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GraphSAGE

Inductive Representation Learning on Large Graphs

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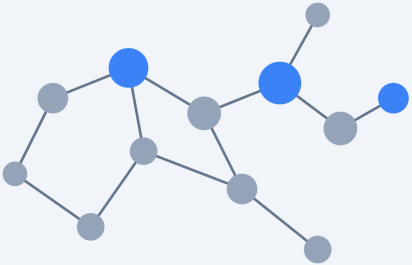

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Introduction

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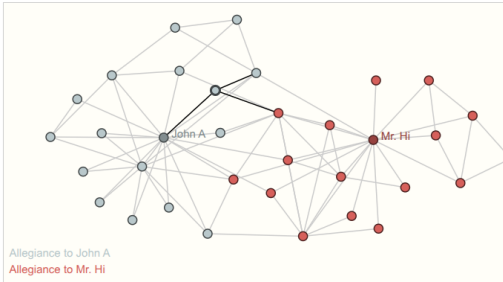
Graph Prediction Tasks

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).

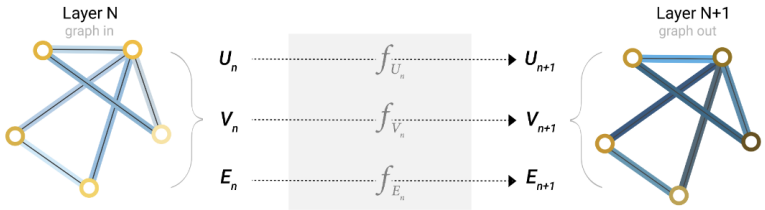


What is a Graph Neural Network?

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)

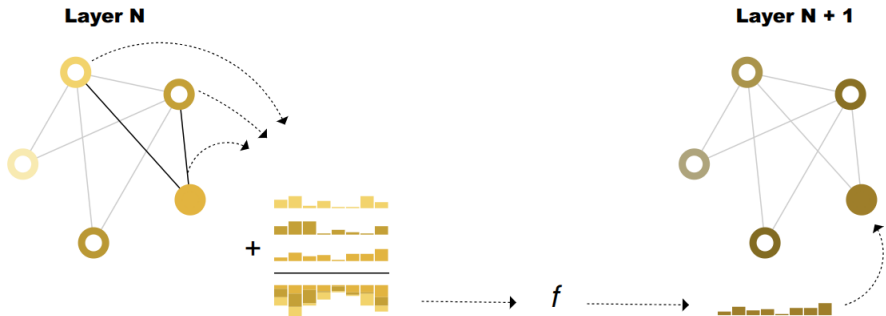


Message Passing: The Core Idea

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

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

- $h_v^{(k)}$ — Node v repr. at layer k
- h_u — Neighbor node u repr.
- $N(v)$ — Neighbors of v
- k — Layer index (hops)
- $\text{AGG}(\cdot)$ — 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

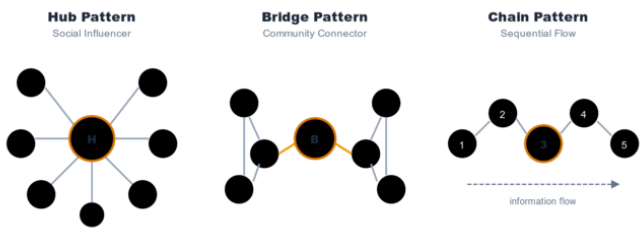
The Key Insight

The Key Insight

Don't learn embeddings for each node...

