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D-INFK

Natural Graph Networks

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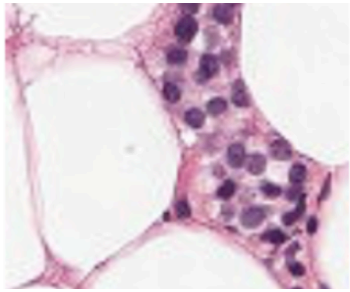
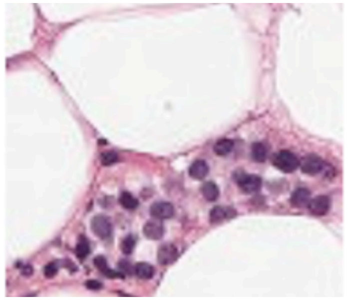
Motivation
How powerful are GNNs?

What is Invariance?

$f($  $)$ → Pathological

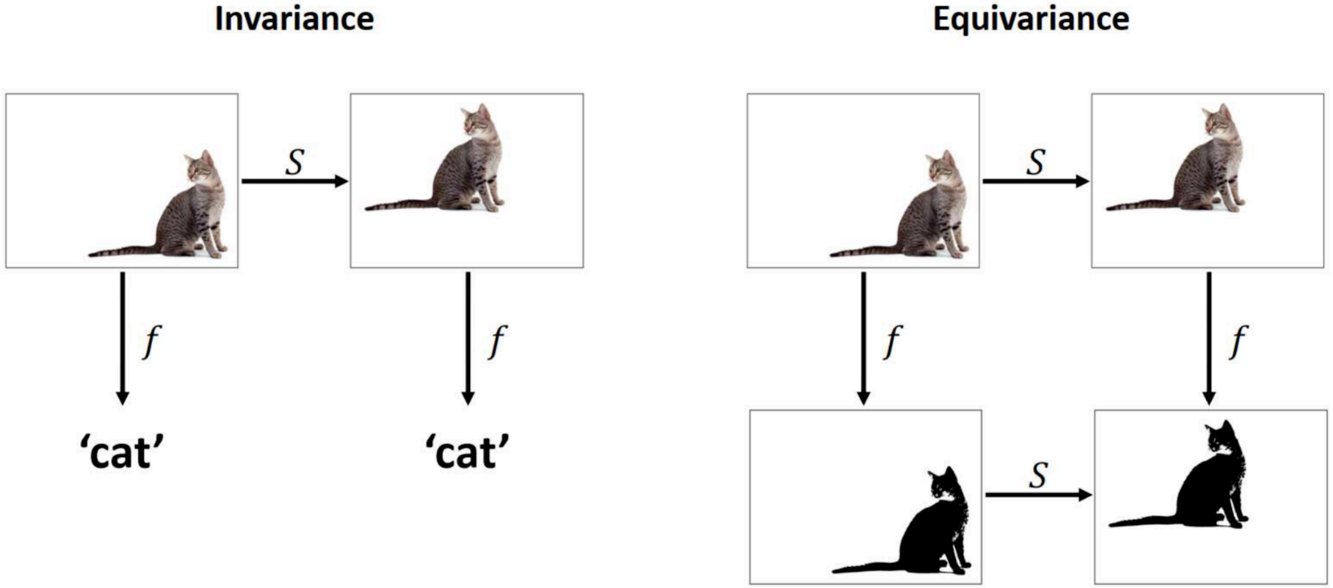
$f($  $)$ → Pathological

For any symmetry operation $S: \; f(x) = f \circ S(x)$

The Picasso problem

Invariance is too restrictive!

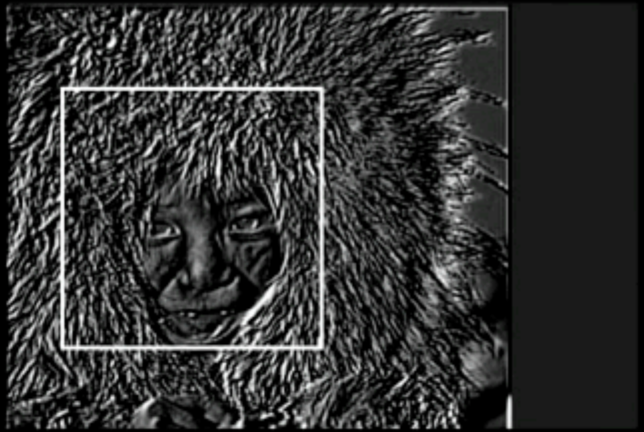
Invariance vs Equivariance



- Invariance $\longrightarrow$ the output stays constant no matter how the input is transformed
    - $f(x) = f \circ S(x)$
- Equivariance $\longrightarrow$ the output undergoes the exact same transformation as the input
    - $S \circ f(x) = f \circ S(x)$

