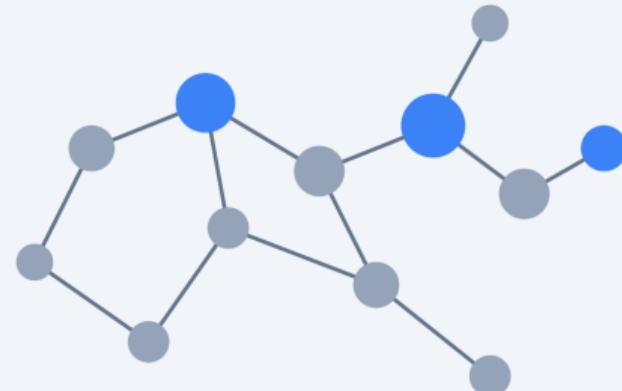


GRAPH SAGE

INDUCTIVE REPRESENTATION LEARNING ON LARGE GRAPHS

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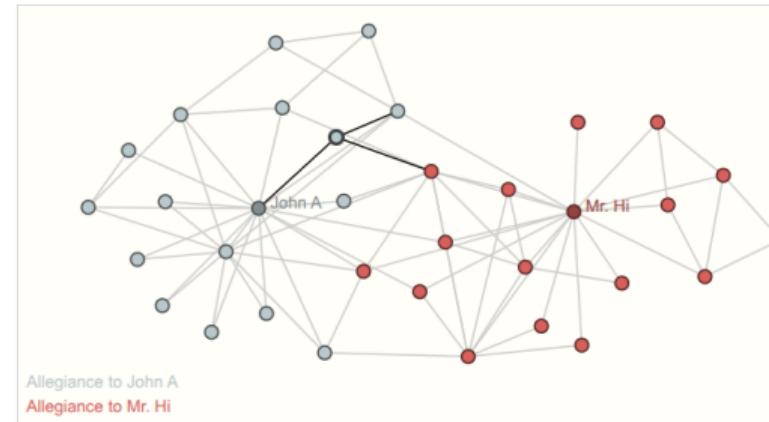
Introduction

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).

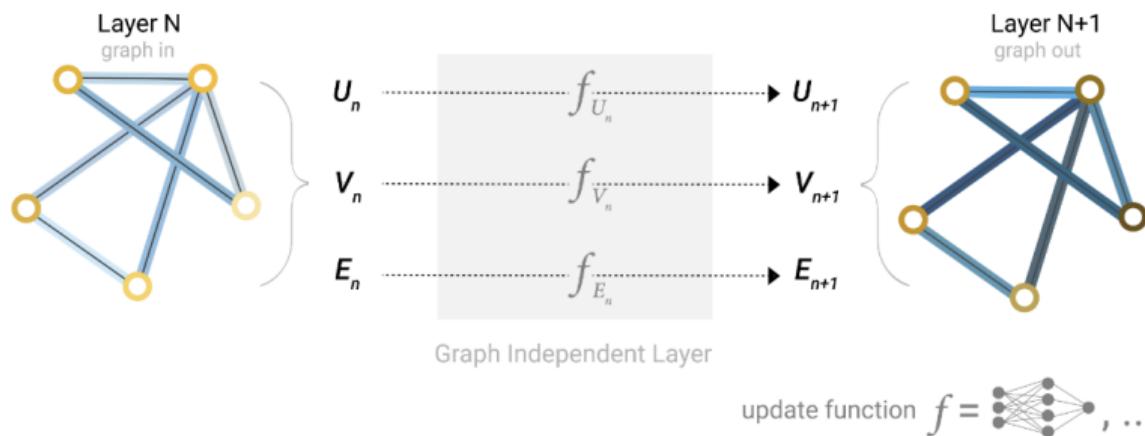


What is a Graph Neural Network?

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)

