Universal Invariant and Equivariant GNNs [1]

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Introduction

Universal Approximation

Universal Approximation Theorem

MLPs with a single hidden layer are universal approximators

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- **Are *equivarient* GNNs universal approximators of *equivariant* continuous functions on graphs?**

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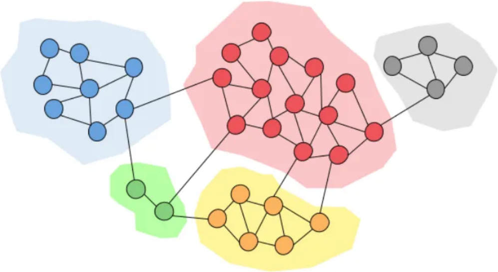
Equivalance vs Invariance

- Community detection

$$G = (V, E) \quad y : V \to \{1, \cdots, C\}$$



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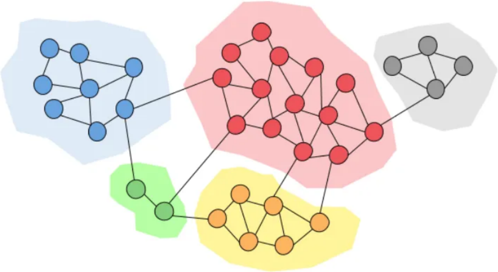

- Recommender Systems

Equivalence vs Invariance

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- Recommender Systems

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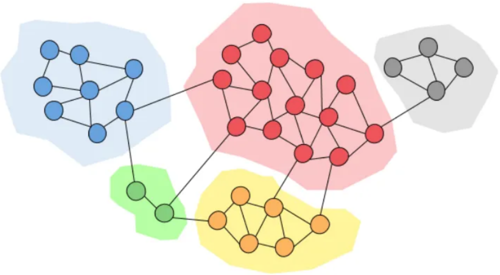

One-Layer GNN

- $f(G) = \sum_{s=1}^{S} H_s[\rho(F_s[G] + B_s)] + b$

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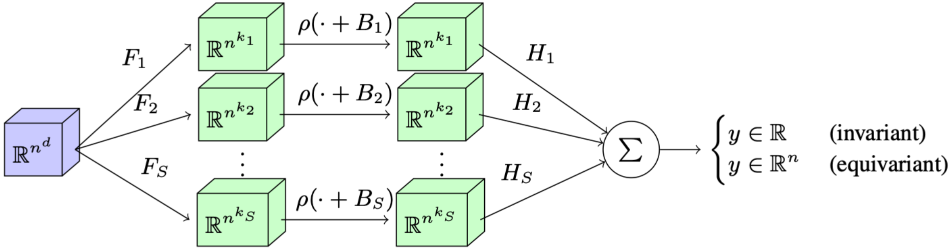
- $B_s = \sigma B_s$: equivariant Bias

Model of GNN


$\mathbb{R}^{n^d}$
F_1
F_2
F_S
$\mathbb{R}^{n^{k_1}}$
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$\rho(\cdot + B_1)$
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H_1
H_2
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Σ
$\begin{cases} y \in \mathbb{R} & \text{(invariant)} \\ y \in \mathbb{R}^n & \text{(equivariant)} \end{cases}$

Number of parameters

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- We want to show that a GNN approximates a continuous function uniformly well for several n at once

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8
Proof for Invariant Case

Proof Idea: Dense subsets

- If $\mathcal{A} \subset \mathcal{B}$ is dense in $\mathcal{B}$, then $\forall b \in \mathcal{B}, \forall \epsilon > 0, \exists a \in \mathcal{A}$ such that $\|a - b\| < \epsilon$

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- Show class of invariant 1-layer GNNs is dense in space of real-valued continous invariant functions on graphs

Alternate Proof for [2]

Show class of invariant 1-layer GNNs is dense in space of real-valued continous invariant functions on graphs

- Equivalence class of isomorphic graphs
  $\mathcal{G}_{\mathsf{inv}} := \left\{ \mathcal{O}(G);\, G \in \mathbb{R}^{n^d} \text{ with } n \leq n_{\max},\, \|G\| \leq R \right\}$

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Isomorphism

G_1, G_2 isomorphic if $G_1 = \sigma \star G_2$

Invariance

$f(G_1) = f(\sigma \star G_2) = f(G_2)$

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- $\mathcal{O}$: set of permutations $\sigma : [n] \to [n]$
- $\mathcal{O}(G) := \{\sigma \star G; \sigma \in \mathcal{O}\}$

Edit Distance

- Graph edit distance

$$d_{\textsf{edit}}(\mathcal{O}(G_1), \mathcal{O}(G_2)) := \min_{(o_1, o_2, \cdots, o_k) \in \mathcal{P}(G_1,\, G_2)} \sum_{i=1}^{k} c(o_i)$$

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  - $c(\texttt{edge\_weight\_modification}) = |w - w'|$

