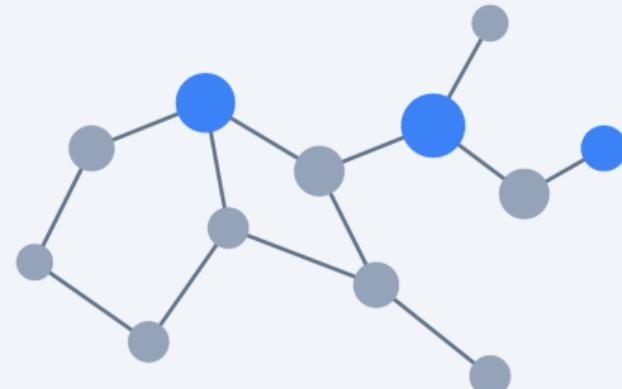


GRAPH SAGE

INDUCTIVE REPRESENTATION LEARNING
ON LARGE GRAPHS

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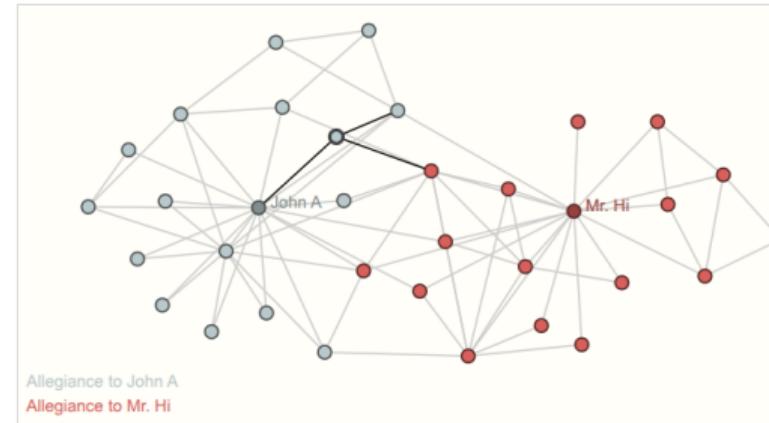
Introduction

Graph Prediction Tasks

Introduction

Primary focus: Node-level prediction — predict properties of individual nodes (classification, regression).

- **Node-level (focus):** Predict node attributes or labels using features and neighbor information.
- **Edge-level:** Predict relationships between node pairs (link prediction, edge classification).
- **Graph-level:** Predict properties of whole graphs (e.g., molecule properties).

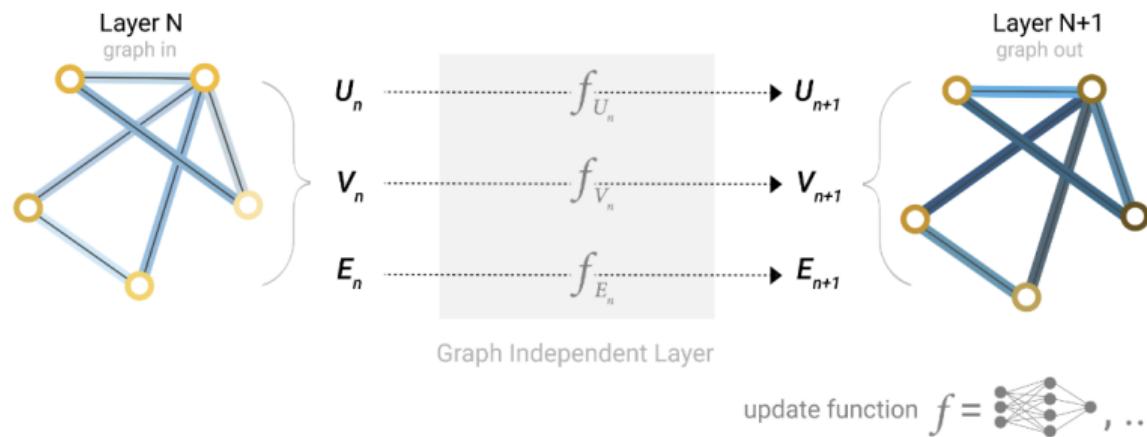


What is a Graph Neural Network?

