Universal Invariant and Equivariant Graph Neural Networks

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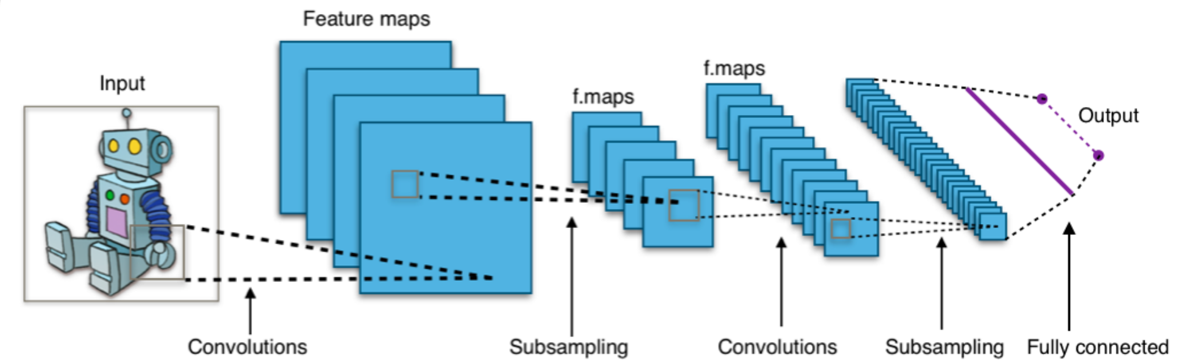
GdR Isis, 2019 Oct. 17th

Deep NN



« Alternate linearities and non-linearities »

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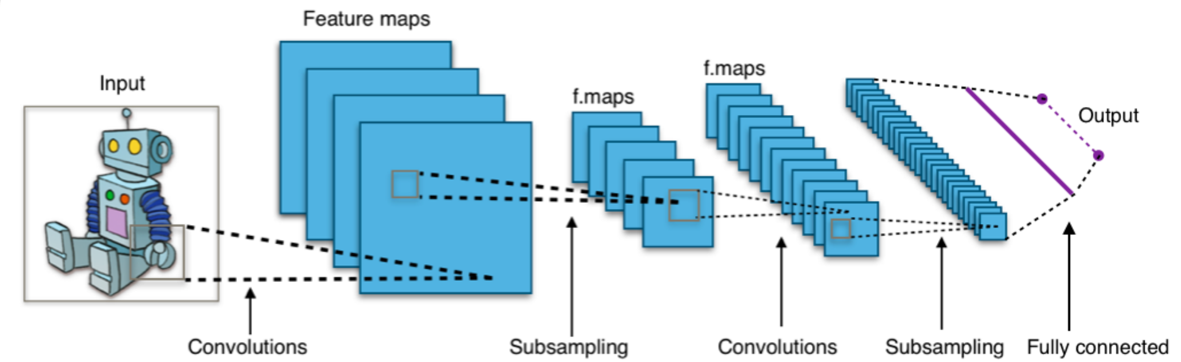

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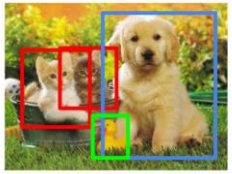
State-of-the-art in: **most everything ?** *(with sufficient data and domain knowledge…)*

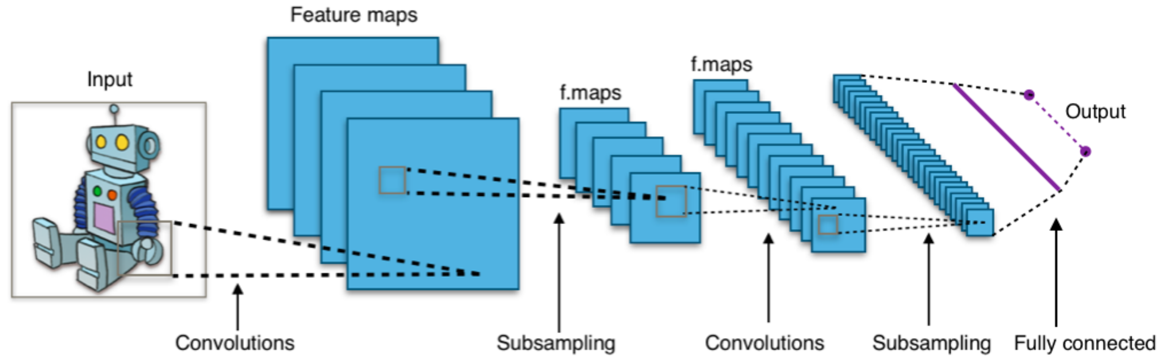
- Computer vision
- Speech recognition
- Natural Language Processing (NLP)
- Recommender systems
- Reinforcement learning (sequential learning)
- Etc etc etc.