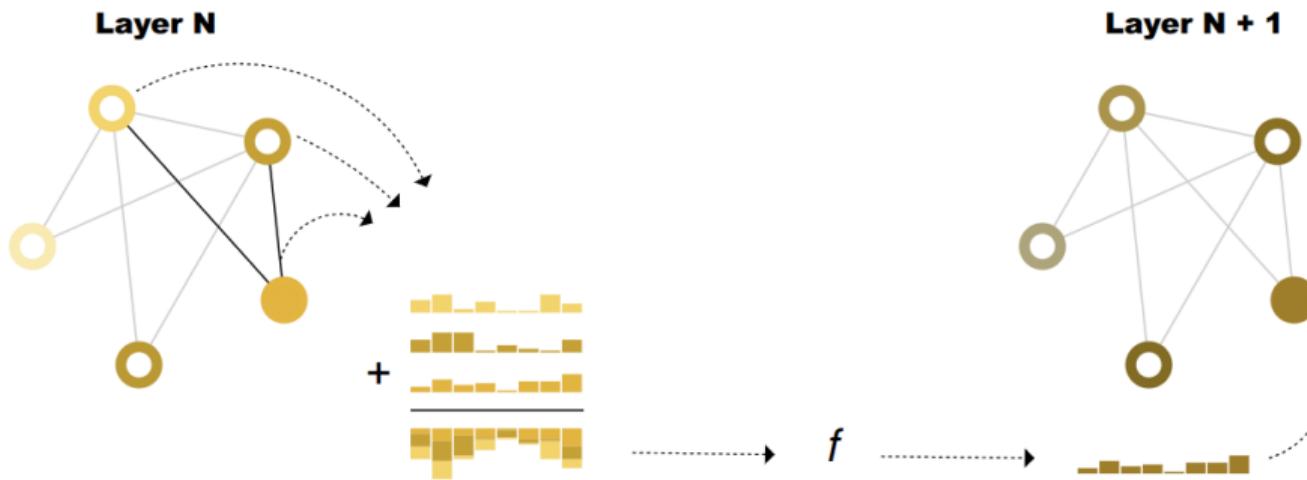


Message Passing: The Core Idea

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

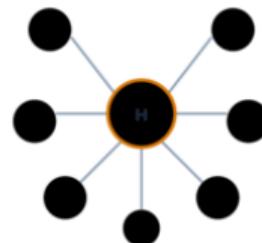
The Key Insight

Don't learn embeddings for each node...

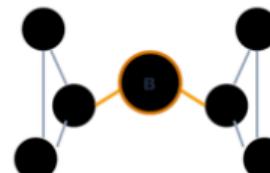
Learn a **FUNCTION** that generates embeddings

By sampling & aggregating neighborhood features

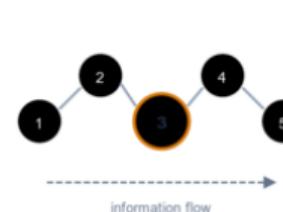
Hub Pattern
Social Influencer



Bridge Pattern
Community Connector



Chain Pattern
Sequential Flow



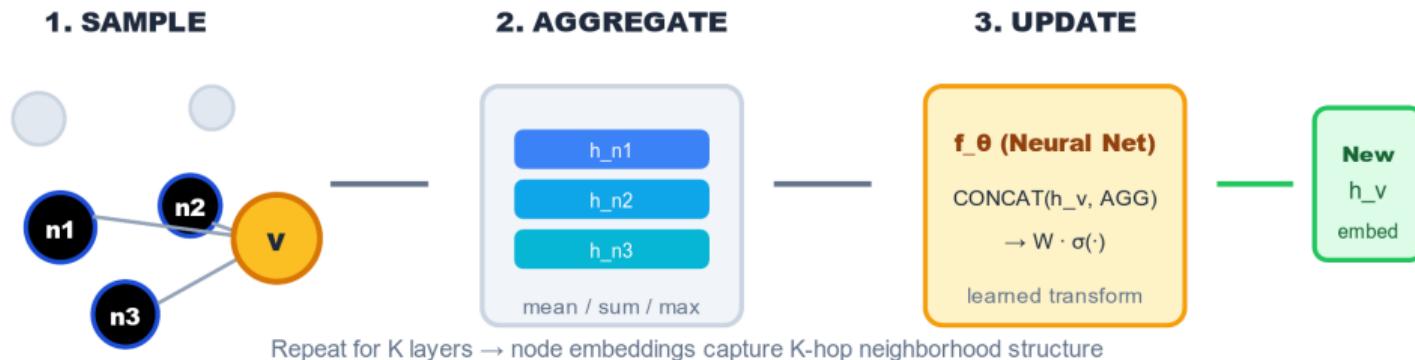
GraphSAGE Framework

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

System Architecture Overview

Implementation

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

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

Training Environment:

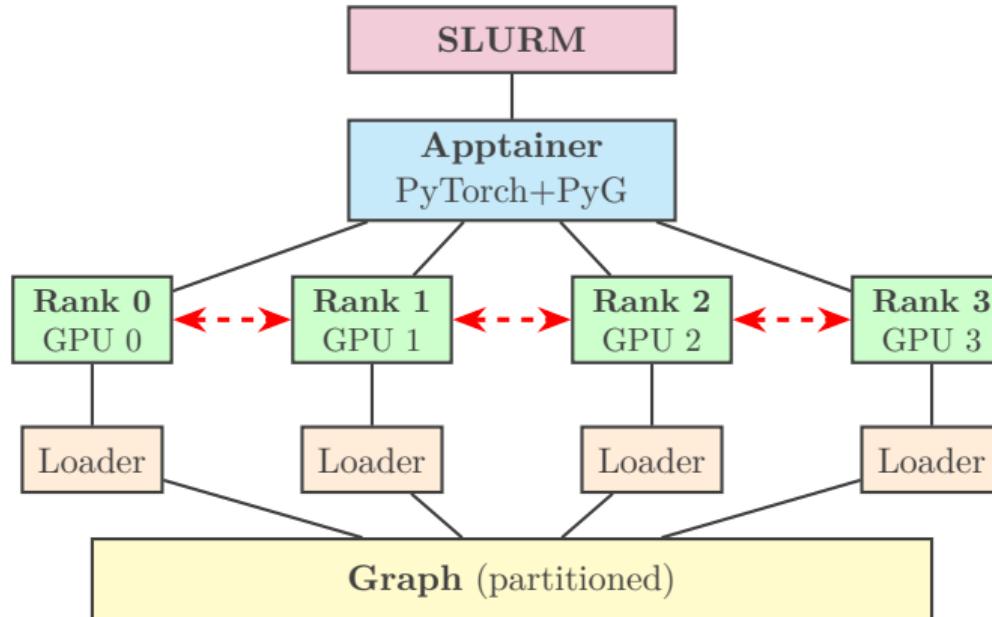
- **HPC Cluster:** MeluXina (Luxembourg National Supercomputer)
- **GPUs:** Up to 4x NVIDIA A100 (40GB) per node
- **Framework:** PyTorch 2.1.2 + PyTorch Geometric
- **Containerization:** Apptainer/Singularity for reproducibility

Model Architecture:

- 5-layer GraphSAGE (SAGEConv + LayerNorm + ReLU)
- Hidden dimension: 256, Dropout: 0.5

System Architecture Diagram

Implementation



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

Execution Model: Distributed Data Parallel

Implementation

Process Initialization:

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

Data Distribution:

- Training set (250k nodes) partitioned: 62.5k per rank
- No overlap between ranks → each processes unique subset
- Each rank has independent NeighborLoader for k-hop sampling

Gradient Synchronization:

- DDP automatically wraps model: synchronizes gradients after backward()
- All-reduce operation: averages gradients across all GPUs
- Learning rate scaled linearly: $lr_{\text{eff}} = lr_{\text{base}} \times N_{\text{GPUs}}$

Execution Model: Training Workflow

Implementation

1. Data Loading (Parallel):

- Each rank: 4-8 worker processes prefetch batches
- NeighborLoader samples k-hop subgraphs
- Pinned memory → GPU transfer (non-blocking)

2. Forward + Backward (Parallel):

- Each GPU: processes batch independently
- 5-layer message passing: aggregate → transform → activate
- Compute loss (cross-entropy), backpropagate gradients

3. Gradient Synchronization:

- DDP all-reduce: average gradients across 4 GPUs (NCCL)
- Optimizer step with synchronized gradients

4. Evaluation (Rank 0 Only):

- Every 5 epochs: validation accuracy on full validation set
- Checkpoint best model, early stopping (patience = 10)

Code Structure & Containerization

Implementation

Main Python Scripts:

- `train_graphsage.py` — Single-GPU training baseline
- `train_graphsage_ddp.py` — Multi-GPU DDP training (enhanced)
- `plot_batch.py` — Batch size benchmarking analysis
- `plot_neighbor.py` — Neighbor sampling strategy analysis

Apptainer Container:

- **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. Scale of the Problem:

- Dataset cannot fit in single GPU
- Neighbor sampling: Each batch node samples 5-hop neighborhoods
- Fanout [15,10,10,10,10] → 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 (40 GB) cannot handle large batches → slow training

3. Solution: Multi-GPU Parallelism

- Split data across 4 GPUs → 4x memory capacity
- Effective batch size: 2048 nodes (faster convergence)
- Training time: **hours instead of days**

Hyperparameters

Hyperparameters

Hyperparameters

Hyperparameter tuning details coming soon...