Introduction

A learnable transformation on graph attributes that:

- Updates node/edge/graph features using **neural networks**
- **Respects graph structure** by aggregating information from neighbors
- Is **permutation invariant** (order of nodes doesn't matter)

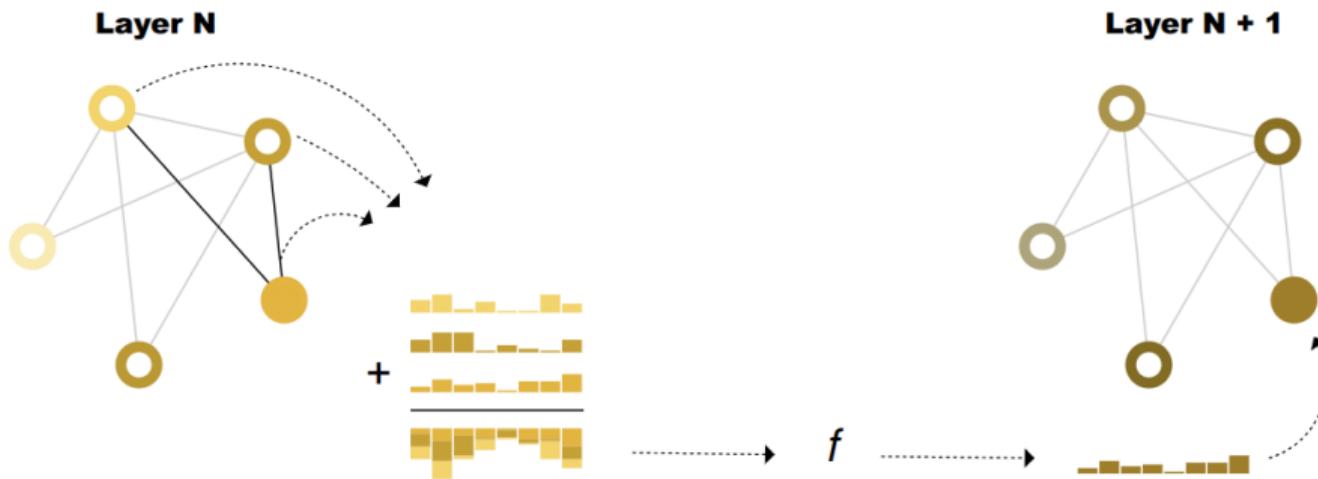


Message Passing: The Core Idea

Introduction

Three steps repeated at each layer:

1. **Gather:** Collect embeddings from neighboring nodes
2. **Aggregate:** Combine neighbors' info (sum / mean / max)
3. **Update:** Apply learned transform using the aggregated vector



Message Passing: Notation

Introduction

Message Passing Equation

$$h_v^{(k)} = \sigma \left(W \cdot \left[h_v^{(k-1)}, \text{AGG}(\{h_u : u \in N(v)\}) \right] \right)$$

- $h_v^{(k)}$ — Node v repr. at layer k
- h_u — Neighbor node u repr.
- $N(v)$ — Neighbors of v
- k — Layer index (hops)
- AGG(\cdot) — Aggregator (mean, sum, max)
- W — Learnable weight matrix
- σ — Activation (ReLU, tanh)

Before GraphSAGE: The Problem

Introduction

Let's audit the limitations of existing approaches...

- **DeepWalk / node2vec:** Transductive: embed every node; new nodes need full retraining.
 - ▷ Not GNNs — random-walk based embeddings, no message passing
- **GCNs:** Often require access to the full graph during training/inference; can be costly to scale.
 - ▷ GNNs — but transductive: fixed node set at training
- **Result:** No compact parametric function to generate embeddings for unseen nodes.

This motivates GraphSAGE's key insight...

The Key Insight

The Key Insight

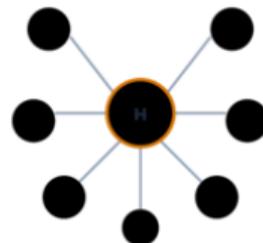
The Key Insight

Don't learn embeddings for each node...

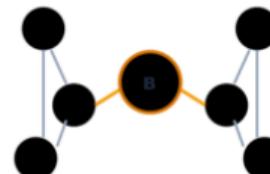
Learn a **FUNCTION** that generates embeddings