CAT, DOG, DUCK

Many specialized *architectures for each application*

Deep NN



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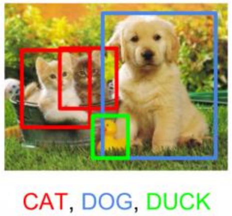

***Many specialized** architectures for each application*

Theory ?

- Approximation theory
  - **Universal Approximation Theorem** *[Hornik 1989, Cybenko 1989, Pinkus 1999…]*
  - Approximation rate / smoothness space *[Cohen, Kutyniok, Gribonval…]*
- Generalisation / Sample complexity *[Barnett, Arora, Neyshabur…]*
- Optimisation / Regularization *[Du, Lee, Bach, Jordan, Montanari…]*

Graph NN

Adapting DNN to graph inputs…

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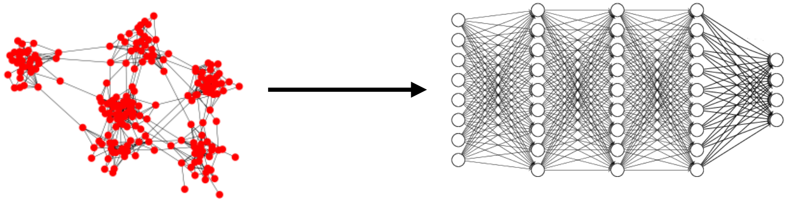

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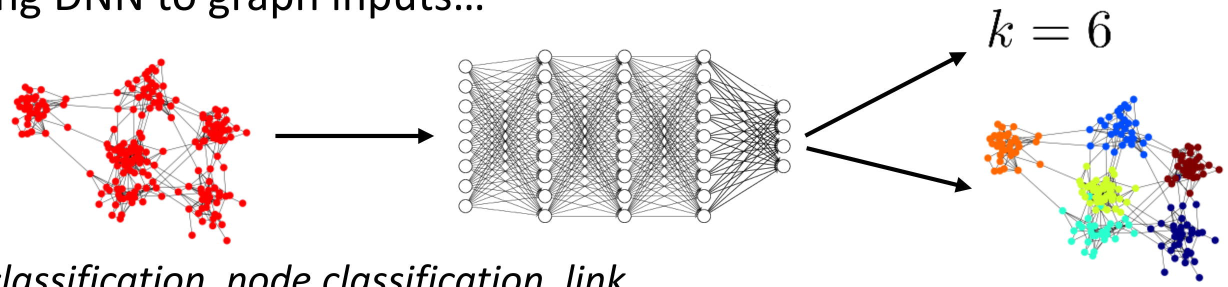

Graph classification, node classification, link prediction…

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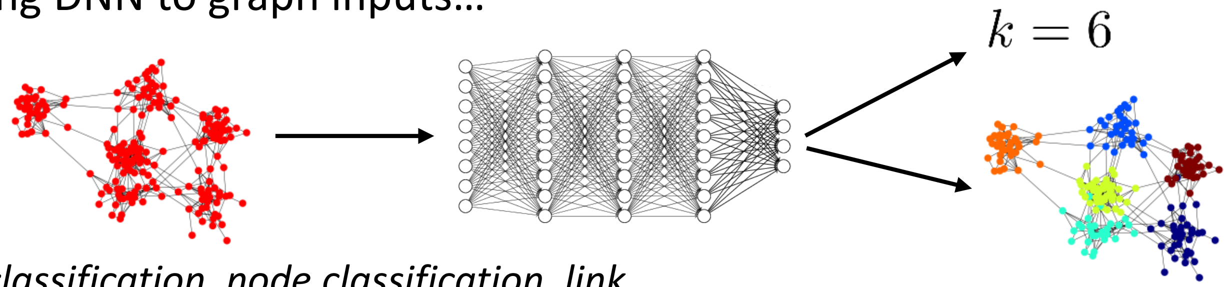

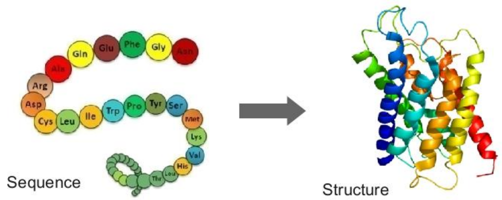

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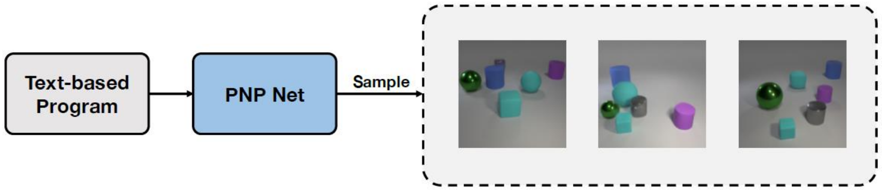

