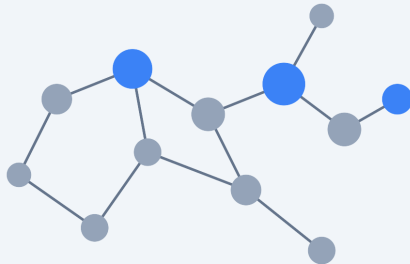# GraphSAGE

Inductive Representation Learning on Large Graphs

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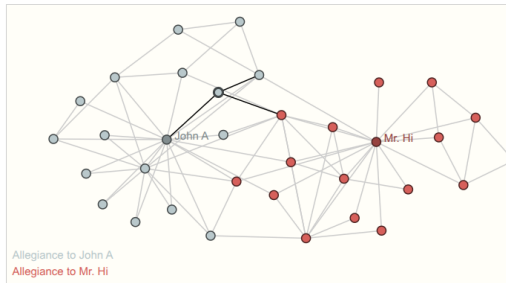Jan Marxen

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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
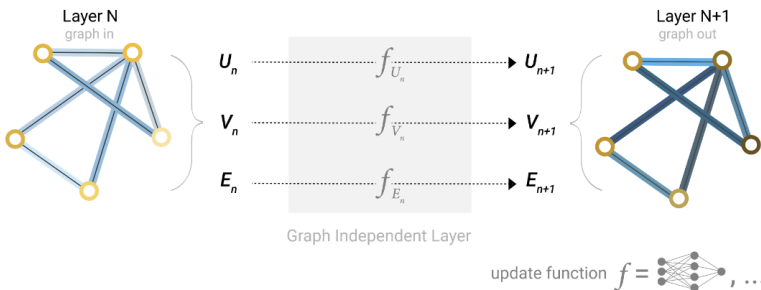 whole graphs (e.g., molecule properties).

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
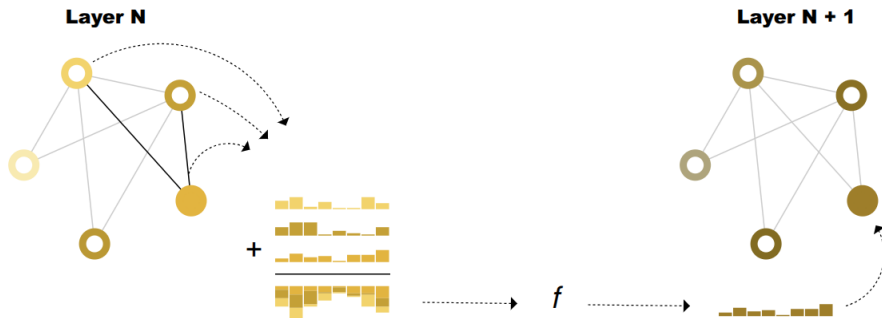- Is **permutation invariant** (order of nodes doesn't matter)

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

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

- $h_v^{(k)}$ — 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)

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

Don't learn embeddings for each node...

Learn a FUNCTION that generates embeddings

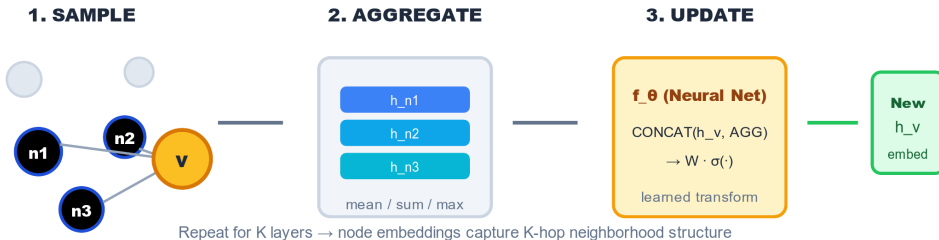*By sampling & aggregating neighborhood features*

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

1. SAMPLE   **2. AGGREGATE**   **3. UPDATE**

h_n1
h_n2
h_n3

mean / sum / max

f_θ (Neural Net)

CONCAT(h_v, AGG)

→ W · σ(·)

learned transform

New h_v embed

Repeat for K layers → node embeddings capture K-hop neighborhood structure

Implementation

Implementation details coming soon...

Hyperparameters

Hyperparameter tuning details coming soon...

Results

Experimental results coming soon...

Any Question?

References

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