By sampling & aggregating neighborhood features

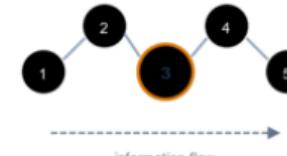
Hub Pattern
Social Influencer



Bridge Pattern
Community Connector



Chain Pattern
Sequential Flow



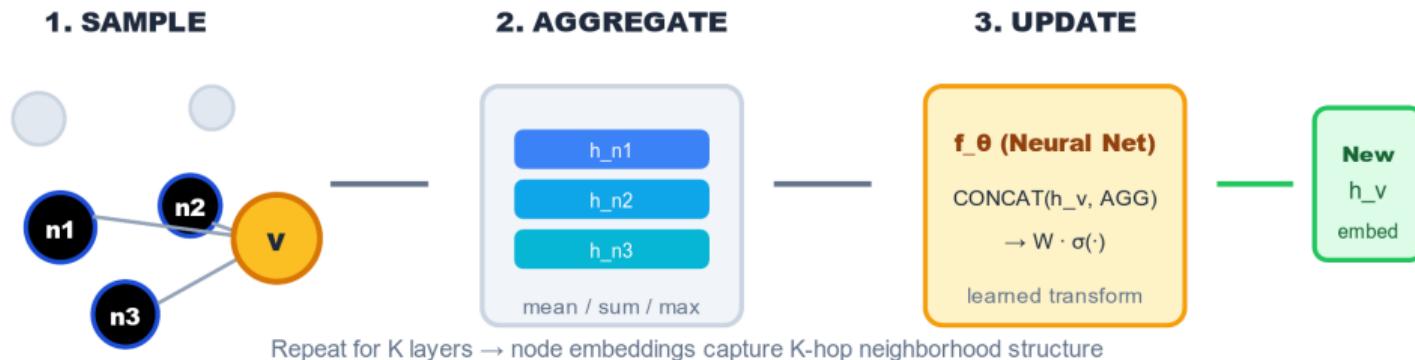
GraphSAGE Framework

GraphSAGE: Inductive Framework

GraphSAGE Framework

Core Principle: Sample + Aggregate

- Learn **aggregator functions** (not node embeddings)
- For any node v : sample **neighbors**, aggregate their features
- Pass through learned neural networks
- **Inference:** Apply same function to unseen nodes



Implementation

Training GraphSAGE: The Challenge

Implementation

Dataset: ogbn-products (Amazon co-purchase network)

- 2.4M nodes (products), 61M edges, 47 classes
- 8% train / 2% val / 90% test split

The Problem:

- Cannot fit entire graph in GPU memory
- Cannot do full message passing on 2.4M nodes
- **Solution:** Mini-batch training + neighbor sampling

Mini-Batch and Neighbor Sampling

Implementation

1. Mini-Batch Sampling:

- Select small subset of seed nodes per iteration (e.g., 128 nodes)
- Only compute embeddings for these nodes + their neighborhoods
- Update model parameters based on batch loss

2. Neighbor Sampling (k-hop):

- For each seed node, sample neighbors recursively for k layers
- **Fanout:** number of neighbors sampled per layer [L₁, L₂, ..., L_k]
- Example: [15, 10, 10, 10, 10] = 15 neighbors at layer 1, 10 at layers 2-5

Why this matters:

- Fanout grows **exponentially**: ~150k neighbors per seed node
- 128 seed nodes × 150k expansion = **19.2M nodes per batch**
- Memory bottleneck: sampled subgraphs » model parameters

Neighbor Sampling: Visual Example

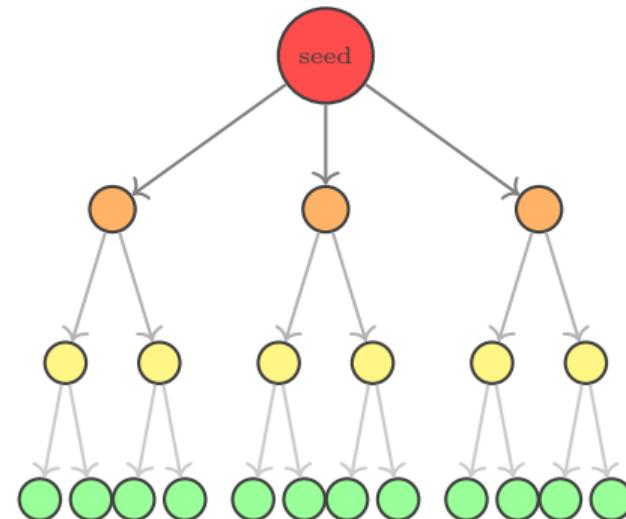
Implementation

K-Hop Expansion:

- Start with 1 seed node
- Sample neighbors recursively
- Fanout: [3, 2, 2] (simplified)

Growth per layer:

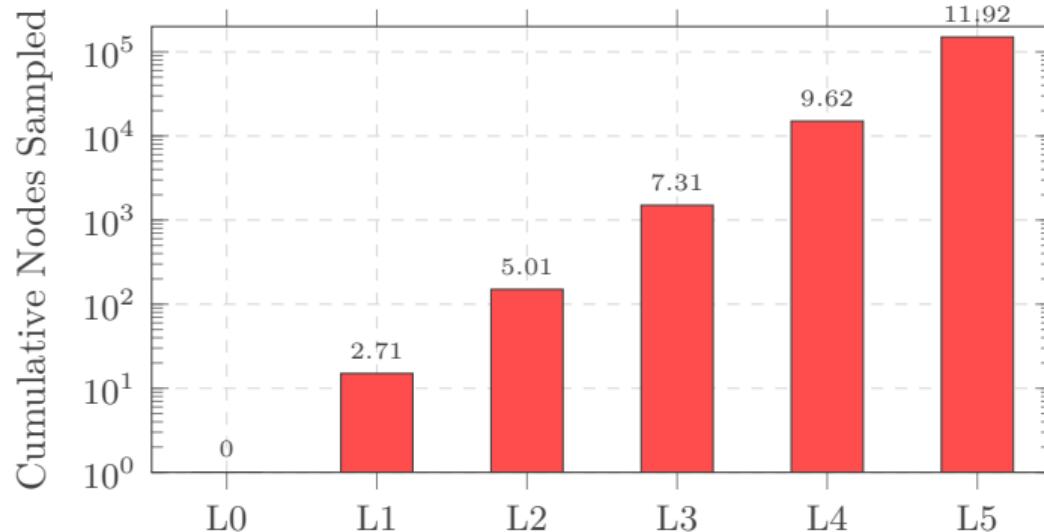
- Layer 0: 1 seed
- Layer 1: $1 \times 3 = 3$
- Layer 2: $3 \times 2 = 6$
- Layer 3: $6 \times 2 = 12$



The Memory Explosion

Implementation

Real Configuration: [15, 10, 10, 10, 10]



Combined: 128 seed nodes \times 150k neighbors = **19.2M nodes/batch**

Training Environment

Implementation

HPC Infrastructure:

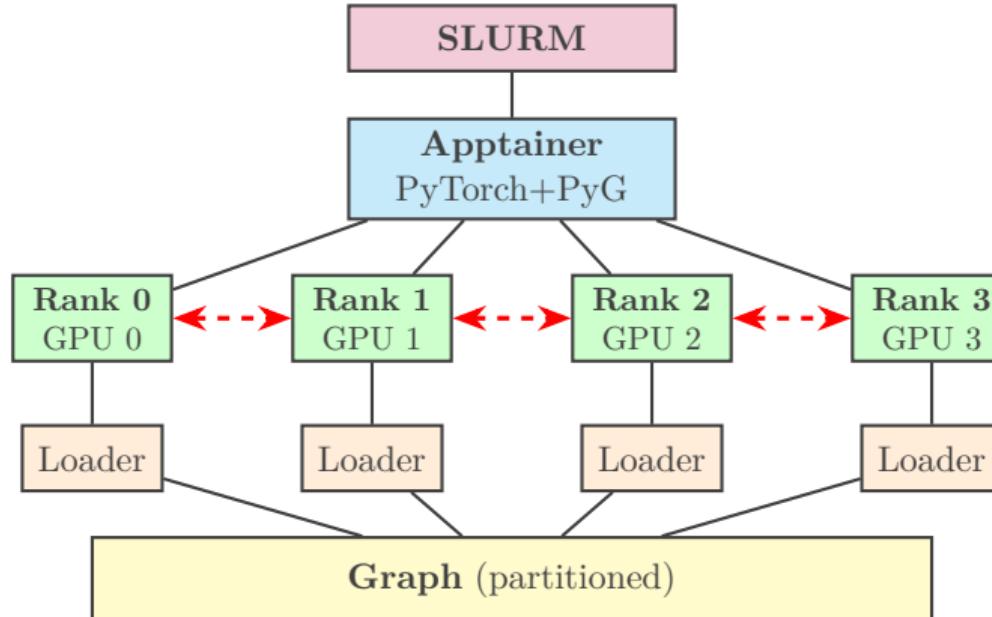
- **Cluster:** MeluXina (Luxembourg National Supercomputer)
- **GPUs:** Up to 4x NVIDIA A100 (40GB) per node
- **Framework:** PyTorch 2.1.2 + PyTorch Geometric
- **Containerization:** Apptainer/Singularity for reproducibility

Why Distributed Training?