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- **NLP**: text classification (semantic graph)
- **Chemistry**: infer molecular properties, protein structure, *synthetize* new compound…

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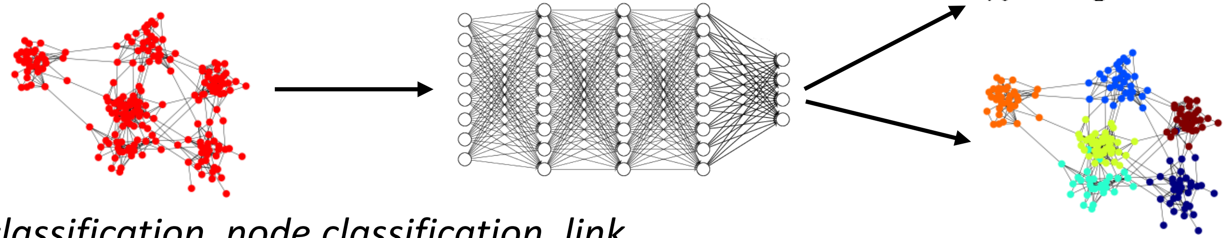

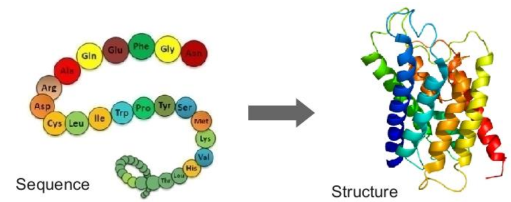

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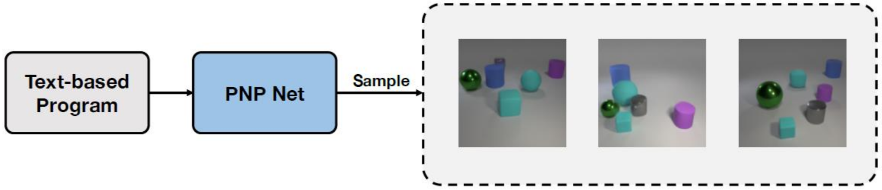

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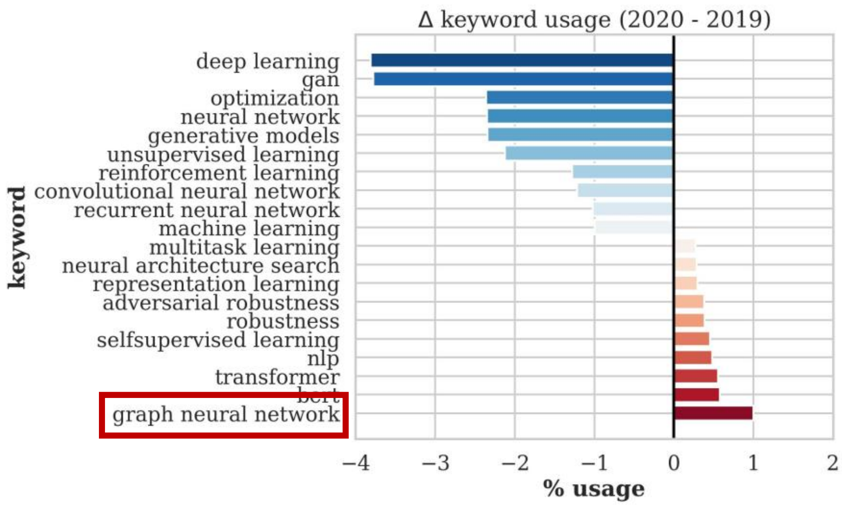

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Theory ? Most of it missing…

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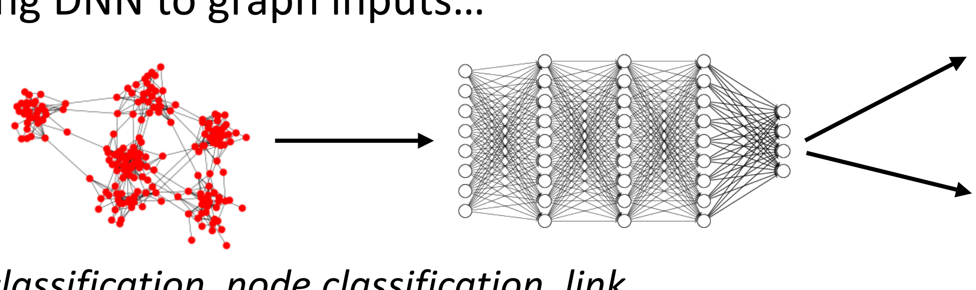

