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GraphSAGE

Inductive Representation Learning on Large Graphs

Thomas Gantz
Alberto Finardi
Tommaso Crippa
Jan Marxen

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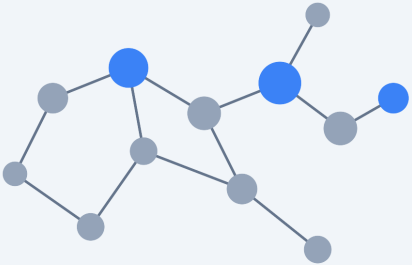

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Introduction

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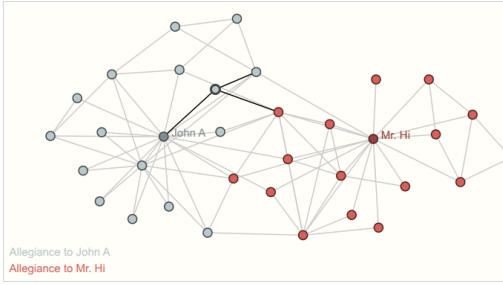
Graph Prediction Tasks

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).

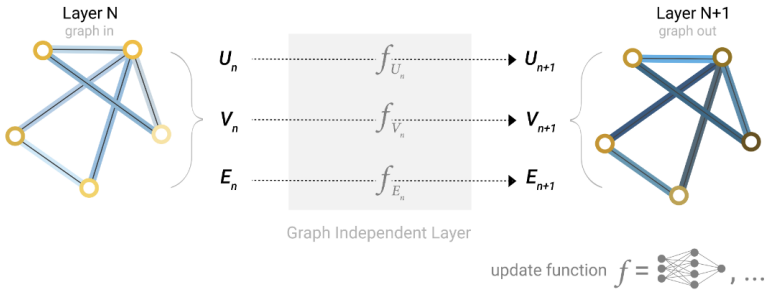


What is a Graph Neural Network?

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)

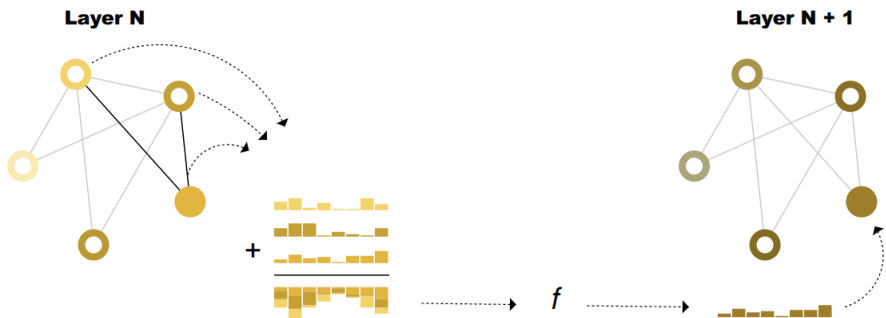


Message Passing: The Core Idea

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



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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)

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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

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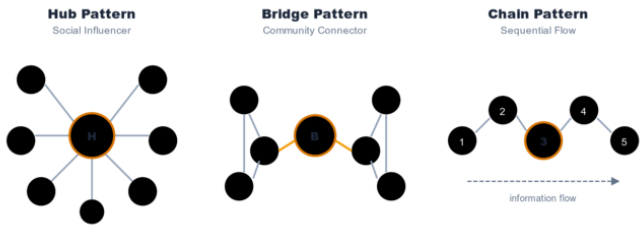
The Key Insight

Don't learn embeddings for each node...

Learn a FUNCTION that generates embeddings

By sampling & aggregating neighborhood features



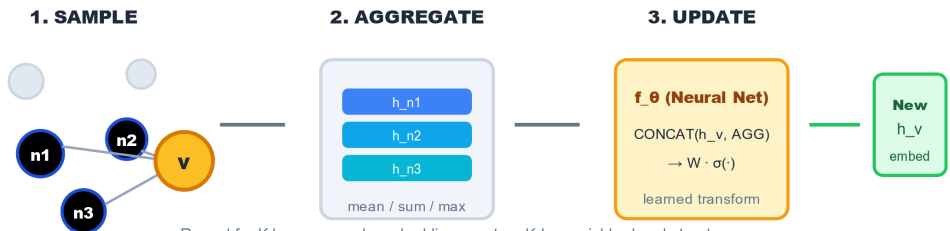
GraphSAGE Framework

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



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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

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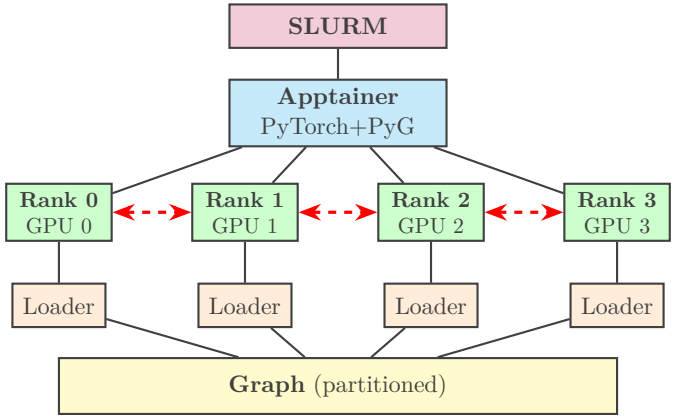
System Architecture Diagram

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

Hyperparameters

Hyperparameters

Hyperparameter tuning details coming soon...

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Results

Results

Results

Experimental results coming soon...

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Any Question?

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