GraphSAGE

Inductive Representation Learning on Large Graphs

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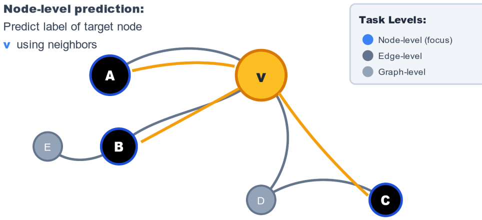
Introduction

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).

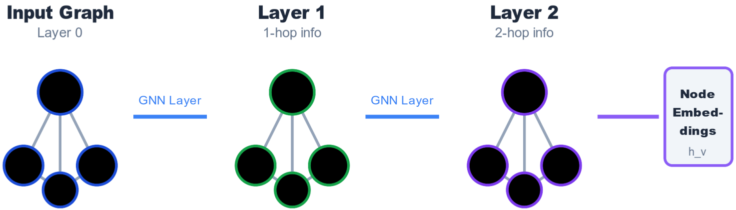


What is a Graph Neural Network?

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)



Each layer aggregates information from neighbors → deeper layers capture larger neighborhoods

Message Passing: The Core Idea

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 Equation

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

Analogy: CNNs aggregate over fixed local pixel neighborhoods; GNNs aggregate over variable-size neighbor sets.

Message Passing: Notation

Introduction

- $h_v^{(k)}$ — Representation of node v at layer k
- h_u — Representation of neighbor node u
- $N(v)$ — Set of neighbor nodes of v
- k — Layer index (message-passing hops)
- $\mathrm{AGG}(\cdot)$ — Aggregator function (mean, sum, max, LSTM)
- W — Learnable weight matrix
- σ — Non-linear activation (ReLU, tanh)

Before GraphSAGE: The Problem

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...

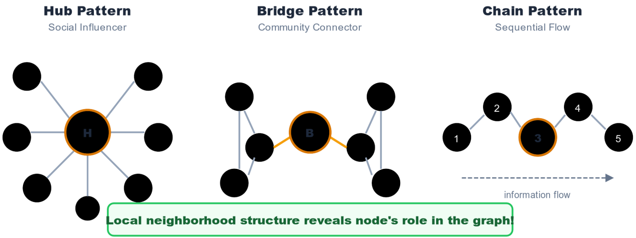
The Key Insight

The Key Insight

Don't learn embeddings for each node...

Learn a FUNCTION that generates embeddings

By sampling & aggregating neighborhood features



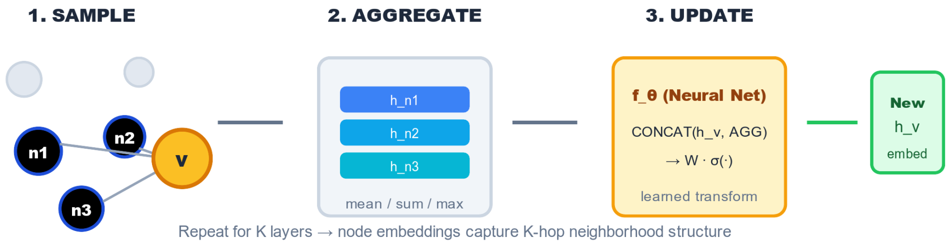
GraphSAGE Framework

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

Implementation

Implementation

Implementation details coming soon...

Hyperparameters

Hyperparameters

Hyperparameters

Hyperparameter tuning details coming soon...

Results

Results

Experimental results coming soon...

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Any Question?

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References

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