- Single GPU: limited batch size due to memory (sampled subgraphs ~30-40GB)
- **Solution:** Distributed Data Parallel (DDP) across multiple GPUs
- Partition training data, synchronize gradients

System Architecture Diagram

Implementation



Multi-GPU DDP: data partitioned across 4 GPUs, gradients synced via NCCL

Containerization

Implementation

- **Base:** pytorch/pytorch:2.1.2-cuda12.1-cudnn8-runtime
- **Dependencies:** PyTorch Geometric, pyg-lib, OGB, torch-scatter/sparse
- **Why containerize?**
 - Complex dependency graph (CUDA-compiled extensions)
 - Reproducibility across HPC environments
 - Avoid version conflicts on shared cluster

Why HPC and Parallelism?

Implementation

1. Dimension of the Problem:

- Each batch node samples 5-hop neighborhoods
- Fanout → exponential growth: ~150k neighbors per seed node
- Batch 128 nodes × 150k expansion = 19.2M nodes per batch

2. Memory Bottleneck:

- Model parameters: only ~8 MB
- Sampled subgraphs + intermediate activations: **30-40 GB** per batch
- Single GPU cannot handle large batches → slow training

3. Solution: Data Parallelism with DDP

- More GPUs with fixed batch size ⇒ bigger effective batch size ⇒ faster convergence
- **DeepSpeed** overkill

Distributed Data Parallel (DDP) Training

Implementation

1. Process Initialization:

- SLURM launches 4 processes (1 per GPU)
- Each process: independent Python interpreter + CUDA context
- NCCL backend for GPU-to-GPU communication

2. Data Partitioning:

- Training set split across ranks (no overlap)
- Each rank: independent NeighborLoader for k-hop sampling
- 4-8 worker processes prefetch batches per GPU

3. Forward + Backward (Parallel):

- Each GPU independently processes its batch
- Compute loss, backpropagate gradients

4. Gradient Synchronization:

- DDP all-reduce: average gradients across all GPUs
- Optimizer step with synchronized gradients

Hyperparameters

Overview

Hyperparameters

◎ **Goal:** Scalable and reproducible hyperparameter optimization

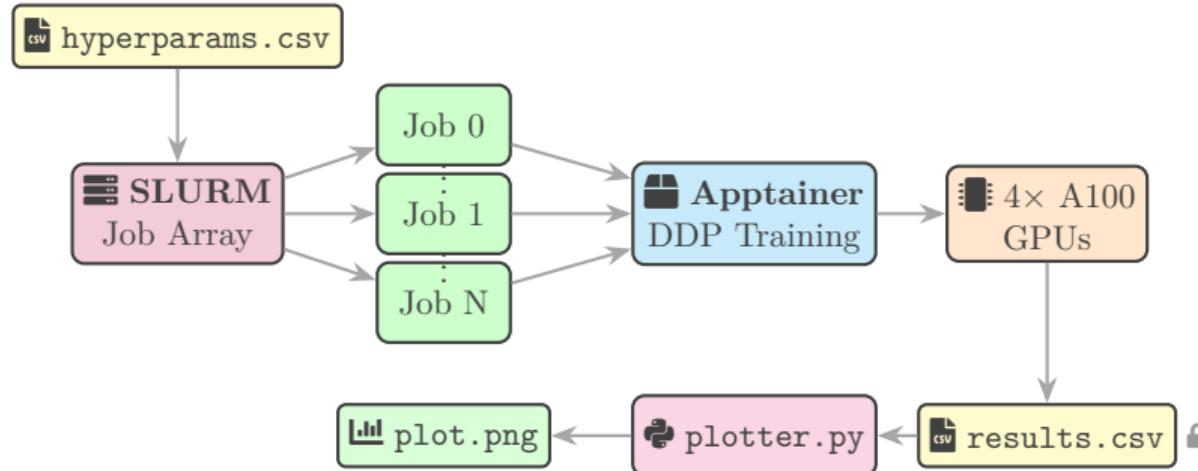
Model Architecture: GraphSAGE (SAGEConv + LayerNorm + ReLU)

Approach:

- █ **Apptainer containers:** reproducible environments
- █ **SLURM job arrays:** parallel execution across configs
- █ **CSV-driven pipeline:** configuration & result logging