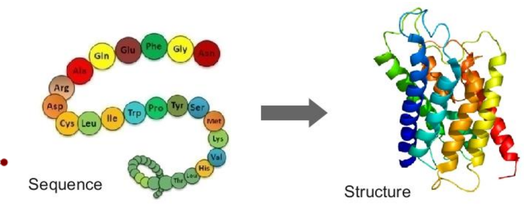

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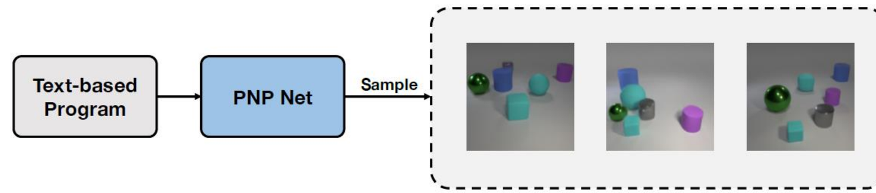

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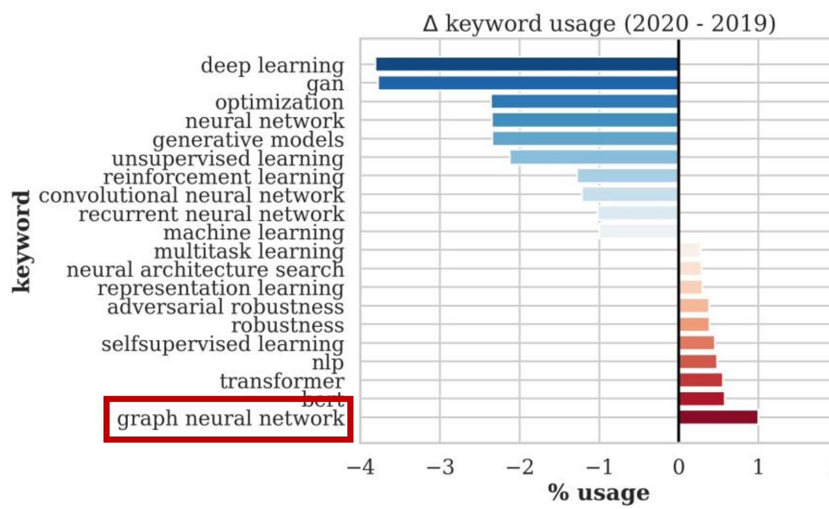

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*In this talk: **Universal Approximation Theorem***

A zoology of Graph NN

- **Convolutional GNN** : takes inspiration from ***Convolutional*** *NN*

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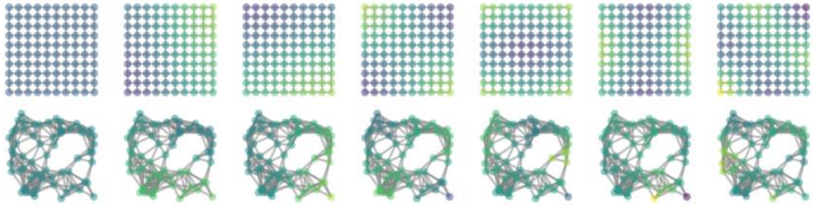
    - **Spectral** : convolution in Fourier domain (successive filtering using graph Laplacian)
    - **Spatial** : « convolution » in graph domain



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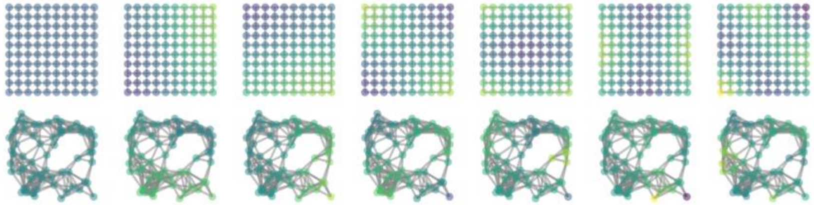

- **Recursive GNN** : defined as equilibrium state (inspired by physics, message-passing algorithms…)
- **Dynamic GNN** : temporal graphs, use random walks…
- **Graph Auto Encoders** : graph embedding, graph generation…

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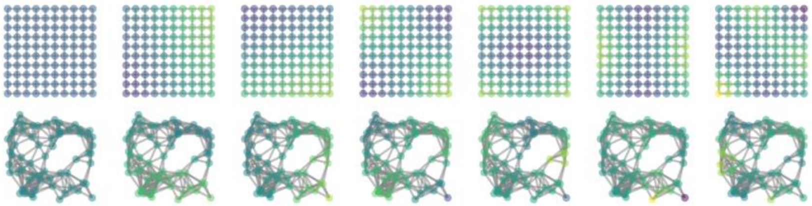