Results

Experimental Setup

Results

Hardware: MeluXina Supercomputer (Luxembourg National Supercomputer)

- 4× NVIDIA A100 (40GB) per node
- HDR200 InfiniBand (400 Gb/s aggregate bandwidth)

Benchmarking Focus:

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?

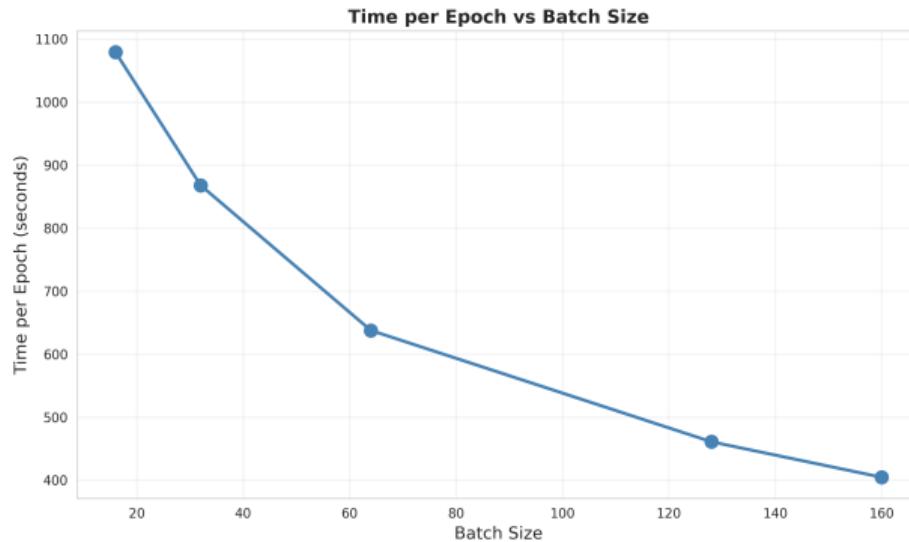
How does **batch size** and **gradient accumulation** affect:

- 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

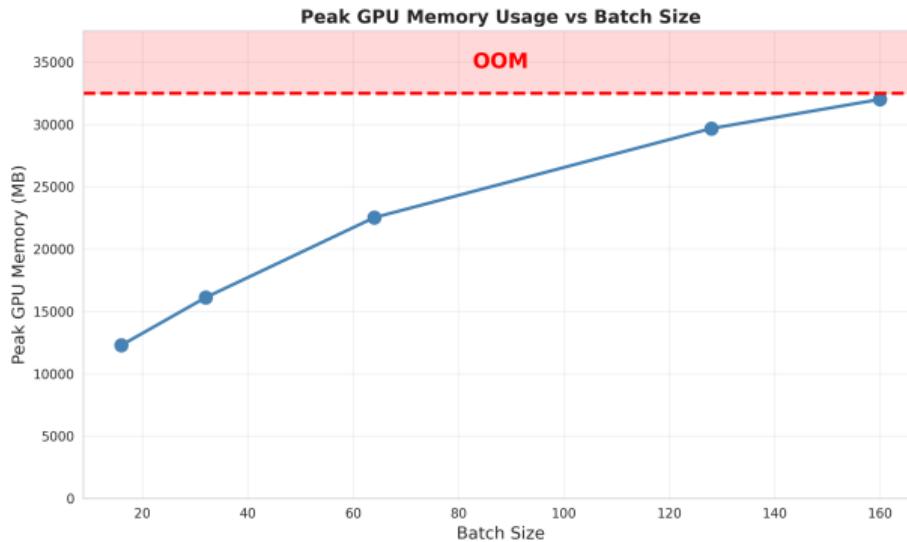


Key Findings:

- 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 \sim 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

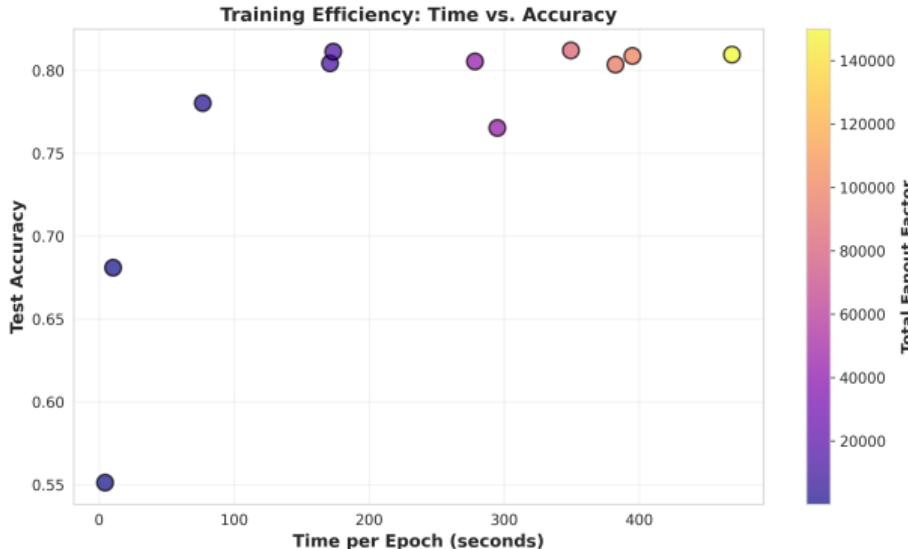
Total Fanout = product across all layers