Learn a FUNCTION that generates embeddings

By sampling & aggregating neighborhood features



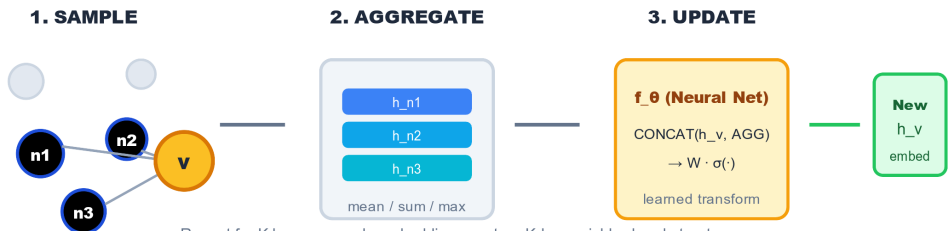
GraphSAGE Framework

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

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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:

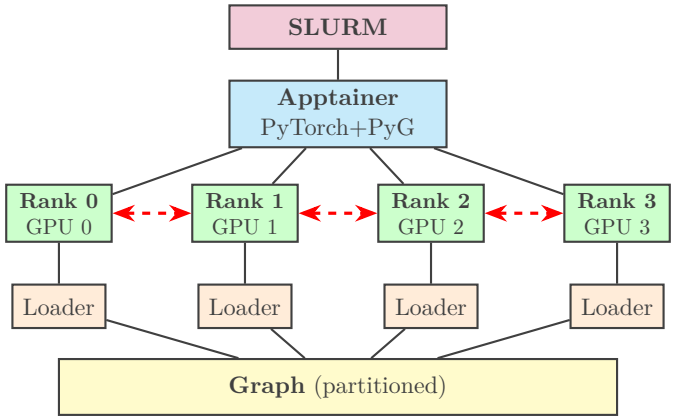
- **HPC Cluster:** MeluXina (Luxembourg National Supercomputer)
- **GPUs:** Up to 4x NVIDIA A100 (40GB) per node
- **Framework:** PyTorch 2.1.2 + PyTorch Geometric
- **Containerization:** Apptainer/Singularity for reproducibility

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

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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: $\text{lr}_{\text{eff}} = \text{lr}_{\text{base}} \times N_{\text{GPUs}}$

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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)

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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

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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

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Overview

Hyperparameters

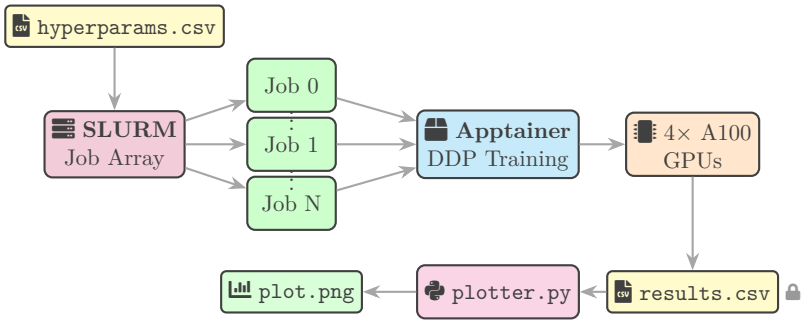
Goal: Scalable and reproducible hyperparameter optimization

Approach:

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

Benchmark Pipeline

Hyperparameters



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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:

batch_size × accum_steps × world_size

Configs tested: 34

15 batch · 15 neighbor · 4 scaling

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

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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

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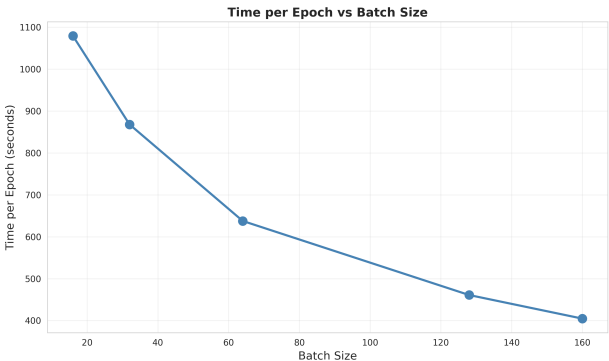
Batch Size: Training Time

Results

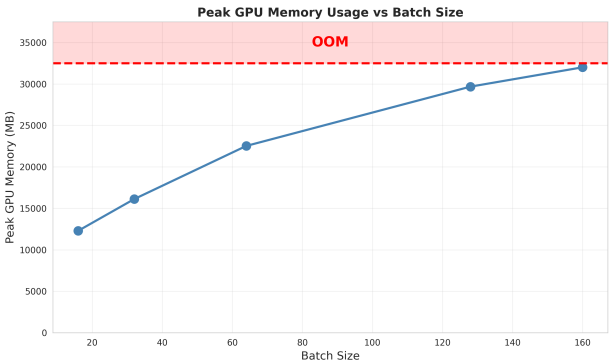


Key Findings:

- 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

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Neighbor Sampling: Configurations

Results

What's being tested?