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Review papers :

- *Bronstein et al (2017) : Geometric Deep Learning: Going beyond Euclidean data*
- *Hamilton et al (2017) : Representation learning on graphs: Methods and applications*
- *Wu et al (2019) : A Comprehensive Survey on Graph Neural Networks*

A simple architecture: Invariant and Equivariant layers

Input

Weight matrix $W \in \mathbb{R}^{n \times n}$

Multi-graph $W \in \mathbb{R}^{n^\ell}$

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For $\sigma \in \Sigma_n$, denote $\sigma \star W$ perm. of nodes

Ex: $P_\sigma W P_\sigma^\top$ for $\ell = 2$

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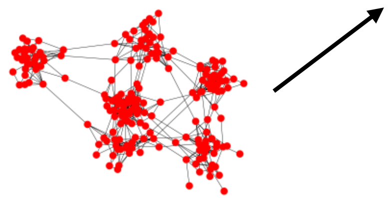

$k = 6$

Invariant

$f(\sigma \star W) = f(W)$

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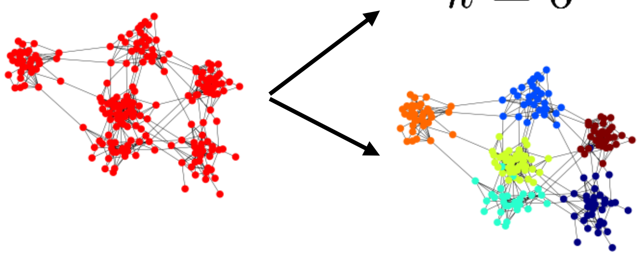

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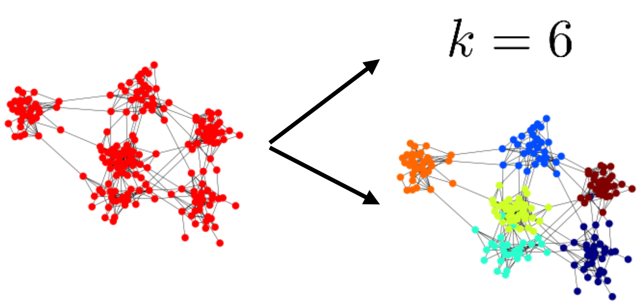

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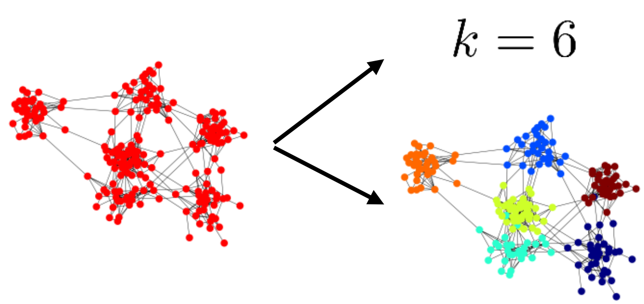

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Thm *(Maron et al. 2018)*:

Bell number

There is a basis of $b(k+\ell)$ possible **equivariant** linear operators $F : \mathbb{R}^{n^k} \to \mathbb{R}^{n^\ell}$

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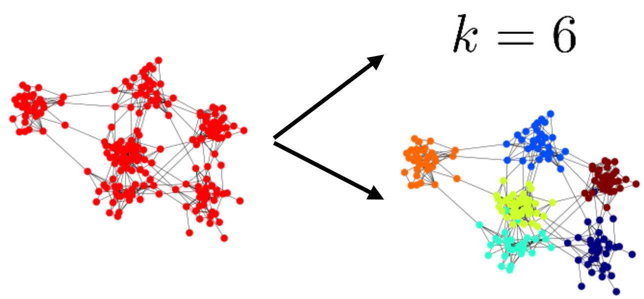

