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Reducing Communication in Graph Neural Network Training

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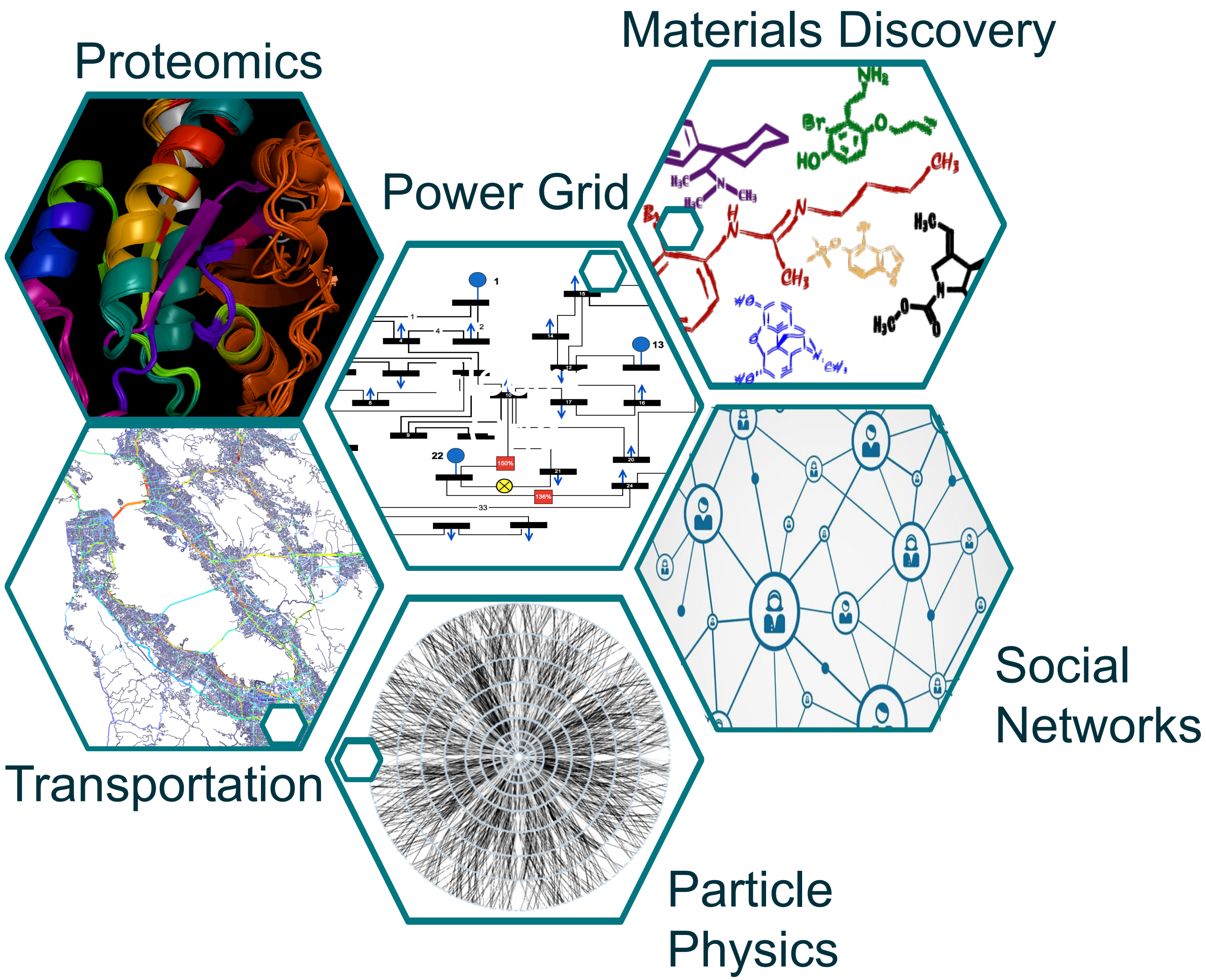
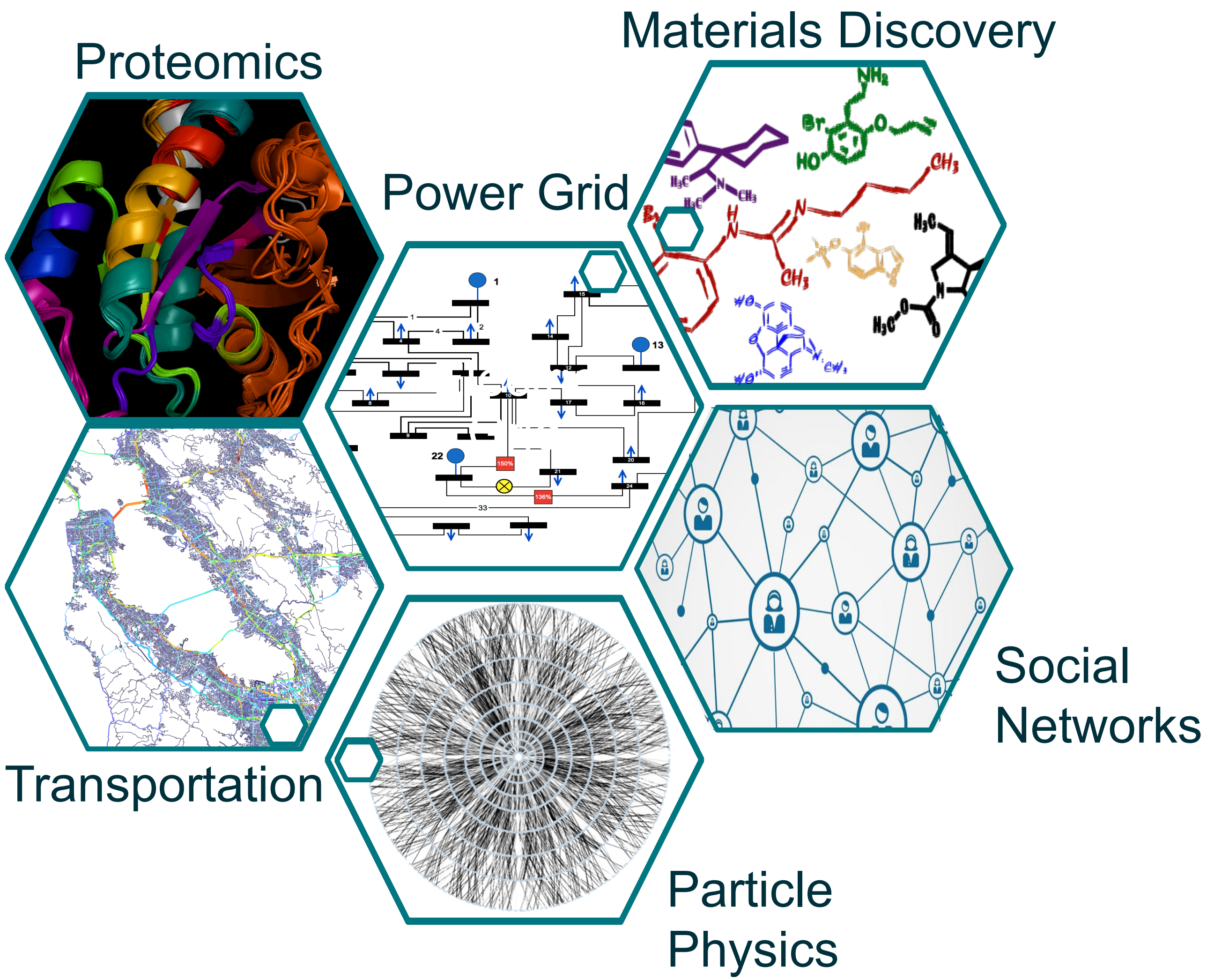
Why focus on graphs?

