Universal Invariant and Equivariant Graph Neural Networks

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This presentation is a review of Keriven & Peyré (2019).

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Overview

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2. Background
3. Results
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The Problem and its Importance

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- Since permutation of nodes doesn't affect graph structure, graph neural networks should be invariant or equivariant.
- Classical universal approximation theorem (Cybenko 1989, Hornik et al. 1989, Pinkus 1999) states that a single layer MLP can approximate any continuous function on a compact set.
- Universality is important because it ensures that a model does not have "gaps" in its learning capabilities.
- Are GNNs still universal under equivariance or invariance?

Prior Work

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- Work on equivariance has mainly been limited to translation as it relates to convolution (Cohen & Welling 2016).
- Many applications demand equivariance, e.g., community detection (Chen et al. 2017), recommender systems (Ying et al. 2018).

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Universality

Definition

Given an activation function $\rho : \mathbb{R} \to \mathbb{R}$, a one-layer MLP is a neural network of the form

$$f : \mathbb{R}^n \to \mathbb{R}, x \mapsto \sum_s c_s \rho(\langle a_s, x \rangle + b_s).$$

The set of such MLPs is denoted $N_{\mathrm{MLP}}(\rho)$.

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The set of such MLPs is denoted $N_{\mathrm{MLP}}(\rho)$.

Theorem (The Universal Approximation Theorem (Pinkus 1999))

For any $\rho \in C[a, b]$ that is not a polynomial, $N_{MLP}(\rho)$ is a dense subspace of $C[a, b]$.

Equivariance/Invariance

Definition

Given a hypergraph $G \in \mathbb{R}^{n^d}$ represented as a tensor and a permutation $\pi \in S_n$, denote by

$$(\pi \cdot G)_{i_1,\ldots,i_d} := G_{\pi^{-1}(i_1),\ldots,\pi^{-1}(i_d)}$$

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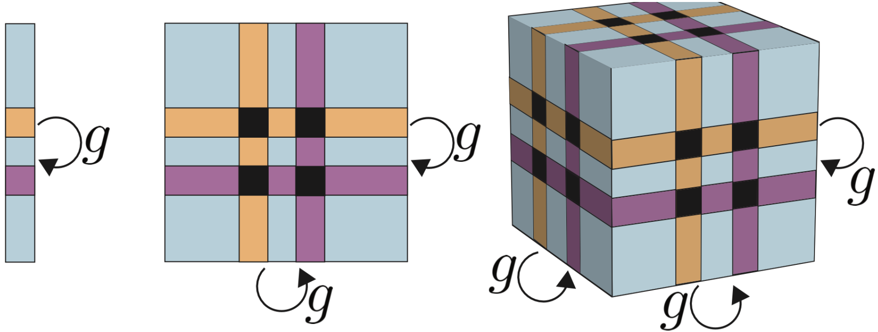
A map $f : \mathbb{R}^{n^k} \to \mathbb{R}^{n^\ell}$ is called equivariant if $f(\pi \cdot G) = \pi \cdot f(G)$ for all π and G.

Equivariant and Invariant GNNs



(Maron et al. 2019)

Equivariant and Invariant GNNs

Definition

A one-layer invariant (equivariant) GNN with activation function $\rho : \mathbb{R} \to \mathbb{R}$ is

$$f : \mathbb{R}^{n^d} \to \mathbb{R}(\mathbb{R}^n), G \mapsto \sum_s H_s(\rho(F_s G + B_s)) + b$$

where each $F_s : \mathbb{R}^{n^d} \to \mathbb{R}^{n^{k_s}}$ is a linear equivariance, each $H_s : \mathbb{R}^{n^{k_s}} \to \mathbb{R}(\mathbb{R}^n)$ is an linear invariance (equivariance), and each bias term satisfies the equivariance relation $B_s = \pi \cdot B_s$. The set of these invariant networks is denoted $N_{\mathrm{inv}}(\rho)$ and the equivariant networks are denoted $N_{\mathrm{eq}}(\rho)$.

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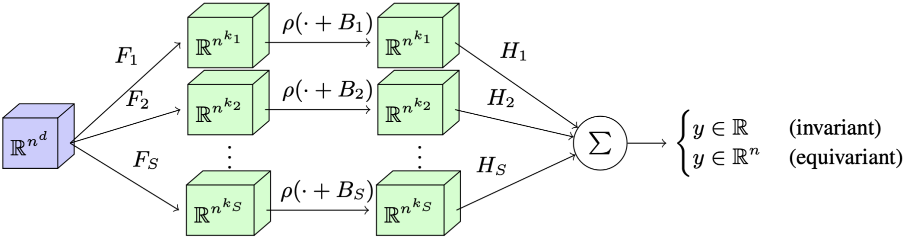

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Universality of Invariant GNNs

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Theorem

Let $\mathcal{G}_{N,R} := \{G \in \mathbb{R}^{n^d} : n \leq N, ||G|| \leq R\}$ and let $C_{inv}(\mathcal{G}_{N,R})$ denote the set of continuous and invariant functions $f : \mathcal{G}_{N,R} \to \mathbb{R}$. Then, for any locally Lipschitz non-polynomial ρ, $N_{inv}(\rho)$ is dense in $C_{inv}(\mathcal{G}_{N,R})$.