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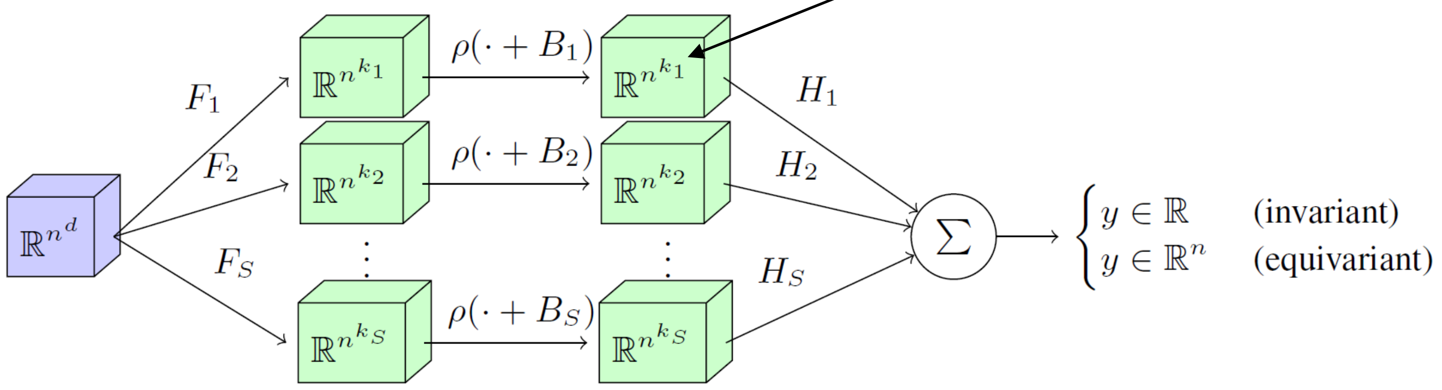
Does not depend on n !! *Ex: there are only 15 equivariant linear operators* $\mathbb{R}^{n \times n} \to \mathbb{R}^{n \times n}$

Universality for Invariant NN

One-layer: $f(W) = \sum_s H_s \rho(F_s W + B_s)$

Can increase the order of the tensor !



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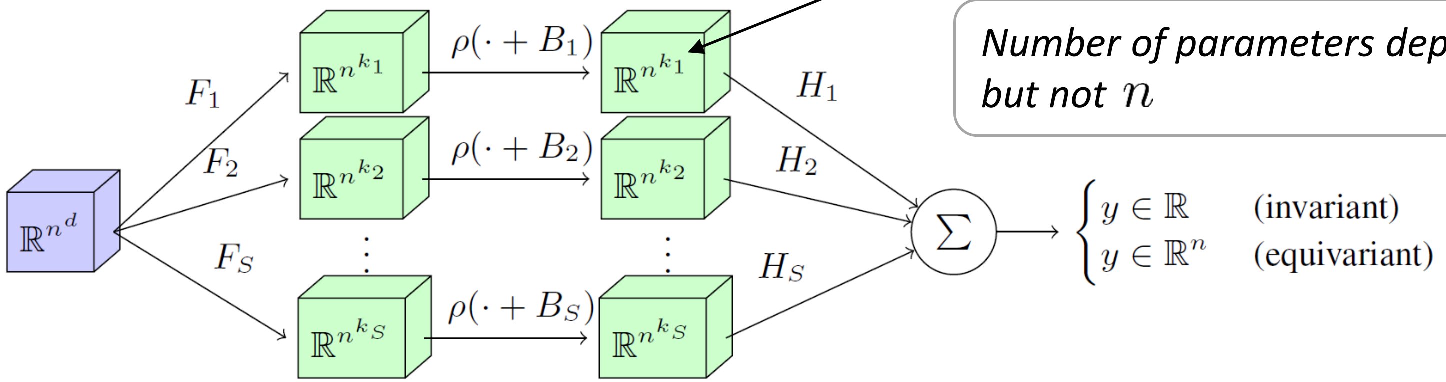

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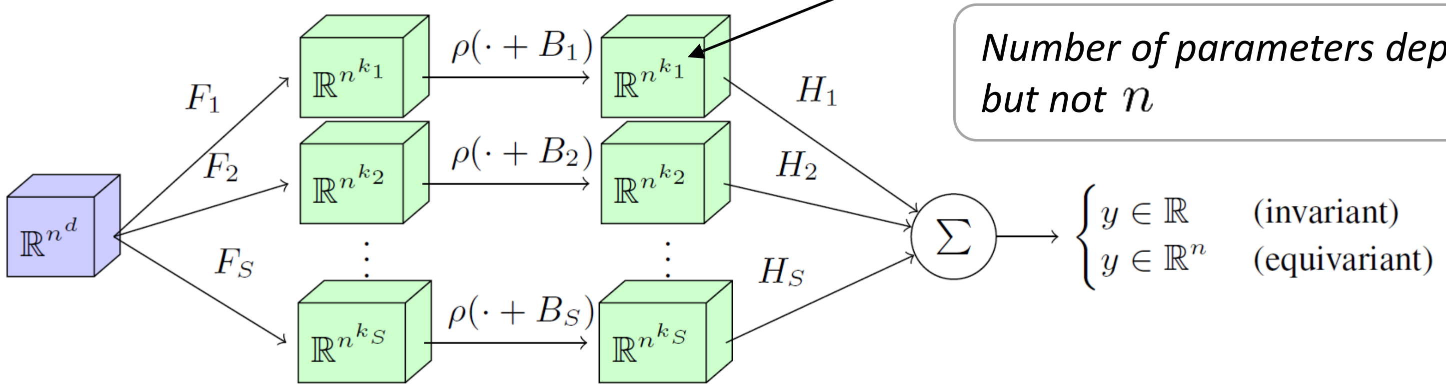

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When $S, k_s \to \infty$, can approximate **any continuous invariant function**.