Existing CNNs: Translation Equivariance

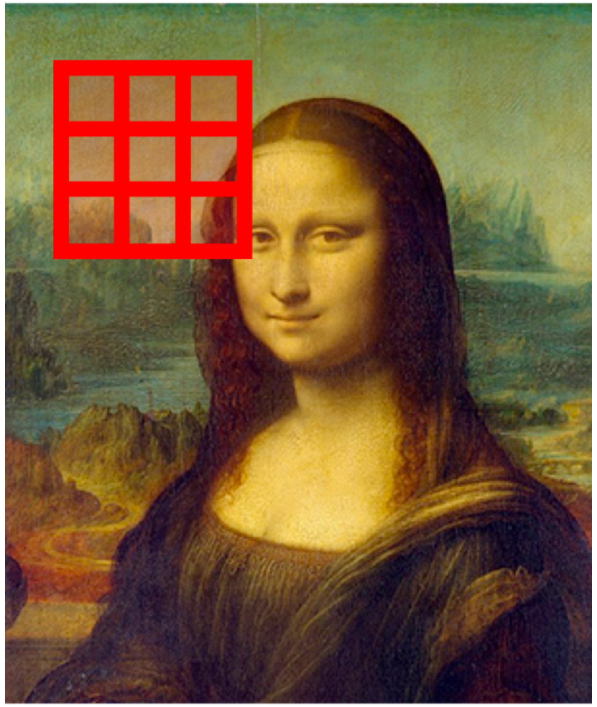
Input

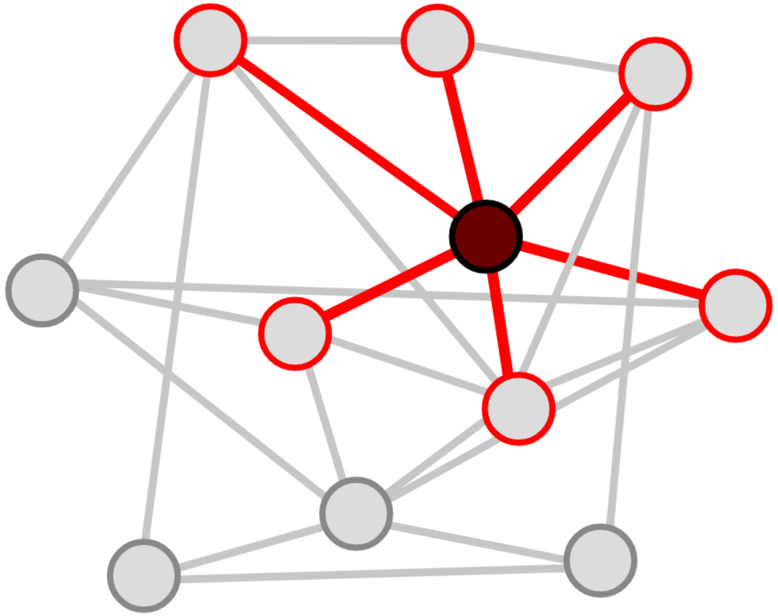


Features

Windowed view

Images vs Graphs



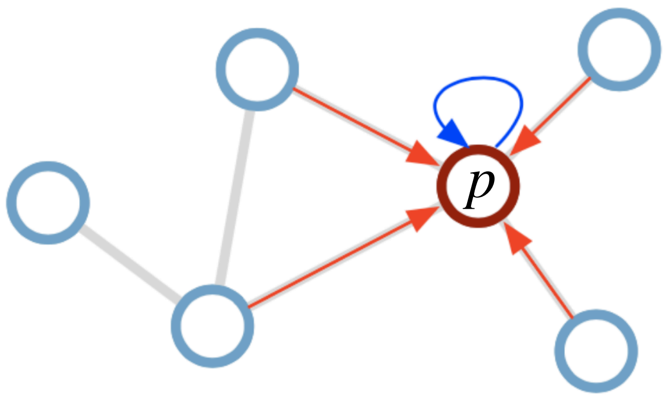


- Constant number of neighbours
- Fixed ordering of neighbours
- Traslation invariance