How do different **fanout strategies** affect:

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

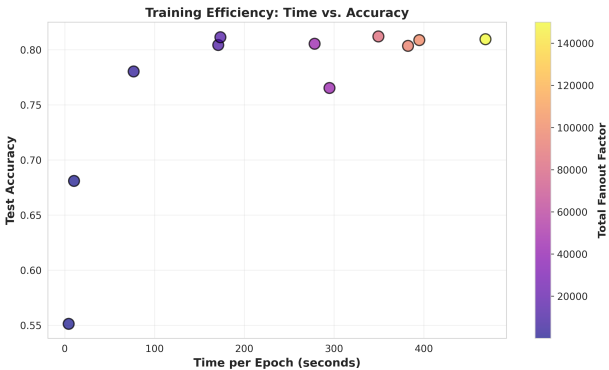
Fanout = neighbors sampled per layer
Total Fanout = product across all layers

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

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

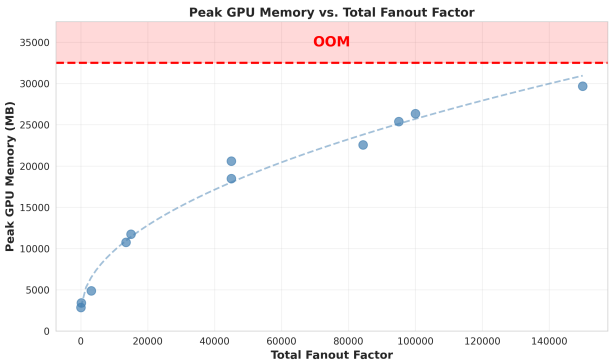


Key Findings:

- 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

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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

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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

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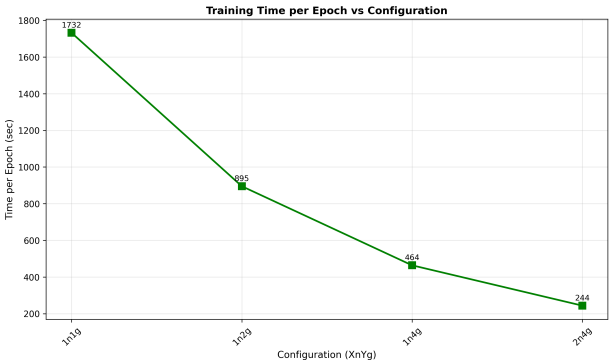
GPU Scaling: Training Time

Results

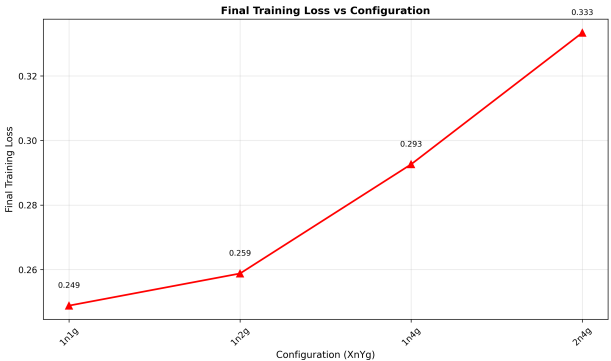


Key Findings:

- **1→2 GPUs:** 1.93× (96.5% efficiency)
- **1→4 GPUs:** 3.73× (93% efficiency)
- **1→8 GPUs:** 7.1× (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

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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 × 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

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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× (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 -¿ accuracy, speed, memory, communication always compete
3. **Reproducibility matters:** Containerization and fixed seeds essential for scientific HPC work

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Any Question?

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References

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