Proof: uses invariant polynomials, density of polynomials, and classical universality theorem.

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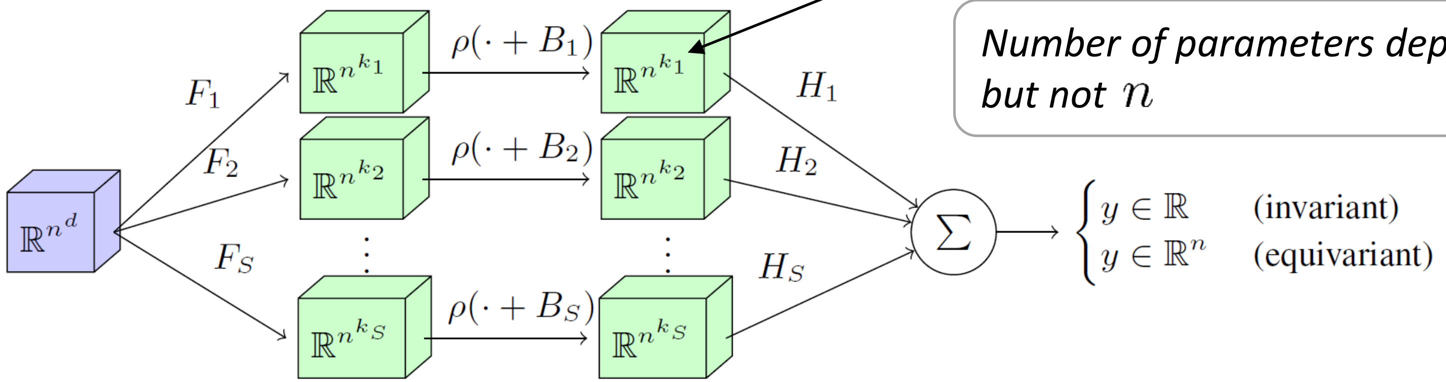

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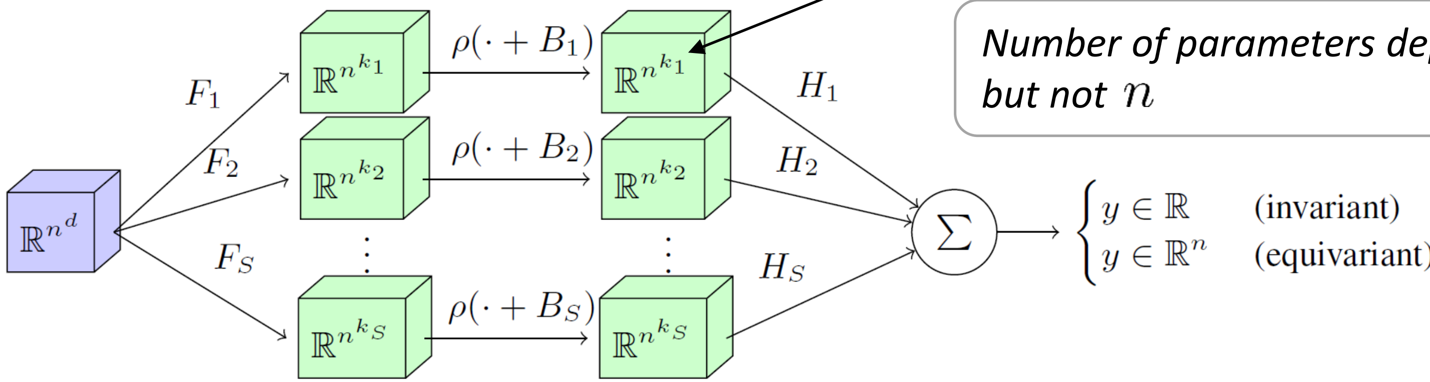