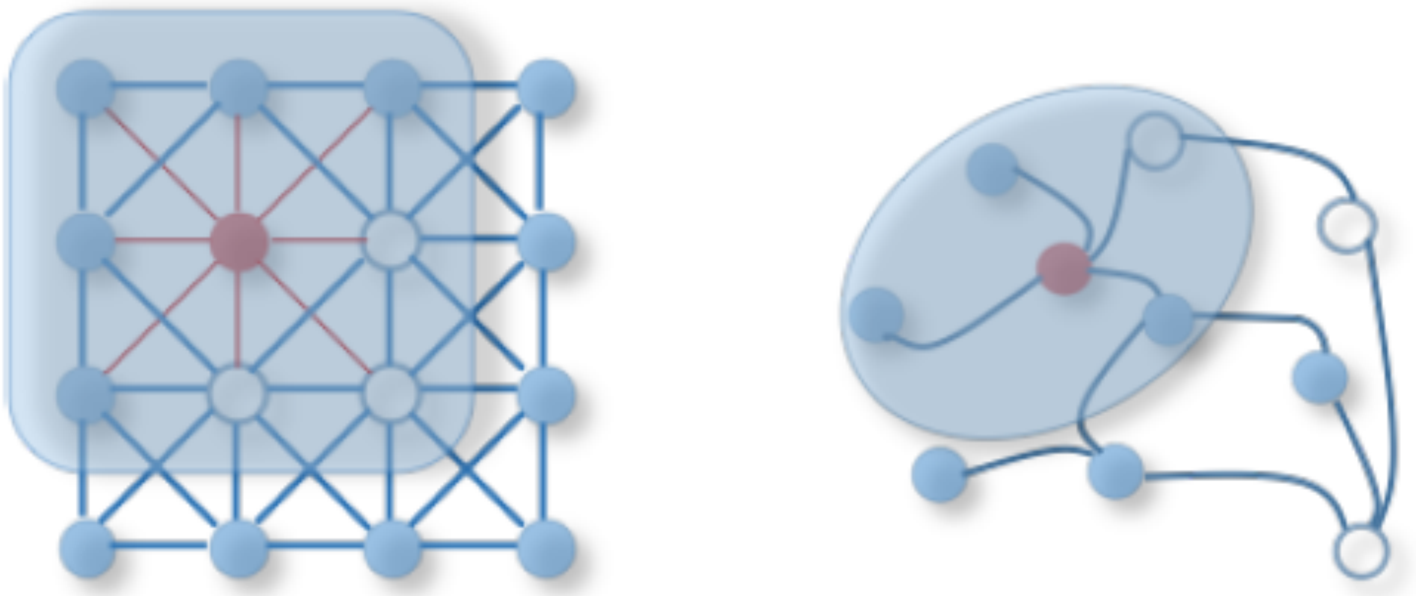


Learning problems on graphs



- Graph classification
- Edge classification
- **Node classification**

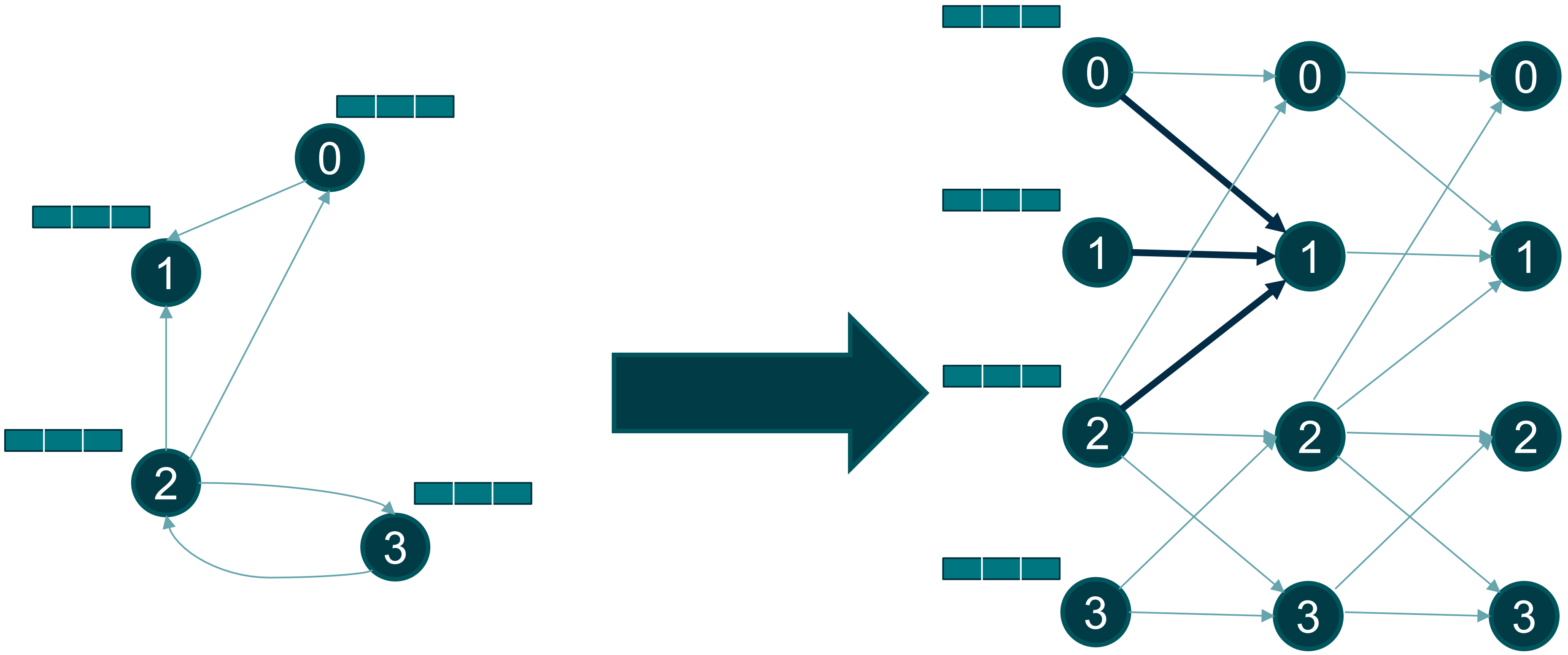
Why not use CNNs?



- Must generalize convolution

[1] Z. Wu, S. Pan, F. Chen, G. Long, C. Zhang, and P. S. Yu, “A comprehensive survey on graph neural networks,” arXiv preprint arXiv:1901.00596, 2019.