Edit Distance Example

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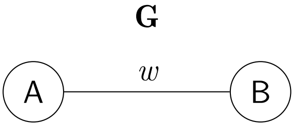
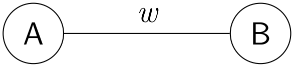


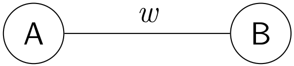
cost accumulated: c

Edit Distance Example

$\mathbf{G}$



$\mathbf{G'}$



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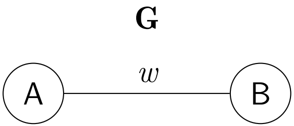

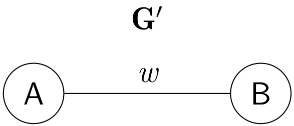

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$$d_{\text{edit}}(G, G') = c + w$$

Edit Distance Observations

Assume $d_{\text{edit}}(\mathcal{O}(G_1), \mathcal{O}(G_2)) < c$. Then the following hold:

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- This shows any continuous invariant function is *uniformly* well-approximated by a GNN on $\mathcal{G}_{\mathsf{inv}}$

Stone-Weierstrass Theorem

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Hasudorff

Separate points have separate neighborhoods
✓ all metric spaces are Hausdorff

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  - Therefore $G \mapsto \mathcal{O}(G)$ is continuous

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Subalgebra

a vector subspace closed under the multiplication of vectors

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Separability

For all $x \neq y$ in X, there exists $f \in A$ such that $f(x) \neq f(y)$

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For two distinct classes of isomorphic graphs in $\mathcal{G}_{\text{inv}}$ $(\mathcal{O}(G_1) \neq \mathcal{O}(G_2))$, there is a class of 1-layer GNNs $f \in \mathcal{N}^{\otimes}{}_{\text{inv}}$ with $f(\mathcal{O}(G_1)) \neq f(\mathcal{O}(G_2))$.

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- Proof by contradiction and graphs G_1, G_2 are permutations of each other if $f(\mathcal{O}(G_1)) = f(\mathcal{O}(G_2))$ for $f \in \mathcal{N}_{\text{inv}}^{\otimes}(\rho_{\text{sig}})$

Stone-Weierstrass Theorem

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  - ✓ $(\mathcal{G}_{\mathsf{inv}}, d_{\mathsf{edit}})$ compact, Hausdorff
  - ✓ $\mathcal{N}_{\mathsf{inv}}^{\otimes}$ subalgebra of $\mathcal{C}(\mathcal{G}_{\mathsf{inv}}, d_{\mathsf{edit}})$
  - $\mathcal{N}_{\mathsf{inv}}^{\otimes}(\rho_{\mathsf{sig}})$ separates points in $\mathcal{C}(\mathcal{G}_{\mathsf{inv}}, d_{\mathsf{edit}})$
- Then $\mathcal{N}_{\mathsf{inv}}^{\otimes}(\rho_{\mathsf{sig}})$ is dense in $\mathcal{C}(\mathcal{G}_{\mathsf{inv}}, d_{\mathsf{edit}})$

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Wrapping up Theorem 1

- So far proved $\mathcal{N}^{\otimes}_{\text{inv}}(\rho_{\text{sig}})$ is dense in $\mathcal{C}(\mathcal{G}_{\text{inv}}, d_{\text{edit}})$
- Can go from $\mathcal{N}^{\otimes}_{\text{inv}}(\rho_{\text{sig}})$ to $\mathcal{N}_{\text{inv}}(\rho)$
- Show $\mathcal{N}_{\text{inv}}(\rho)$ dense in $\mathcal{N}^{\otimes}_{\text{inv}}(\rho_{\text{sig}})$
- Have re-proved results from [2] but without fixing n

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Proof for Equivariant Case

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Equivariance

For isomorphic G_1, G_2, $(G_1 = \sigma \star G_2)$ we have

$$f(G_1) = f(\sigma \star G_2) = \sigma \star f(G_2) \neq f(G_2)$$

Equivariant Case

- Isomorphic graphs aren't equivalent anymore
- So define

$$\mathcal{G}_{\text{eq}} := \left\{ G \in \mathbb{R}^{n^d} ; n \leq n_{\max}, \|G\| \leq R \right\}$$

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- H_s equivariant output operators

Theorem 2

For any $\rho \in \mathcal{F}_{\mathsf{MLP}}, \mathcal{N}_{\mathsf{eq}}(\rho)$ is dense in $\mathcal{C}(\mathcal{G}_{\mathsf{eq}}, d)$

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$\mathcal{C}(\mathcal{G}_{\mathsf{eq}}, d)$ is a particular subset of continuous functions

Classical Stone-Weierstrass theorem doesn't apply!

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Solution

Define specialized version of Stone-Weierstrass theorem for equivariant functions

Stone-Weierstrass for equivariant functions

- Additional condition: self-separability
- $f(G)$ can have different values on different coordinates
- Rest of the proof similar to invariant case

Conclusion

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