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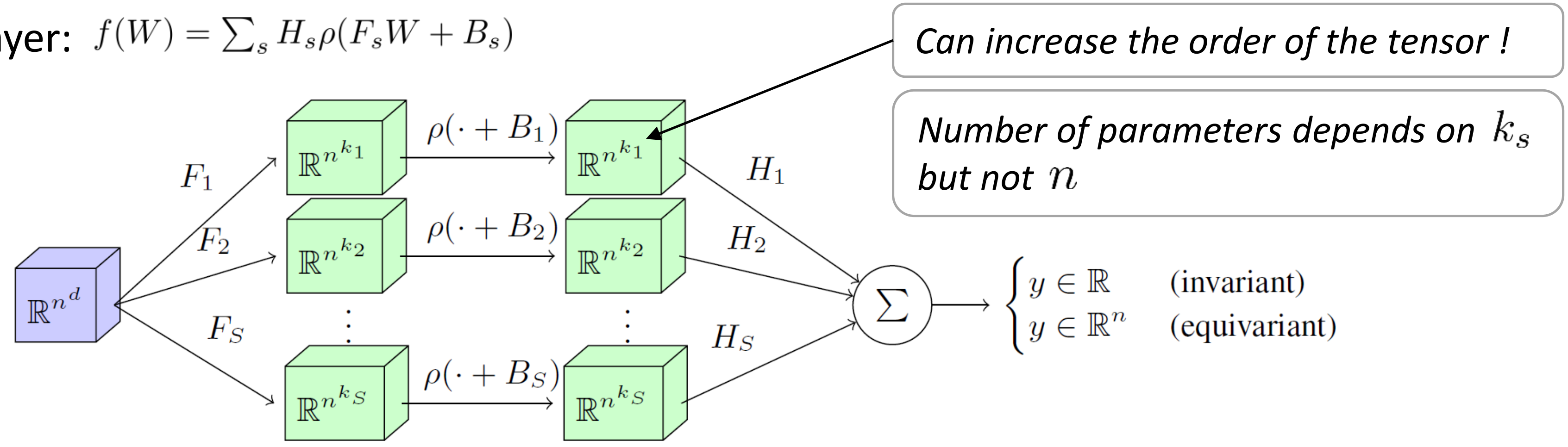

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- Alternative proof based on Stone-Weierstrass (SW) theorem.

- With a ***single set of parameters***, can approximate a function defined on **graphs of varying size** $n \leq n_{\max}$ *(continuous for the edit distance)*

Our proof : SW theorem for graphs

Apply Stone-Weierstrass theorem in the space of graphs quotiented by permutations.

Thm *(Stone-Weierstrass)*

On a compact space, an **algebra** of continuous real-valued functions that **separates points** is dense in the space of continuous functions.

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Hard ! *(core of the proof)*

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Main contribution:

Thm *(Keriven, Peyré 2019):*

One layer **equivariant** GNNs $\mathbb{R}^{n^d} \to \mathbb{R}^n$ are dense in the space of **continuous equivariant functions**.

(defined on graphs of varying size $n \leq n_{\max}$ *)*

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Thm (SW for equivariant functions)
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An **algebra of equivariant functions** (for coordinate-wise product) that **separates points** and **separates coordinates** is dense in the space of equivariant continuous functions.

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Universality for Equivariant NN

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Thm *(Keriven, Peyré 2019):*

One layer **equivariant** GNNs $\mathbb{R}^{n^d} \to \mathbb{R}^n$ are dense in the space of **continuous equivariant functions.**

(defined on graphs of varying size $n \leq n_{\max}$ *)*

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- Not valid for **output** $\mathbb{R}^{n^k}$
- Not valid for subgroups of Σ_n

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Conclusion

Summary

- Defined a class of Universal Invariant and Equivariant GNNs
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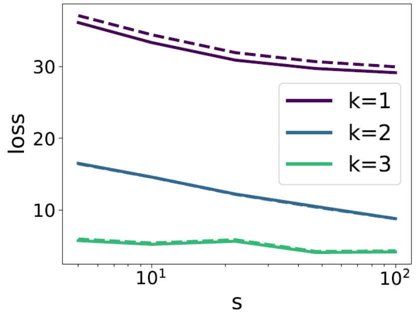

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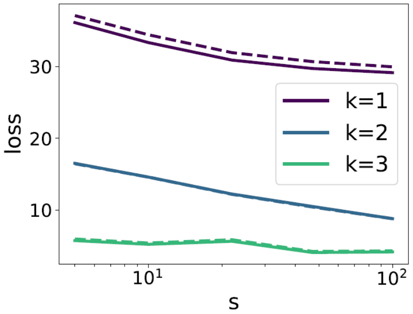

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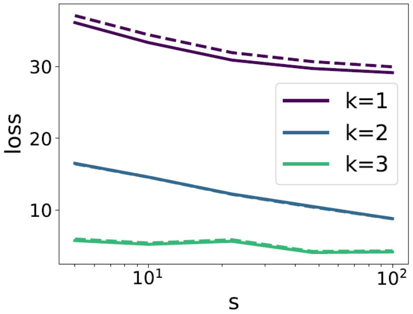

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Take-home msg: GNNs are still in their infancy, both theoretically and in practice. Scalability and stability remain challenging. Many opportunities !

Thank you !

Keriven, Peyré. **Universal Invariant and Equivariant Graph Neural Networks**
NeurIPS 2019, arxiv:1905.04943

More at *nkeriven.github.io*