Sparse-Dense Matrix Multiplication

GNN training as sparse-dense matrix multiplication

Forward Propagation:

$$\mathbf{Z}^l \leftarrow \mathbf{A}^\top \mathbf{H}^{l-1} \mathbf{W}^l$$

$$\mathbf{H}^l \leftarrow \sigma(\mathbf{Z}^l)$$

Backward Propagation:

$$\mathbf{G}^{l-1} \leftarrow \mathbf{A} \mathbf{G}^l (\mathbf{W}^l)^\top \odot \sigma'(\mathbf{Z}^{l-1})$$

$$\mathbf{Y}^{l-1} \leftarrow (\mathbf{H}^{l-1})^\top \mathbf{A} \mathbf{G}^l$$

- \mathbf{A} is stored in sparse format
- All other matrices dense

Symbols and Notations	
Symbol	Description
\mathbf{A}	Modified adjacency matrix of graph ($n \times n$)
\mathbf{H}^l	Embedding matrix in layer l ($n \times f$)
\mathbf{W}^l	Weight matrix in layer l ($f \times f$)
\mathbf{Y}^l	Matrix form of $\frac{\partial \mathcal{L}}{\partial W_{ij}^l}$ ($f \times f$)
\mathbf{Z}^l	Input matrix to activation function ($n \times f$)
\mathbf{G}^l	Matrix form of $\frac{\partial \mathcal{L}}{\partial Z_{ij}^l}$ ($n \times f$)
σ	Activation function
f	Length of feature vector per vertex
f_u	Feature vector for vertex u
L	Total layers in GNN
P	Total number of processes
α	Latency
β	Reciprocal bandwidth

GNN training as sparse-dense matrix multiplication

Forward Propagation:

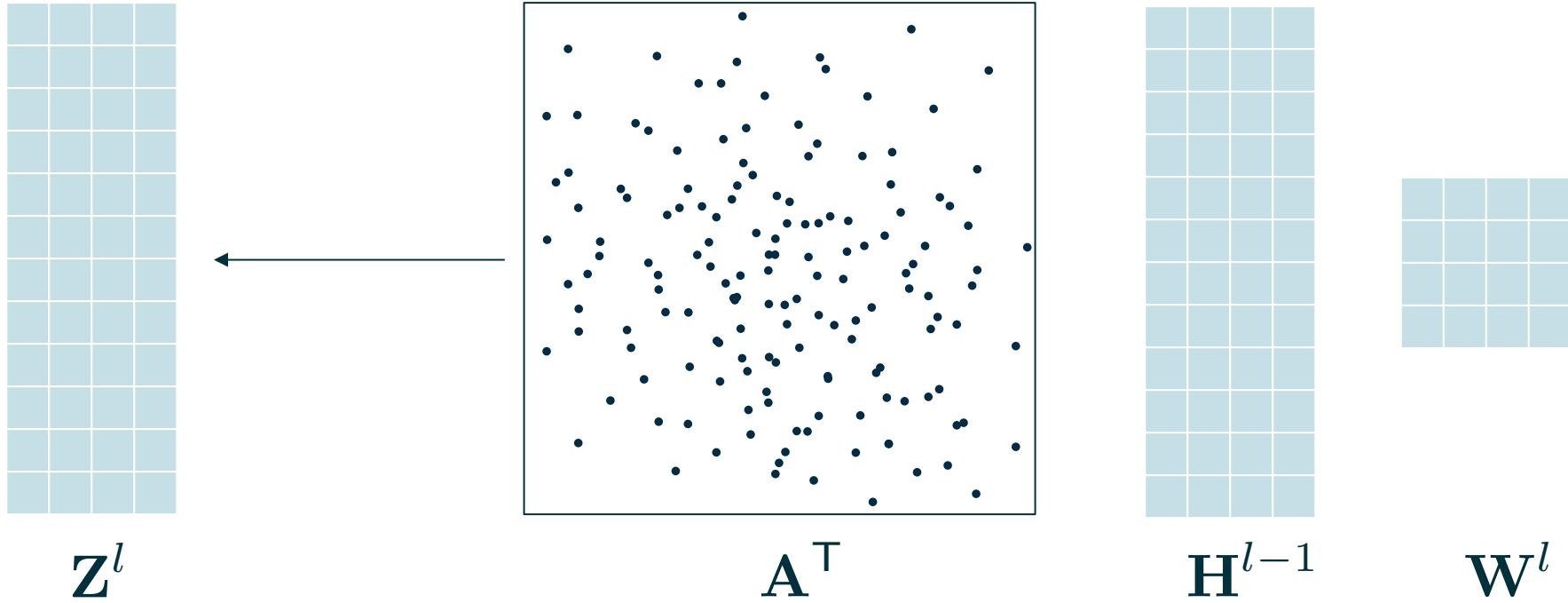
$$\mathbf{Z}^l \leftarrow \mathbf{A}^\top \mathbf{H}^{l-1} \mathbf{W}^l \quad \xleftarrow{\text{SpMM, DGEMM}}$$
$$\mathbf{H}^l \leftarrow \sigma(\mathbf{Z}^l) \quad \xleftarrow{\text{In paper}}$$

