GraphSAGE

Inductive Representation Learning on Graphs

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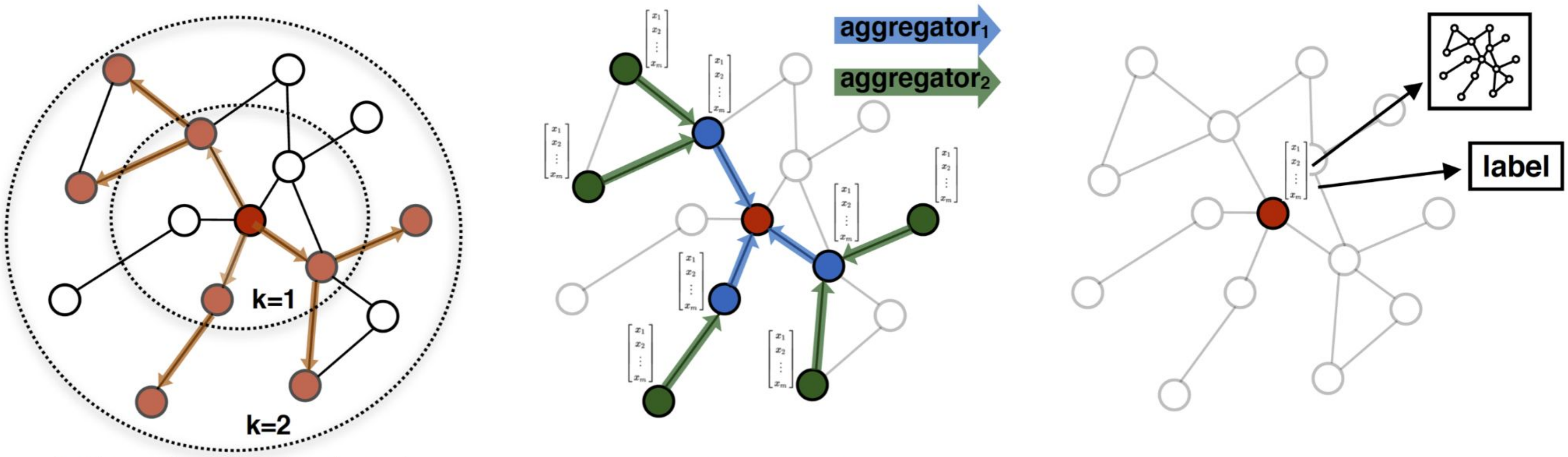
We will go over

1. What is GraphSAGE
2. Results
3. Findings

GraphSAGE



1. Sample neighborhood

2. Aggregate feature information from neighbors

3. Predict graph context and label using aggregated information

Algorithm 1: GraphSAGE embedding generation (i.e., forward propagation) algorithm

Input : Graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$; input features $\{\mathbf{x}_v, \forall v \in \mathcal{V}\}$; depth K; weight matrices $\mathbf{W}^k, \forall k \in \{1, ..., K\}$; non-linearity σ; differentiable aggregator functions $\text{AGGREGATE}_k, \forall k \in \{1, ..., K\}$; neighborhood function $\mathcal{N} : v \rightarrow 2^{\mathcal{V}}$

Output : Vector representations $\mathbf{z}_v$ for all $v \in \mathcal{V}$

$\mathbf{h}_v^0 \leftarrow \mathbf{x}_v, \forall v \in \mathcal{V}$;
for $k = 1...K$ **do**
    for $v \in \mathcal{V}$ **do**
        $\mathbf{h}_{\mathcal{N}(v)}^k \leftarrow \text{AGGREGATE}_k(\{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\})$;
        $\mathbf{h}_v^k \leftarrow \sigma\left(\mathbf{W}^k \cdot \text{CONCAT}(\mathbf{h}_v^{k-1}, \mathbf{h}_{\mathcal{N}(v)}^k)\right)$
    end
    $\mathbf{h}_v^k \leftarrow \mathbf{h}_v^k / \|\mathbf{h}_v^k\|_2, \forall v \in \mathcal{V}$
end
$\mathbf{z}_v \leftarrow \mathbf{h}_v^K, \forall v \in \mathcal{V}$

A PERMUTATION INVARIANT AGGREGATOR

GraphSAGE uses two different types of neighborhood aggregators. Mean and Max pooling which are both permutation invariant.