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Theorem (Stone–Weierstraß)

Let $\mathcal{X}$ be a compact metric space and let $\mathcal{F}$ be a subalgebra of $C(\mathcal{X})$ that contains at least one non-zero constant function. If $\mathcal{F}$ separates points, i.e. $\forall x \neq y$ there is $f \in \mathcal{F}$ s.t. $f(x) \neq f(y)$, then $\mathcal{F}$ is dense in $C(\mathcal{X})$.

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Note: A subalgebra needs to be closed under pointwise multiplication, addition, as well as scalar multiplication.

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- Next, equip the new space with an appropriate metric d_{edit} based on edit distance.
- Can show $d_{\mathrm{edit}}([G_1],[G_2]) \leq ||G_1 - G_2||_1$, meaning the embedding $G \mapsto [G]$ is continuous and thus no loss of generality working in the new space.

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- That is, if Stone–Weierstraß applies to $N_{\mathrm{inv}}^{\otimes}(\sigma)$, then the theorem is proved for $N_{\mathrm{inv}}(\rho)$.

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- Start by showing that $n = n'$.
- Let $\tau \in \mathbb{R}$ be strictly smaller than all elements in G and G' and consider

$$f_\lambda(G) = \sum_{i_1,\ldots,i_d} \sigma(\lambda(G - \tau))_{i_1,\ldots,i_d} \in N_{\mathrm{inv}}^{\otimes}(\sigma).$$

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- As $\lambda \to \infty$, each $\sigma(\dots)_{i_1,\dots,i_d} \to 1$, so $f_\lambda(G) \to n$ and $f_\lambda(G') \to n'$.
- Remainder of argument is more technically involved but proceeds similarly.

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Theorem

Let $C_{eq}(\mathcal{G}_{N,R})$ denote the set of continuous and equivariant functions $f : \mathcal{G}_{N,R} \to \mathbb{R}^n$. Then, for any locally Lipschitz non-polynomial ρ, $N_{eq}(\rho)$ is dense in $C_{eq}(\mathcal{G}_{N,R})$.

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Ideally, the proof should be analogous to the invariant case.

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- Equivariant functions act differently on members of the same equivalence class.
- Thus unlike in the invariant case, we cannot replace $\mathcal{G}$ by the quotient space $\hat{\mathcal{G}}$.
- Therefore we cannot reduce to Stone–Weierstraß and need a brand new version.

A New Stone–Weierstraß

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- Proving self-separability for $N_{\mathrm{eq}}^{\otimes}(\sigma)$ is similar to separation of points.
- Reduction $N_{\mathrm{eq}}(\rho) \mapsto N_{\mathrm{eq}}(\cos) = N_{\mathrm{eq}}^{\otimes}(\cos) \mapsto N_{\mathrm{eq}}^{\otimes}(\sigma)$ same as before.

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Possible Directions

- Universality of invariant networks is proved constructively in Maron et al. (2019), whereas the Stone–Weierstraß approach is non-constructive. Can we generalize to the equivariant case by an explicit constructive method?

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- Universality of invariant networks is proved constructively in Maron et al. (2019), whereas the Stone–Weierstraß approach is non-constructive. Can we generalize to the equivariant case by an explicit constructive method?
- Can we apply the new Stone–Weierstraß tool to more general settings? In particular, can we show universality for equivariant neural networks operating on dynamic graphs where the structure evolves over time?

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Chen, Z., Li, X. & Bruna, J. (2017), 'Supervised community detection with line graph neural networks', *arXiv preprint arXiv:1705.08415* .

Cohen, T. & Welling, M. (2016), Group equivariant convolutional networks, *in* 'International conference on machine learning', PMLR, pp. 2990–2999.

Cybenko, G. (1989), 'Approximation by superpositions of a sigmoidal function', *Mathematics of control, signals and systems* **2**(4), 303–314.

Hornik, K., Stinchcombe, M. & White, H. (1989), 'Multilayer feedforward networks are universal approximators', *Neural networks* **2**(5), 359–366.

Keriven, N. & Peyré, G. (2019), 'Universal invariant and equivariant graph neural networks', *Advances in Neural Information Processing Systems* **32**.

Maron, H., Fetaya, E., Segol, N. & Lipman, Y. (2019), On the universality of invariant networks, *in* 'International conference on machine learning', PMLR, pp. 4363–4371.

References II

Pinkus, A. (1999), 'Approximation theory of the mlp model in neural networks', *Acta numerica* **8**, 143–195.

Yarotsky, D. (2022), 'Universal approximations of invariant maps by neural networks', *Constructive Approximation* **55**(1), 407–474.

Ying, R., He, R., Chen, K., Eksombatchai, P., Hamilton, W. L. & Leskovec, J. (2018), Graph convolutional neural networks for web-scale recommender systems, *in* 'Proceedings of the 24th ACM SIGKDD international conference on knowledge discovery & data mining', pp. 974–983.

Zaheer, M., Kottur, S., Ravanbakhsh, S., Poczos, B., Salakhutdinov, R. R. & Smola, A. J. (2017), 'Deep sets', *Advances in neural information processing systems* **30**.

Thank You

Thank you :)