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

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

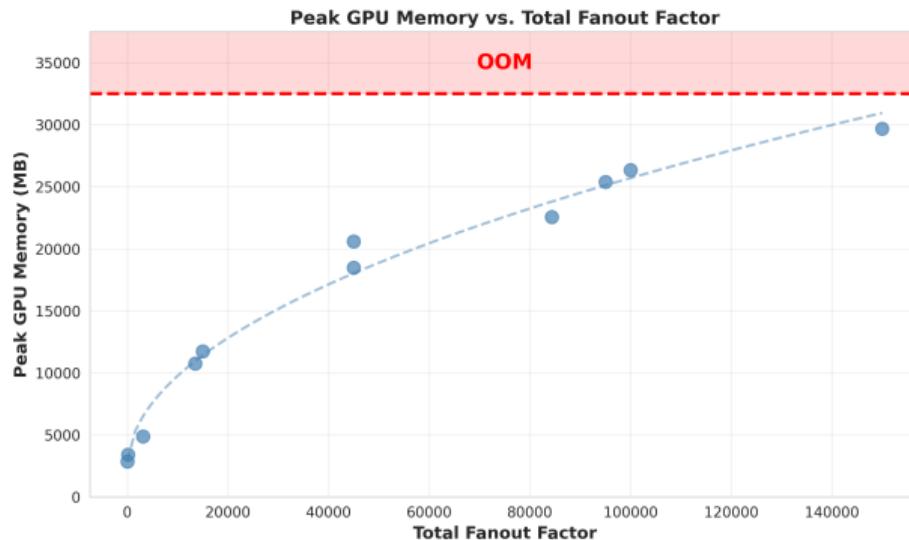


Key Findings:

- 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

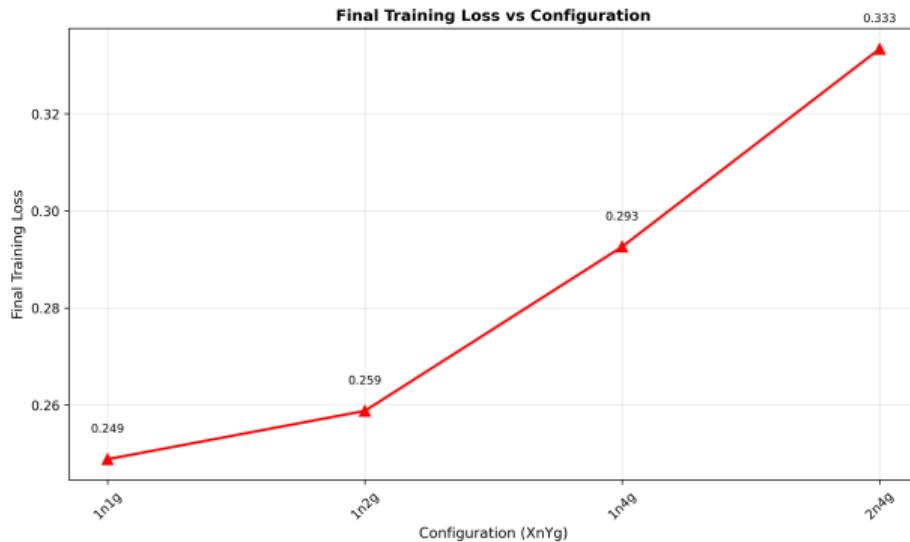


Key Findings:

- **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
- Wider minima, 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
 - Wider minima, 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 was the true bottleneck, not computation
2. **Trade-offs are everywhere:** No free lunch -*i.e.* accuracy, speed, memory, communication always compete
3. **Reproducibility matters:** Containerization and fixed seeds essential for scientific HPC work

Any Question?

References

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- [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>.
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