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Output : Vector representations $\mathbf{z}_v$ for all $v \in \mathcal{V}$

$\mathbf{h}_v^0 \leftarrow \mathbf{x}_v, \forall v \in \mathcal{V}$;

for $k = 1...K$ **do**

  for $v \in \mathcal{V}$ **do**

    $\mathbf{h}_{\mathcal{N}(v)}^k \leftarrow \textsc{aggregate}_k(\{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\})$;

    $\mathbf{h}_v^k \leftarrow \boxed{\sigma\left(\mathbf{W}^k \cdot \textsc{concat}(\mathbf{h}_v^{k-1}, \mathbf{h}_{\mathcal{N}(v)}^k)\right)}$

  end

  $\mathbf{h}_v^k \leftarrow \mathbf{h}_v^k / \|\mathbf{h}_v^k\|_2, \forall v \in \mathcal{V}$

end

$\mathbf{z}_v \leftarrow \mathbf{h}_v^K, \forall v \in \mathcal{V}$

DENSENET BUT GRAPH

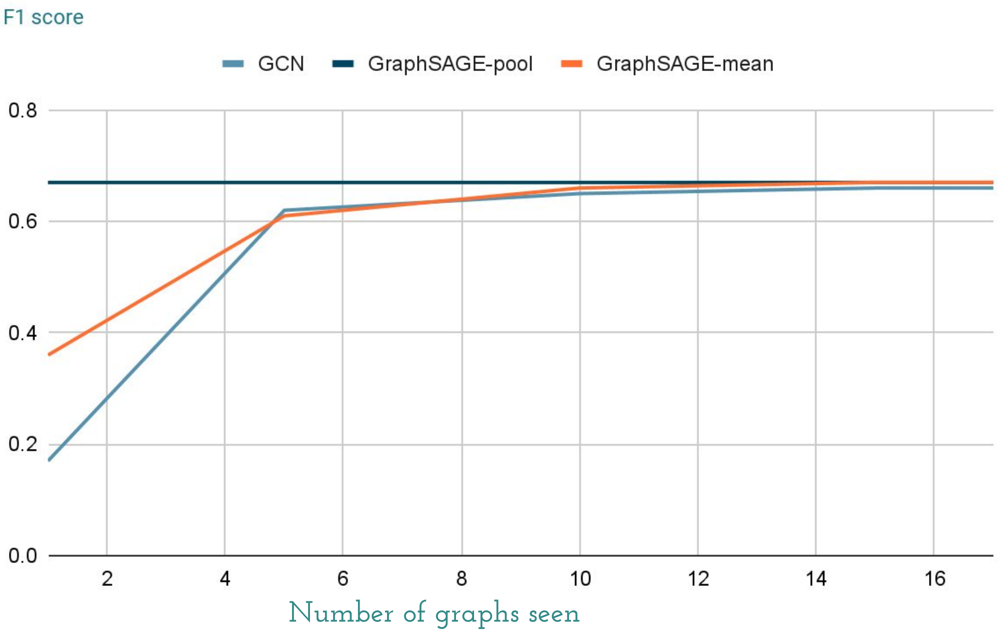
GraphSAGE concatenates features from previous computations in a way that resembles skip connections

Results on CORA 2

	Cora
GCN	78.3
GraphSAGE-mean concat	77.8
GraphSAGE-mean residual	79.8
GraphSAGE-pool concat	75.2
GraphSAGE-pool residual	71.1

F1 scores

Performances were not stable and GraphSAGE does not necessarily present a clear advantage



F1 scores

GraphSAGE-pool generalizes after having seen a single graph

Finding 1

GraphSAGE can work with additions instead of concatenations but loses a bit of its generalization power

Finding 2

The main contribution of GraphSAGE is the ability to generalize quickly and efficiently to unseen graphs

Thanks

Does anyone have any questions?