Backward Propagation:

$$\mathbf{G}^{l-1} \leftarrow \mathbf{A} \mathbf{G}^l (\mathbf{W}^l)^\top \odot \sigma'(\mathbf{Z}^{l-1}) \quad \xleftarrow{\text{SpMM, DGEMM}}$$
$$\mathbf{Y}^{l-1} \leftarrow (\mathbf{H}^{l-1})^\top \mathbf{A} \mathbf{G}^l \quad \xleftarrow{\text{DGEMM}}$$

- **Entirely SpMM, DGEMM calls**

Bottleneck of GNN training



- SpMM >>> DGEMM



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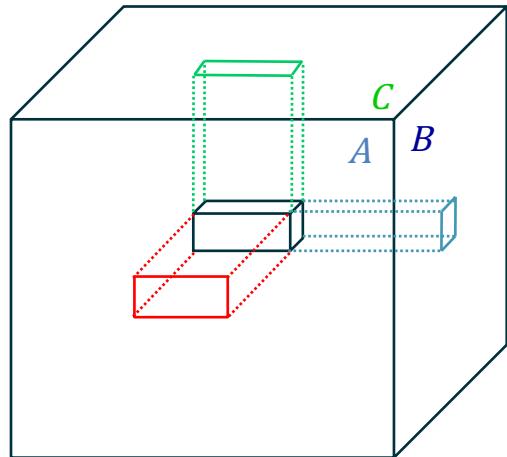
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Distributed Matrix Multiplication Algorithms

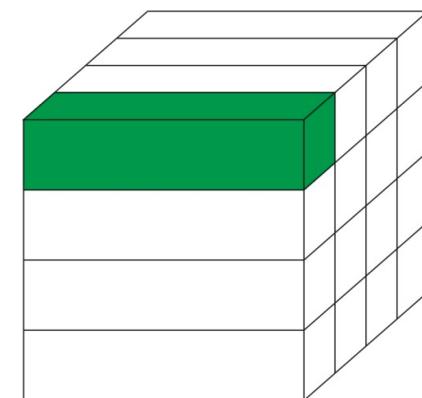
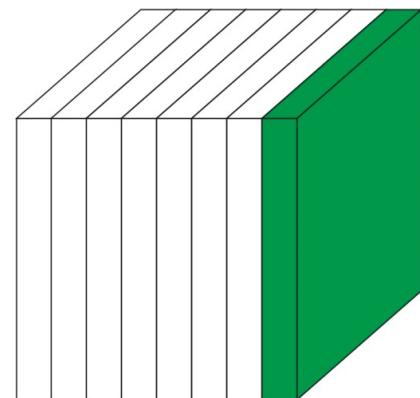
The computation cube of matrix-matrix multiplication

Matrix multiplication: $\forall(i,j) \in n \times n, C(i,j) = \sum_k A(i,k)B(k,j),$



The *computation (discrete) cube*:

- A face for each (input/output) matrix
- A grid point for each multiplication

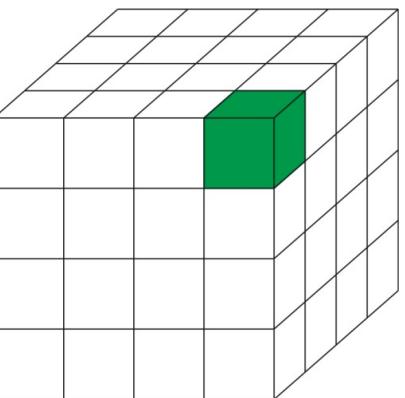


1D algorithms

1.5D algorithms

2D algorithms

3D algorithms



GNN training communication analysis

Communication Analyses			
Algorithm	Latency	Bandwidth	Memory
1D	$\lg P + 2P$	$2nf + f^2$	$\frac{nnz(\mathbf{A})}{P} + \frac{nf}{P}$
1.5D	$2\frac{P}{c^2} \lg \frac{P}{c^2}$	$\frac{2nf}{c} + \frac{2nfc}{P}$	$\frac{nnz(\mathbf{A})c}{P} + \frac{nfc}{P}$
2D	$5\sqrt{P} + 3\lg P$	$\frac{8nf}{\sqrt{P}} + \frac{2nnz(\mathbf{A})}{\sqrt{P}}$	$\frac{nnz(\mathbf{A})}{P} + \frac{nf}{P}$
3D	$4P^{1/3}$	$\frac{2nnz(\mathbf{A})}{P^{2/3}} + \frac{12nf}{P^{2/3}}$	$\frac{nnz(\mathbf{A})}{P} + \frac{nf}{P}$

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- $nnz(\mathbf{A})$ is the number of edges
- C is the replication factor for 1.5D ($C=1$ is 1D)



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GNN Training with Sparse-Dense Matrix Multiplication Results

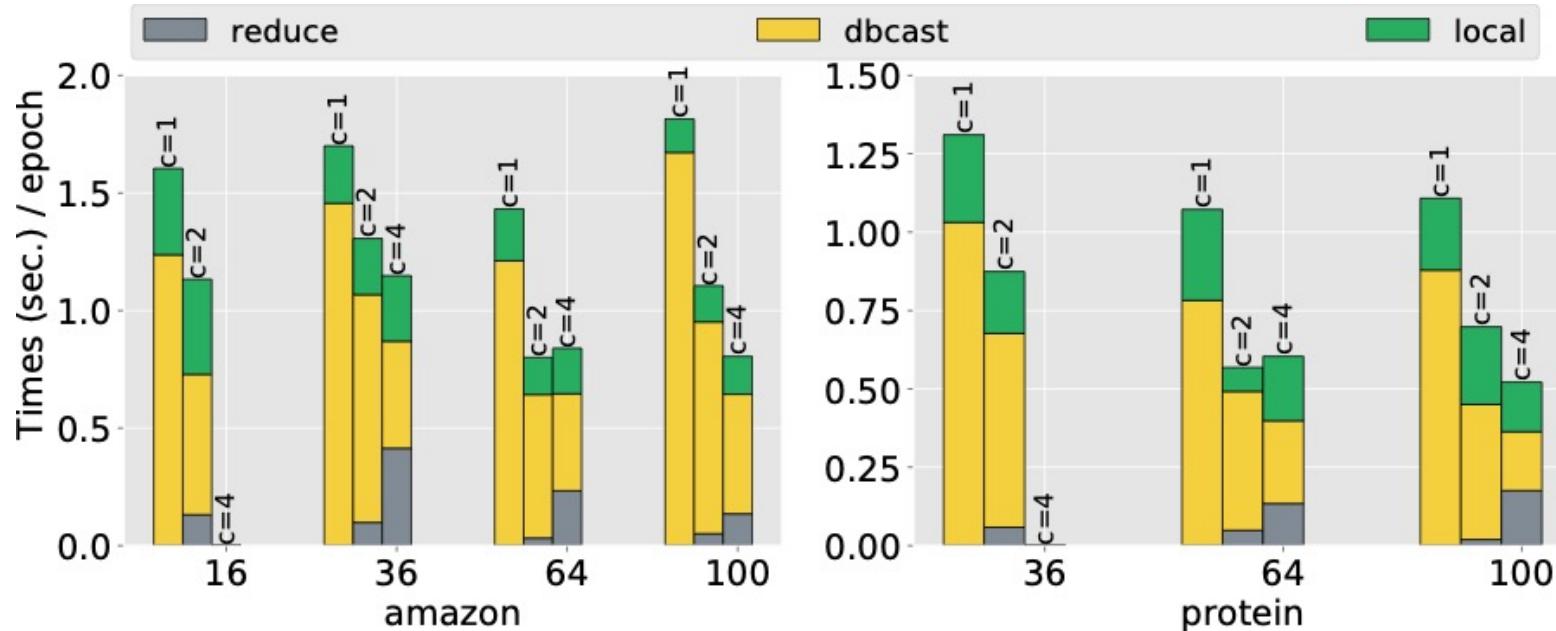
Implementation Details

- PyTorch 1.3 with NCCL 2.0 backend
 - » Kipf-Welling model (3-layers, 16 hidden activations)
- System:
 - » Summit at OLCF
 - » 6 NVIDIA V100s per node
 - » NVLINK 2.0, EDR Infiniband