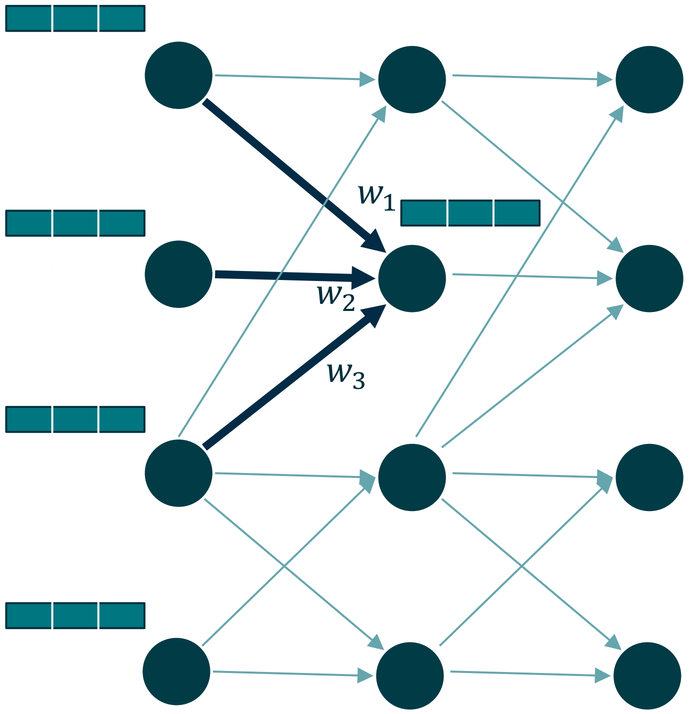
GNN basics



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

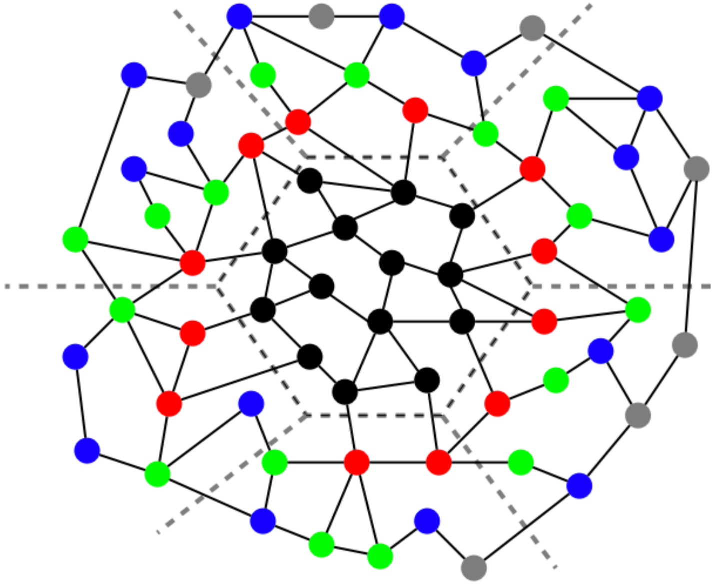
- GNN models are huge: $O(nfL)$
  - » n: number of vertices
  - » f: length of feature vector
  - » L: number of layers

- Need to distribute GNN training + inference

Why not use mini-batch SGD?

sample

No dependencies



Layered dependencies

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

[2] Marghoob Mohiyuddin, Mark Hoemmen, James Demmel, and Katherine Yelick. Minimizing Communication in Sparse Matrix Solvers. In Proceedings of the 2009 ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis(SC), 2009.

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

GNN Training with Sparse-Dense Matrix Multiplication

GNN training as sparse-dense matrix multiplication

Forward Propagation:

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

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

Backward Propagation:

$$\mathbf{G}^{l-1} \leftarrow \mathbf{A}\mathbf{G}^l(\mathbf{W}^l)^\mathsf{T} \odot \sigma'(\mathbf{Z}^{l-1})$$

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

- $\mathbf{A}$ 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 $\frac{\partial \mathcal{L}}{\partial W^l_{ij}}$ $(f \times f)$
$\mathbf{Z}^l$	Input matrix to activation function $(n \times f)$
$\mathbf{G}^l$	Matrix form of $\frac{\partial \mathcal{L}}{\partial Z^l_{ij}}$ $(n \times f)$
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:

$$\mathbf{Z}^l \leftarrow \mathbf{A}^{\mathsf{T}}\mathbf{H}^{l-1}\mathbf{W}^l$$ ← SpMM, DGEMM