Benchmark Pipeline

Hyperparameters



Tunable Hyperparameters

Hyperparameters

	Parameter	Default	Range Tested
	batch_size	128	16–512
	accum_steps	5	1–5
	num_neighbors	[15,10,10,10,10]	various
	num_layers	5	fixed
	hidden_dim	256	fixed
	lr	0.003	fixed
	epochs	150	fixed
	patience	10	fixed
	dropout	0.5	fixed

 Effective batch size:

$$\text{batch_size} \times \text{accum_steps} \times \text{world_size}$$

 Configs tested: 36

$$16 \text{ batch} \cdot 16 \text{ neighbor} \cdot 4 \text{ scaling}$$

Results

Benchmarking Focus

Results

1. **Mini-batch sampling:** Batch size impact on time & memory
2. **Neighbor sampling:** Fanout strategies (accuracy vs. efficiency)
3. **GPU scaling:** 1/2/4/8 GPU distributed training

Section 6.1

Mini-batch Sampling

Mini-batch Benchmarking: Configurations

Results

What's being tested?

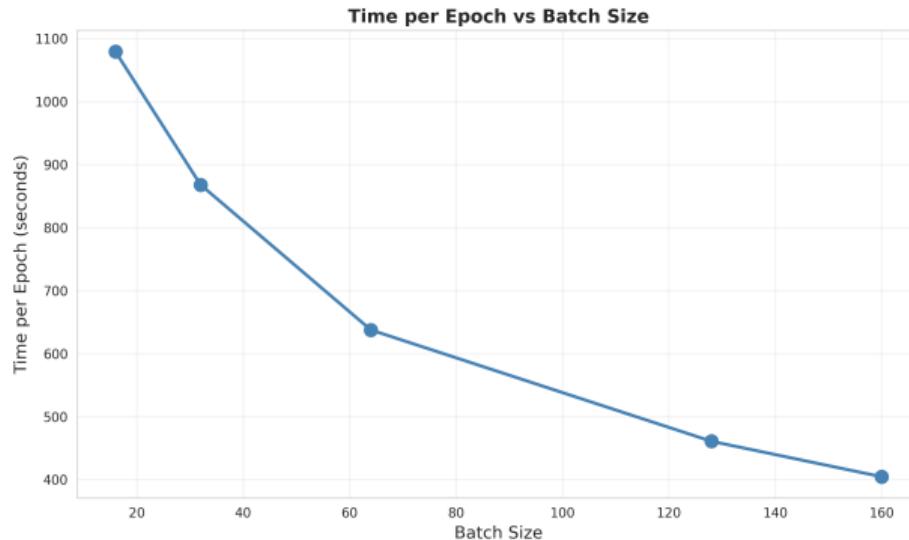
How does **batch size** and **gradient accumulation** affect:

- Training time per epoch
- Peak GPU memory usage
- Overall training efficiency

Batch Size	Accum. Steps
16	5
32	5
64	5
64	1, 2, 3, 4
128	5
128	1, 2, 3, 4
160	5
192	5
256	5
512	5

Batch Size: Training Time

Results

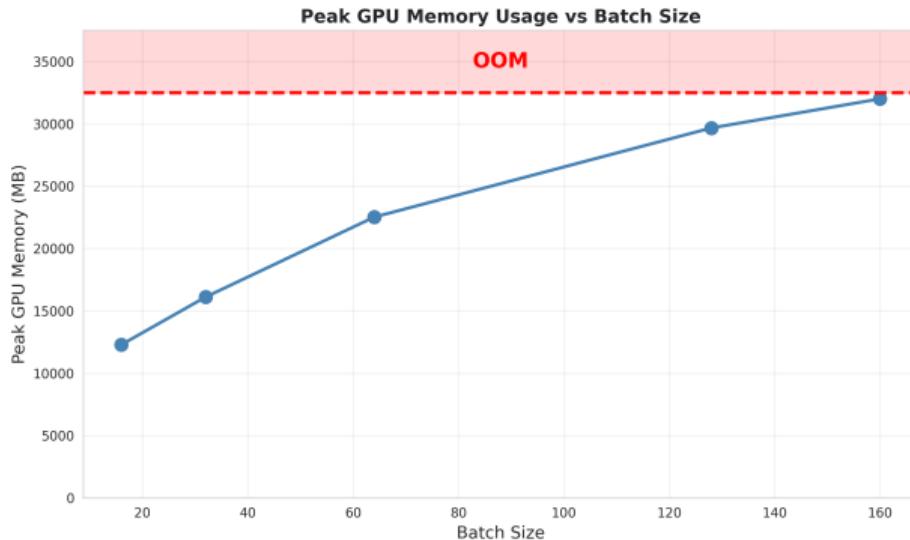


Key Findings:

- Inverse relationship: larger batch = faster training
- Better GPU utilization with larger batches
- Reduced forward pass / backward pass overhead

Batch Size: Memory Consumption

Results



Key Findings:

- Max batch size: 160
- Uses ~32GB (7.5GB system overhead)
- Bigger batches go OOM

Section 6.2

Neighbor Sampling

Neighbor Sampling: Configurations

Results

What's being tested?

