Is uniform expressivity too restrictive? Towards efficient expressivity of GNNs

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GNNs in our work

GNN := SUM-AC GNN

$$\xi^{t+1}(v, G) = \mathrm{comb}_t\left(\xi^t(v, G), \sum_{w \in \mathcal{N}_G(v)} \xi^t(w, G)\right)$$

The question we answer

How does the activation function affect
the expressivity of the GNN?

↑

Expressivity

Trainability

Generability

Queries

$$Q(v) = \forall y \left(E(y, v) \to \exists^{\geq 2} z \, E(z, y) \right)$$

$Q(v, G) = 1$ expresses the following:

in the graph G, every neighbor of the vertex v has at least two neighbors

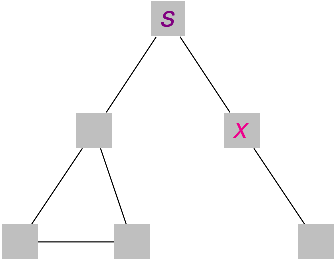
$$\tilde{Q}(v) = \text{Red}(v) \wedge (\forall y \, (E(y, v) \to (\text{Blue}(y) \wedge (\forall z \, (E(z, y) \to \text{Red}(z))))))$$

$\tilde{Q}(v, G) = 1$ expresses the following:

in the graph G, the vertex v is red
and all neighbors of v are blue & have only red neighbors

Queries in Practice I

$$Q(v) = \forall y \left(E(y, v) \to \exists^{\geq 2} z \, E(z, y) \right)$$

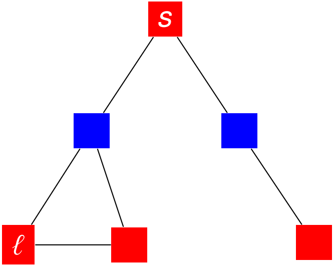


$Q(s) = 1$

$Q(x) = 0$

Queries in Practice II

$$\tilde{Q}(v) = \mathrm{Red}(v) \wedge (\forall y\, (E(y, v) \rightarrow (\mathrm{Blue}(y) \wedge (\forall z\, (E(z, y) \rightarrow \mathrm{Red}(z))))))$$



$\tilde{Q}(s) = 1$

$\tilde{Q}(\ell) = 0$

GC2 Queries

Atomic Queries:

$\mathrm{Col}_i(v)$:= "vertex v has the ith color"

Construction Rules:

Negation:

$\neg\phi(v)$

Conjunction:

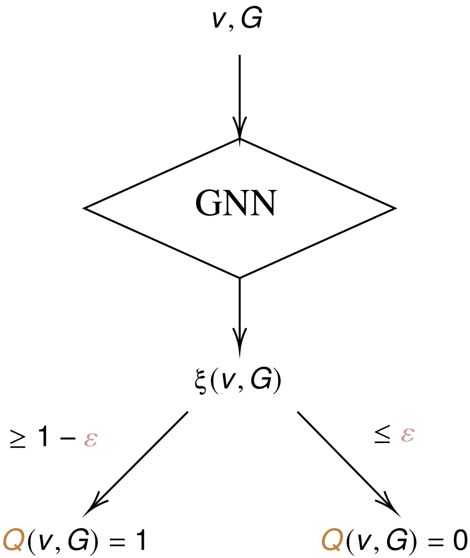
$\phi(v) \wedge \psi(v)$

Restricted Quantification over Neighbors:

$\exists^{\geq N} y\, (E(y, v) \wedge \phi(v))$

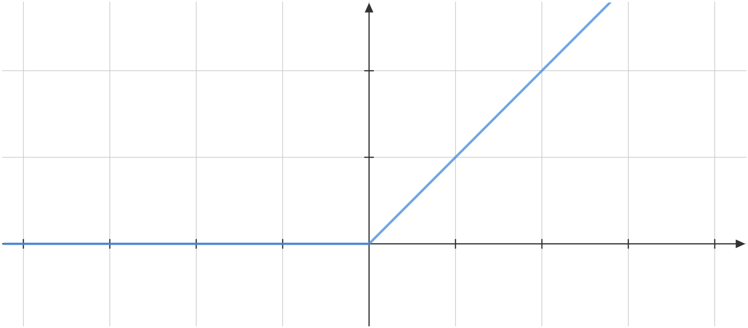
$$\begin{aligned} Q(v) &= \forall y \left(E(y, v) \rightarrow \exists^{\geq 2} z\, E(z, y) \right) \\ &= \neg \left(\exists^{\geq 1} y \left(E(y, v) \wedge \left(\neg \left(\exists^{\geq 2} v\, E(v, y) \right) \right) \right) \right) \end{aligned}$$

GNN Expression of Queries



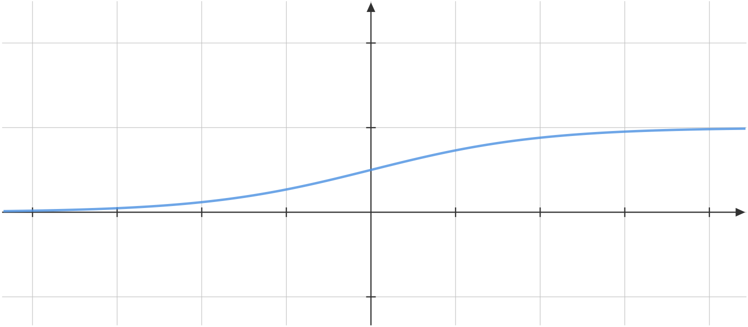
Sigmoid vs ReLU

$$\text{ReLU}(x) := \max\{0, x\}$$



Sigmoid vs ReLU

$$\mathrm{Sigmoid}(x) := \frac{1}{1 + \mathrm{e}^{-x}}$$



State of the Art: ReLU GNNs

Theorem

(Barcelo, Kostylev, Monet, Pérez, Reutter & Silva; 2020)

GC2 query Q of size d

Then:

there is

a ReLU GNN of size $4d$

expressing Q

over all graphs

tldr: GC2 queries are uniformly expressible by ReLU GNNs

A ReLU GNN expressing a first order query expresses a GC2 query

Sigmoid GNNs are less expressive than ReLU GNNs

$$Q(v) = \forall y \left(E(y, v) \rightarrow \exists^{\geq 2} z\, E(z, y) \right)$$

THEOREM
(KH. & T.-C.; ICLR25)
Sigmoid GNN with output ξ
THEN:
for all $\varepsilon > 0$,
there are rooted trees T and T'
with roots s and s'
such that:
(a) $Q(s, T) = 1$ and $Q(s', T') = 0$
(b) $|\xi(s, T) - \xi(s', T')| < \varepsilon$

tldr: Sigmoid GNNs CANNOT express uniformly GC2 queries

Sigmoid GNNs are almost as expressive as ReLU GNNs

Theorem
(Kh. & T.-C.; ICLR25)
GC2 query Q of size d
$\Delta > 0$
Then:
there is
a Sigmoid GNN of size $O(d \log\log(\Delta))$
expressing Q
over all graphs of degree $\leq \Delta$

tldr: Sigmoid GNNs express almost uniformly GC2 queries

Take home message

ReLU GNNs can express a GC2 query for all graphs
with size only depending on the query not on the graph

Sigmoid GNNs cannot express a GC2 query for a class of graphs
with size only depending on the query...

...but dependence on graph size is so small
that does not have practical implications for expressivity

All the details in our paper!