- Different number of neighbours
- No ordering of neighbours
- Permutation invariance

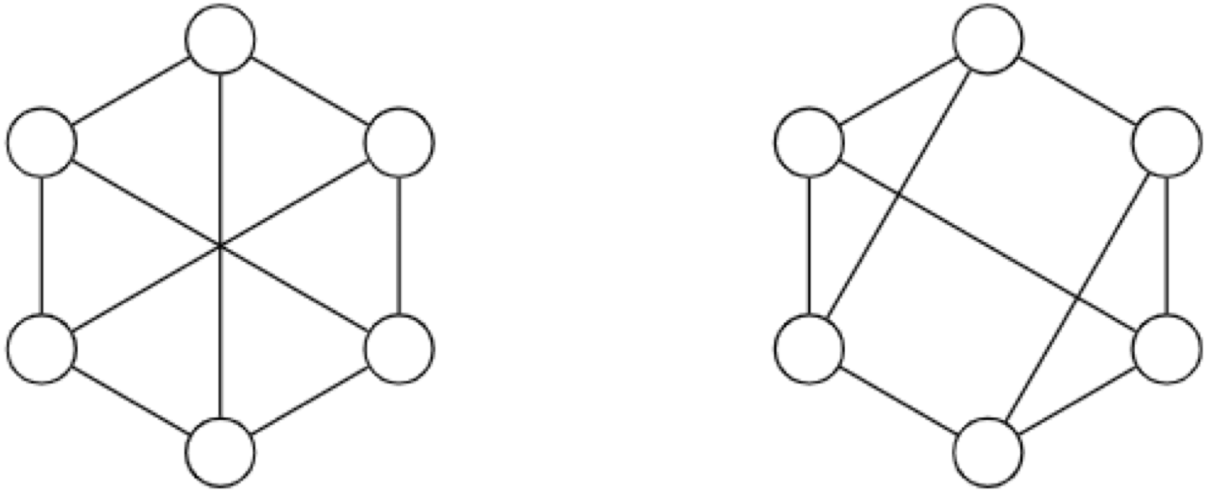
Local Invariant Graph Networks (LIGNs)

$$K(v_p) = \sum_{(p,q)\in E} W \cdot v_q$$



- $K(v_p)$ is invariant under a permutation of its neighbours
- W is a single matrix used on each edge of any graph