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

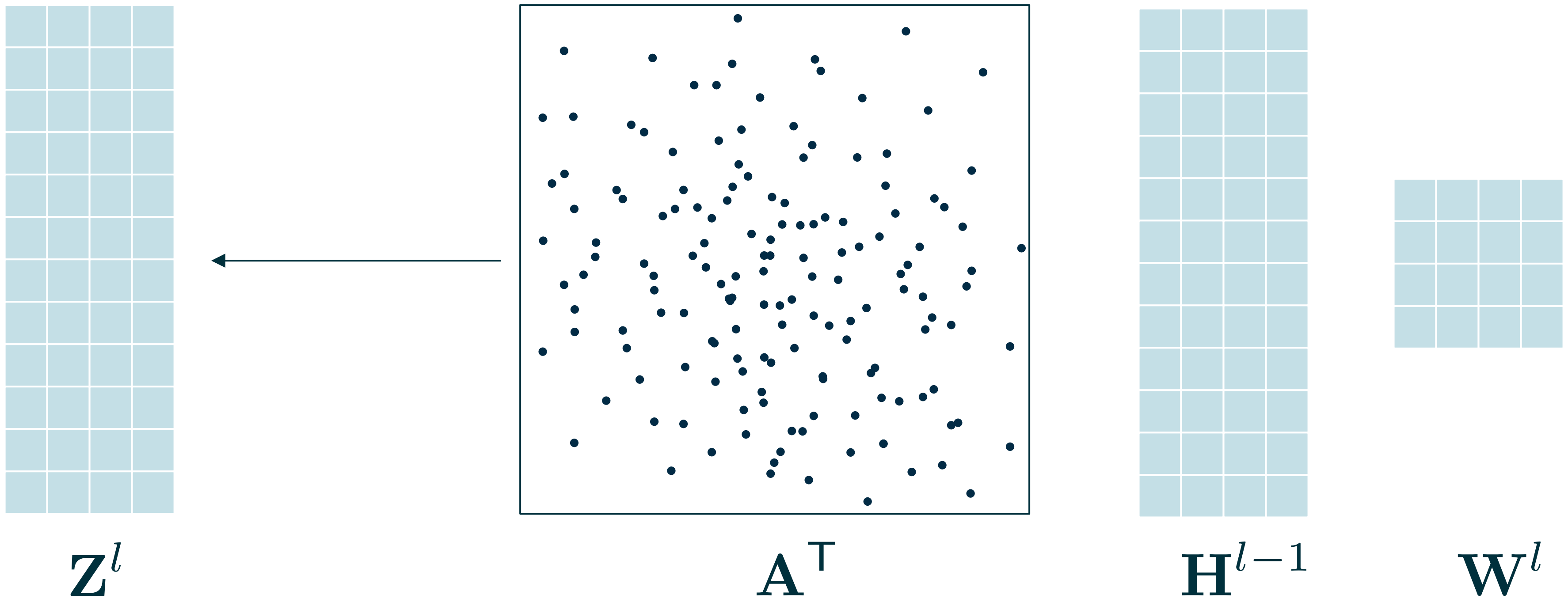
Backward Propagation:

$$\mathbf{G}^{l-1} \leftarrow \mathbf{A}\mathbf{G}^l(\mathbf{W}^l)^{\mathsf{T}} \odot \sigma'(\mathbf{Z}^{l-1})$$ ← SpMM, DGEMM

$$\mathbf{Y}^{l-1} \leftarrow (\mathbf{H}^{l-1})^{\mathsf{T}}\mathbf{A}\mathbf{G}^l$$ ← DGEMM