- Datasets:

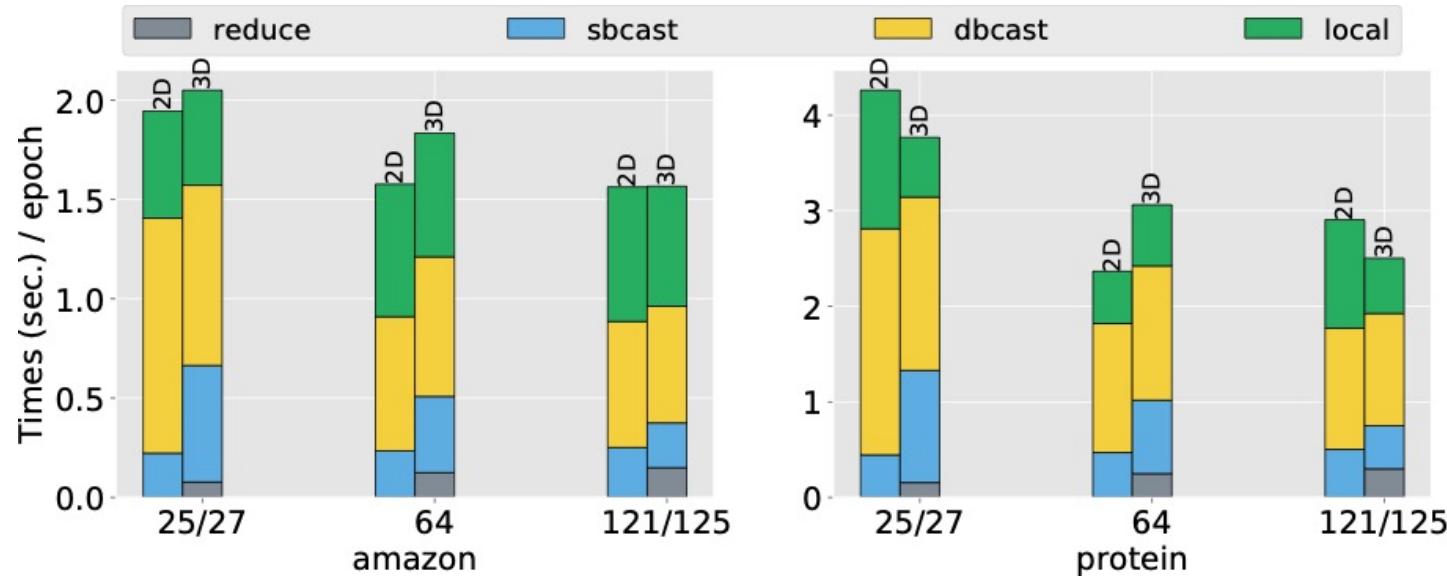
Name	Vertices	Edges	Features	Labels
Amazon	14M	231M	300	24
Reddit	233K	114M	602	41
Protein	8M	2B	128	256

GNN Training with 1.5D Matrix Multiplication



- Scales with both P and c with 1 GPU/node
 - » Summit topology
 - » Full 6GPU/node results in paper
- Expect to scale with all GPUs / node with future architectures
 - » e.g. Perlmutter

GNN Training with 2D/3D Matrix Multiplication



- Other algorithms evaluated in practice
- Communication scales with P , consistent with analysis
- Computation scales less well → explained in paper

Conclusions

- Graphs are everywhere
 - » Lots of deep learning problems on graphs
- Can solve DL on graphs with GNNs
 - » But must distribute training
- Our work
 - » Can formulate GNN training as sparse-dense matrix multiplications
 - » Distribute GNN training with distributed SpMM
 - » Code: <https://github.com/PASSIONLab/CAGNET>
 - » Paper: <https://arxiv.org/pdf/2005.03300.pdf>