Limitations of LIGNs

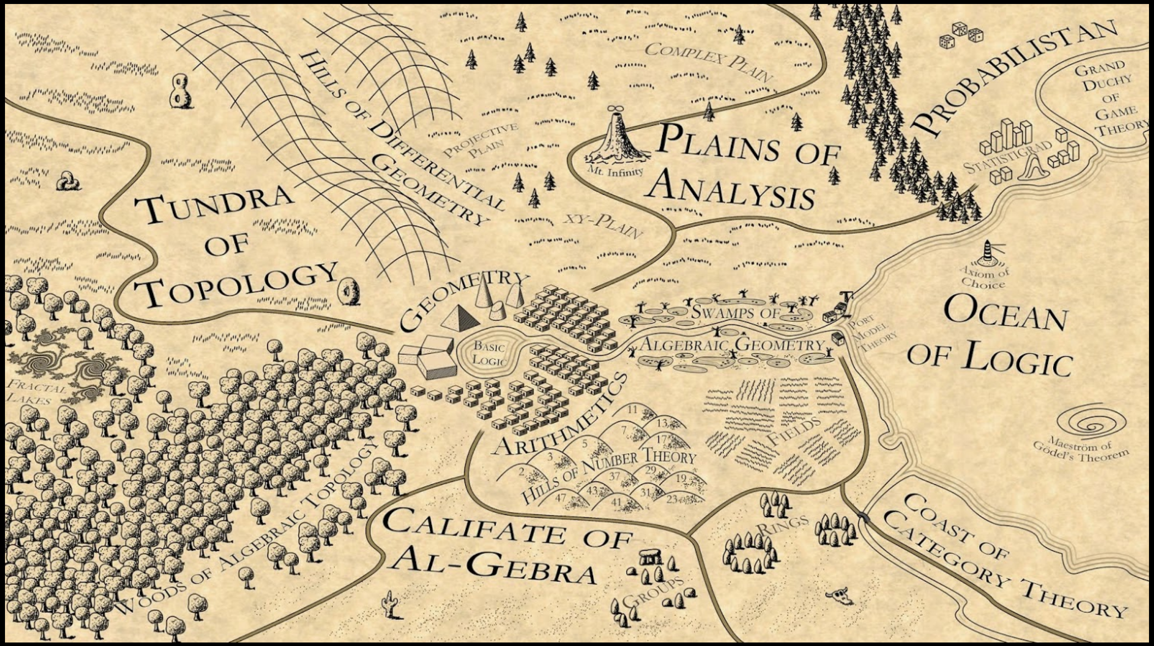


Local invariant graph networks cannot discriminate between these two graphs!

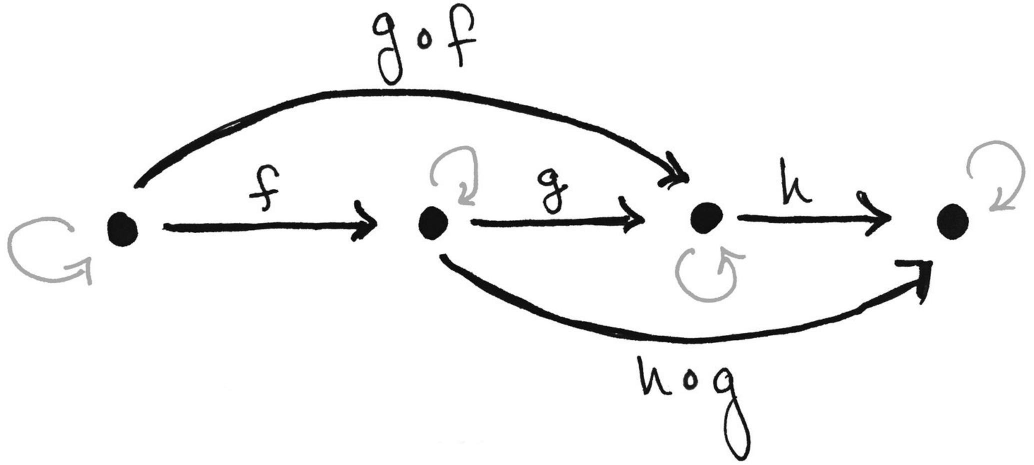
The question arises..

Can we design maximally expressive graph networks that are <u>equivariant</u> to node permutations?

Introduction to Category Theory

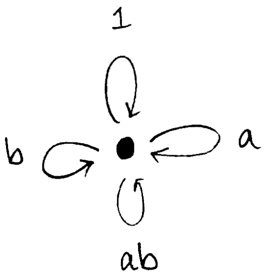


What is a Category?

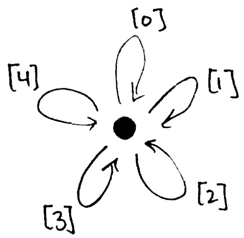


- A category $\mathbf{C}$ consists of three elements:
  - A collection $Ob(\mathbf{C})$ of objects
  - A set of morphisms $\mathbf{C}(c, d)$ for every pair of objects $(c, d) \in Ob(\mathbf{C})$
  - A composition rule: whenever the codomain of one morphism matches the domain of another, there is a morphism that is their composition, i.e. given $x \xrightarrow{f} y$ and $y \xrightarrow{g} z$ there is a morphism $x \xrightarrow{g \circ f} z$
- That satisfy the following properties:
  - Each object $x \in Ob(\mathbf{C})$ has an identity morphism $x \xrightarrow{id_x} x$
  - The composition is associative $(h \circ g) \circ f = h \circ (g \circ f)$ whenever $x \xrightarrow{f} y \xrightarrow{g} z \xrightarrow{h} w$

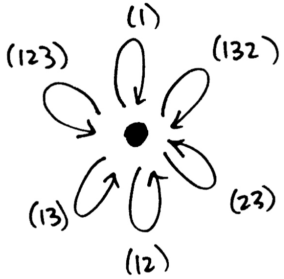
Every group G can be viewed as a category