- **Entirely SpMM, DGEMM calls**

Bottleneck of GNN training

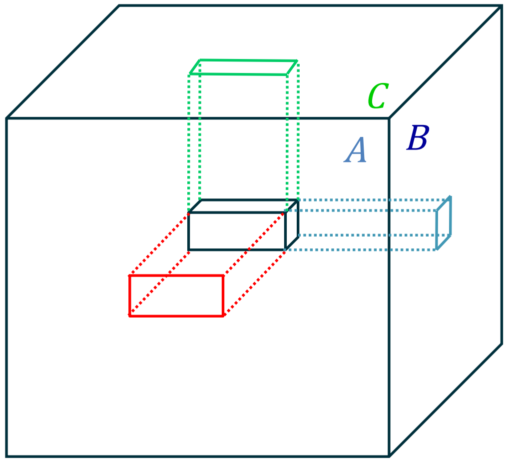


- SpMM >>> DGEMM

Distributed Matrix Multiplication Algorithms

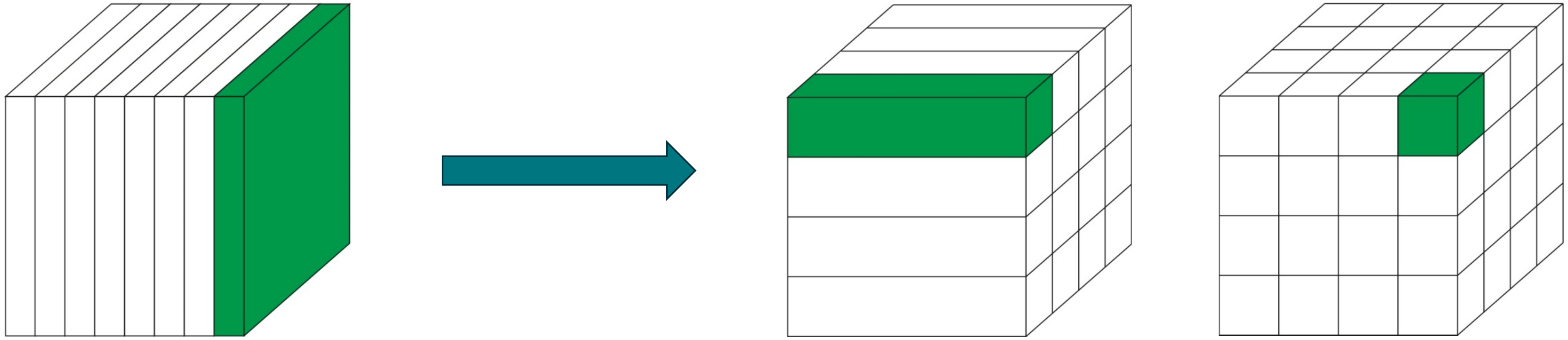
The computation cube of matrix-matrix multiplication

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



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

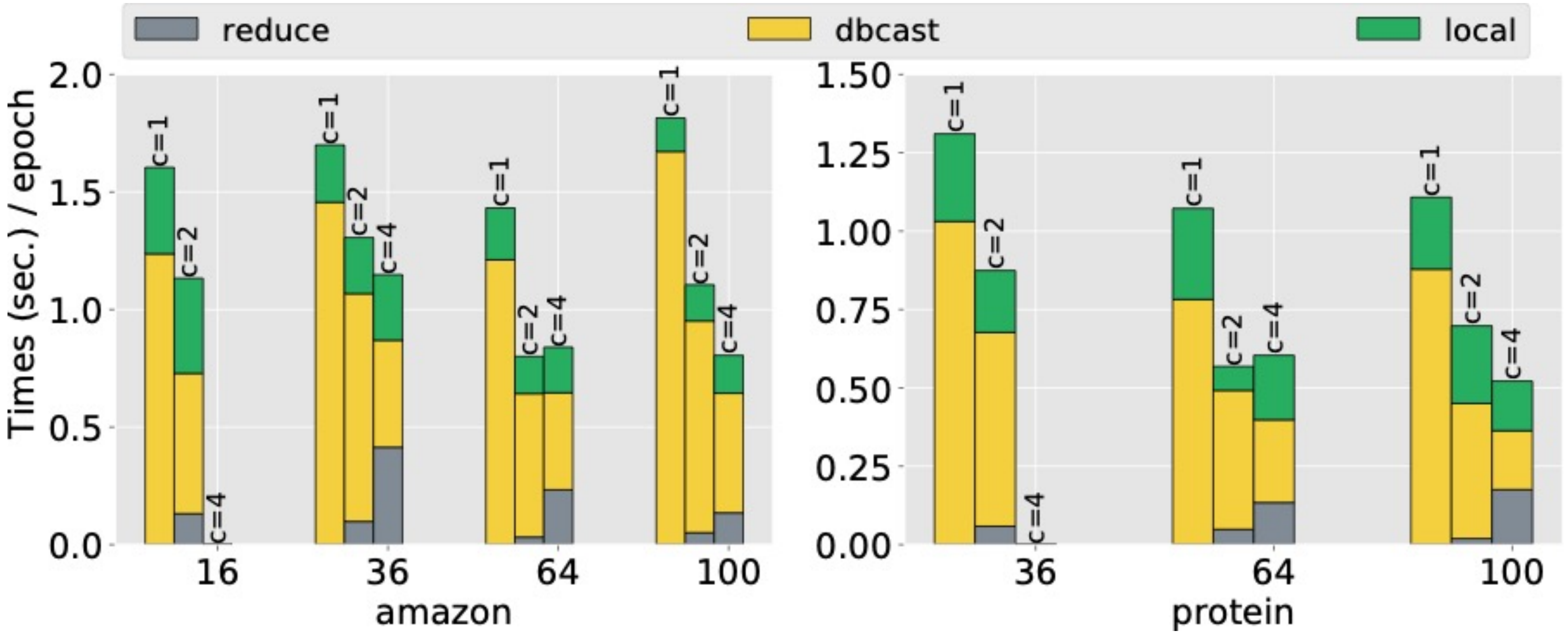
- PyTorch 1.3 with NCCL 2.0 backend
  - » Kipf-Welling model (3-layers, 16 hidden activations)