How do different **fanout strategies** affect:

- Test accuracy
- Training time per epoch
- GPU memory usage

Fanout = neighbors sampled per layer

Total Fanout = product across all layers

$$F_{\text{total}} = \prod_{i=1}^5 L_i$$

L1	L2	L3	L4	L5
50	0	0	0	0
15	0	0	0	0
15	10	0	0	0
15	10	10	0	0
15	10	10	10	0
15	10	10	10	10
10	10	10	10	10
12	12	12	12	12
15	15	15	15	15
20	15	10	5	3
15	15	10	5	5
15	15	15	5	5
12	11	10	9	8
5	5	5	5	5
3	5	10	15	20
30	10	5	3	3

Neighbor Sampling: Accuracy vs. Time

Results

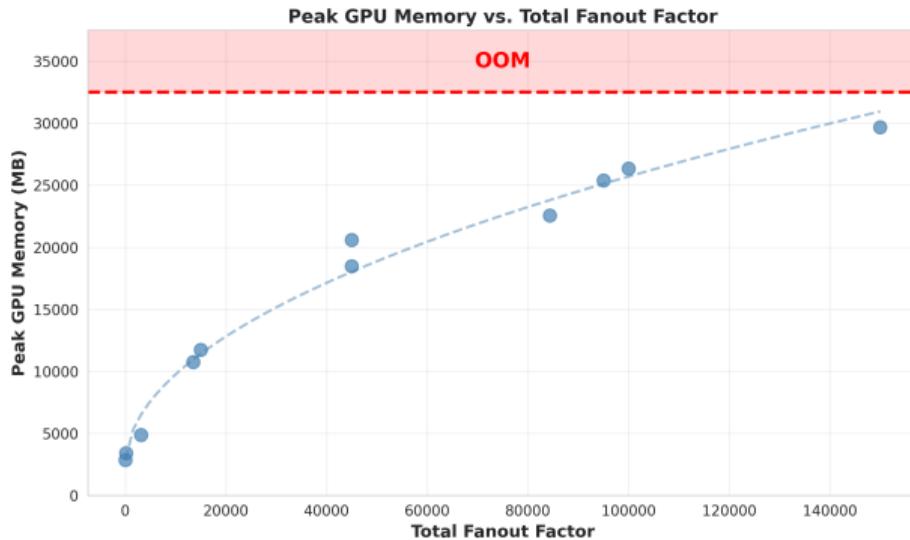


Key Findings:

- Upper-left = optimal
- Moderate fanouts best balance
- Aggressive sampling hurts accuracy or stability
- Very high fanouts: no proportional gains

Neighbor Sampling: Memory vs. Fanout

Results



Key Findings:

- Rapid memory growth with fanout
- Must balance receptive field vs. memory
- High fanouts hit memory limits and go OOM

Top 5 Neighbor Configurations

Results

Rank	Neighbor Sampling	Test Acc	Time (h)
1	[15, 15, 15, 5, 5]	0.8121	14.56
2	[15, 10, 10, 10, 0]	0.8114	7.22
3	[15, 10, 10, 10, 10]	0.8096	19.53
4	[10, 10, 10, 10, 10]	0.8088	16.46
5	[20, 15, 10, 5, 3]	0.8055	11.60

Key insight: [15,10,10,10,0] nearly matches accuracy, and **2.7× faster**

Section 6.3

GPU Scaling

GPU Scaling: Configurations

Results

What's being tested?