BK_4



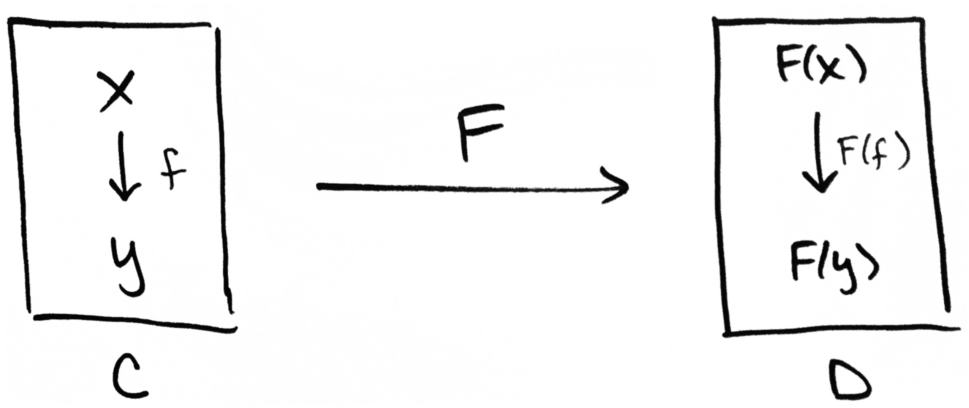
$B\mathbb{Z}_5$



BS_3

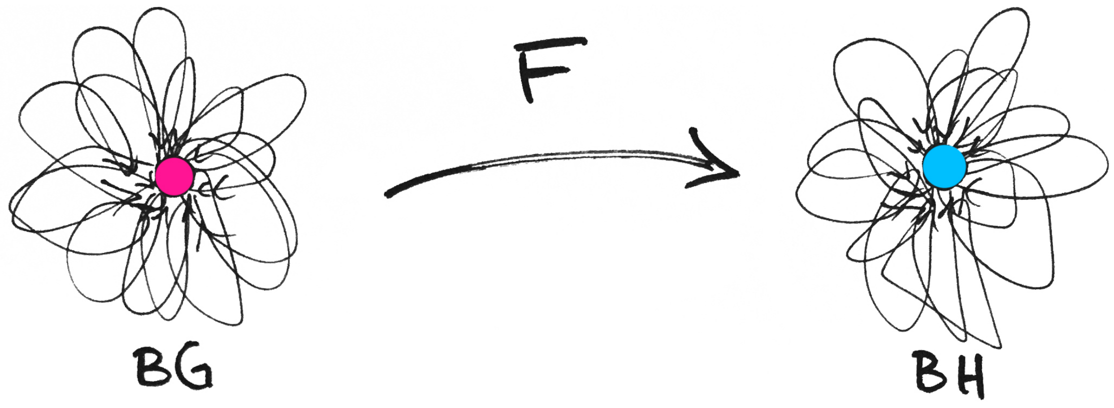
- A single object denoted by $\bullet$
- A morphism $\bullet \xrightarrow{g} \bullet$ for each element $g \in G$
- Composition holds since G is closed under the group operation
- The group identity $e \in G$ serves as the identity morphism for $\bullet$
- Associativity holds because the group operation is associative

What is a Functor?



- A functor $F : \mathbf{C} \to \mathbf{D}$ consists of:
  - An object $F(x) \in Ob(\mathbf{D})$ for every object $x \in Ob(\mathbf{C})$
  - A morphism $F(x) \xrightarrow{F(f)} F(y)$ for every morphism $x \xrightarrow{f} y$
- That satisfy the following properties:
  - F respects composition, i.e. $F(g \circ f) = F(g) \circ F(f)$
  - F sends identities to identities, i.e. $F(id_x) = id_{F(x)}$

A Functor between groups



- $F : BG \longrightarrow BH$
- It sends the single object 🟣 of BG to the single object 🔵 of BH
- It sends any morphism 🟣 $\xrightarrow{g}$ 🟣 to a morphism 🔵 $\xrightarrow{F(g)}$ 🔵
  - In particular, the identity of BG is sent to the identity of BH
- It is precisely a group homomorphism from group G to group H!