- 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

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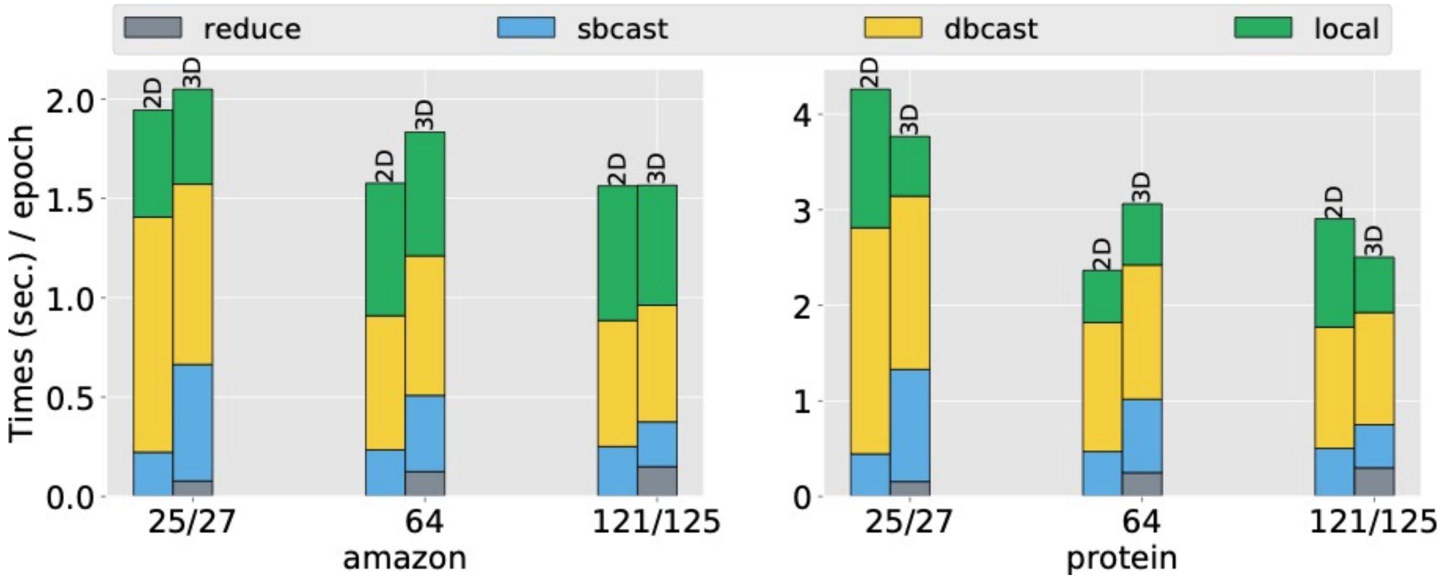
GNN Training with 2D/3D Matrix Multiplication



- Other algorithms evaluated in practice (with 6GPUs/node)
- Communication scales with P, consistent with analysis
- Computation scales less well → explained in paper

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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

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