How does **distributed training** scale across:

- 1/2/4 GPUs per node
- 4 GPUs across 2 nodes (8 GPUs total)

Configuration	Setup
1 GPU	1 node
2 GPUs	1 node
4 GPUs	1 node
8 GPUs	2 nodes
Fixed Hyperparameters	
Batch size	128
Neighbors	[15,10,10,10,10]
Epochs	10

GPU Scaling: Training Time

Results

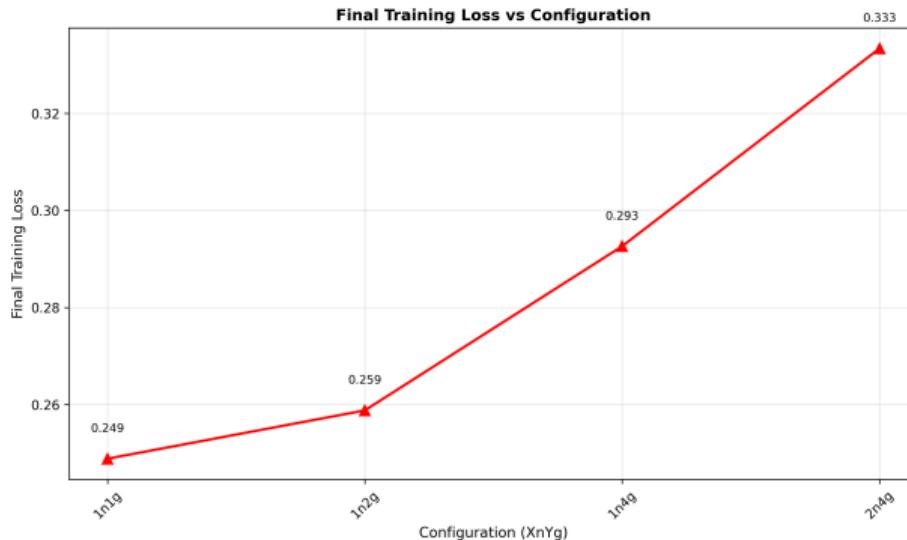


Key Findings:

- **1→2 GPUs:**
 $1.93 \times$ (96.5% efficiency)
- **1→4 GPUs:**
 $3.73 \times$ (93% efficiency)
- **1→8 GPUs:**
 $7.1 \times$ (89% efficiency)

GPU Scaling: Training Loss

Results



Key Findings:

- Loss increases with more GPUs
- Cause: larger effective batch size
- Reduced gradient noise

Discussion

Bottlenecks Discovered

Discussion

- **Memory wall:** Neighbor sampling expansion dominates memory usage
 - Fanout [15,10,10,10,10] = 150k neighbors per seed node
 - 128 batch size \times 150k expansion = 19.2M nodes per batch
 - Sampled subgraph + activations » model parameters (8MB)
- **Inter-node communication:** InfiniBand NCCL all-reduce overhead
 - 4 GPUs (1 node): 93% efficiency
 - 8 GPUs (2 nodes): 89% efficiency (4% degradation)
- **Loss convergence trade-off:** Larger effective batch sizes hurt convergence
 - Training loss increases with GPU count
 - Reduced gradient noise

What Worked Well

Discussion

- **DDP implementation:** Seamless gradient synchronization across GPUs
 - PyTorch DDP handles all-reduce automatically
 - Minimal code changes from single-GPU baseline
- **Strong intra-node scaling:** Excellent up to 4 GPUs
 - Linear speedups: 1→4 GPUs = $3.73\times$ (93% efficiency)
 - PCIe/NVLink bandwidth sufficient for this dataset size
- **Containerization:** Reproducibility & portability
 - Apptainer/Singularity ensures consistent environment
 - Complex PyG dependencies properly managed

Lessons Learned

Discussion

Implementing High-Performance Systems:

1. **Profile first, optimize second:** Memory bound, not compute
2. **Trade-offs are everywhere:** No free lunch → accuracy, speed, memory, communication always compete
3. **Reproducibility matters:** Containerization and fixed seeds essential for scientific HPC work

Any Question?

References

References

- [1] Aditya Grover and Jure Leskovec. “node2vec: Scalable Feature Learning for Networks”. In: *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. 2016, pp. 855–864.
- [2] William L. Hamilton, Rex Ying, and Jure Leskovec. “Inductive Representation Learning on Large Graphs”. In: *Advances in Neural Information Processing Systems (NeurIPS)*. Vol. 30. 2017, pp. 1024–1034. URL: <https://arxiv.org/abs/1706.02216>.
- [3] Thomas N. Kipf and Max Welling. “Semi-Supervised Classification with Graph Convolutional Networks”. In: *arXiv preprint arXiv:1609.02907* (2016).
- [4] Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. “DeepWalk: Online Learning of Social Representations”. In: *Proceedings of the 20th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. 2014, pp. 701–710.