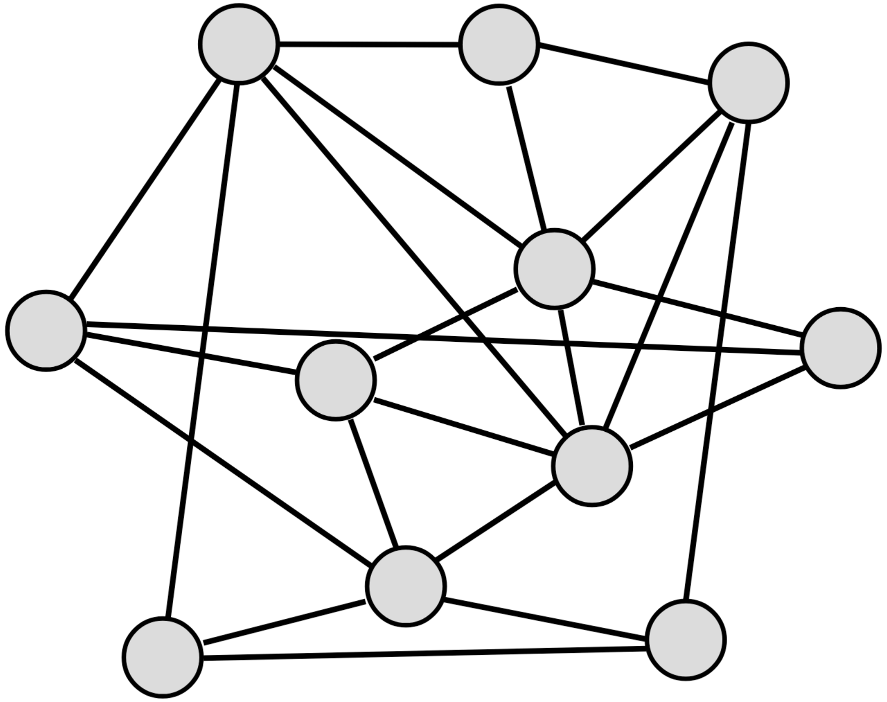
What is a Natural Transformation?

- Given two functors F and $G : \mathbf{C} \to \mathbf{D}$, from natural transformation $\eta : F \implies G$ consists of:
  - A morphism $F(x) \xrightarrow{\eta_x} G(x)$ for each object in category $\mathbf{C}$
  - η is the totality of all morphisms: $\eta = (\eta_x)_{x \in Ob(\mathbf{C})}$
- That satisfies the following property:
  - Whenever $x \xrightarrow{f} y$ is a morphism in $\mathbf{C}$:
    - $G(f) \circ \eta_x = \eta_y \circ F(f)$

$$
\begin{tikzcd}
F(x) \arrow[r, "\eta_x"] \arrow[d, "F(f)"'] & G(x) \arrow[d, "G(f)"] \\
F(y) \arrow[r, "\eta_y"'] & G(y)
\end{tikzcd}
$$

Global Natural Networks

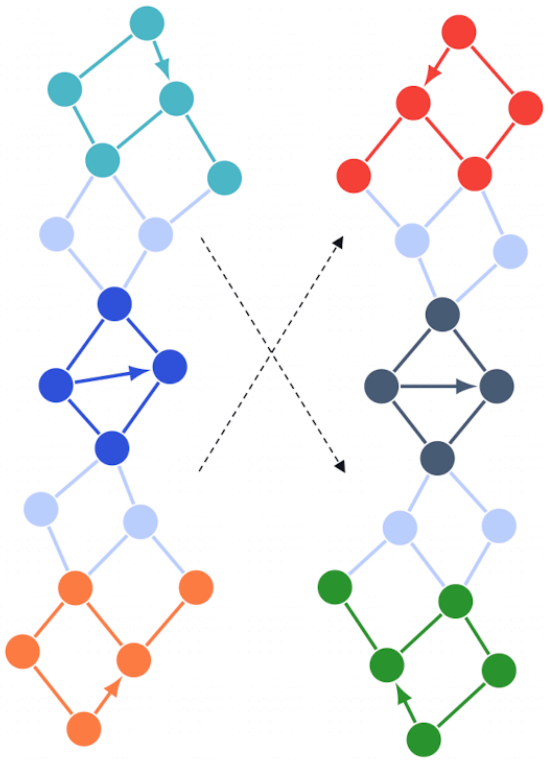
Graphs



- A finite set of nodes: $V = \{1, \ldots, n\}$
- A set of edges: $E = \{(i, j) : i, j \in V\}$

Graph Isomorphisms

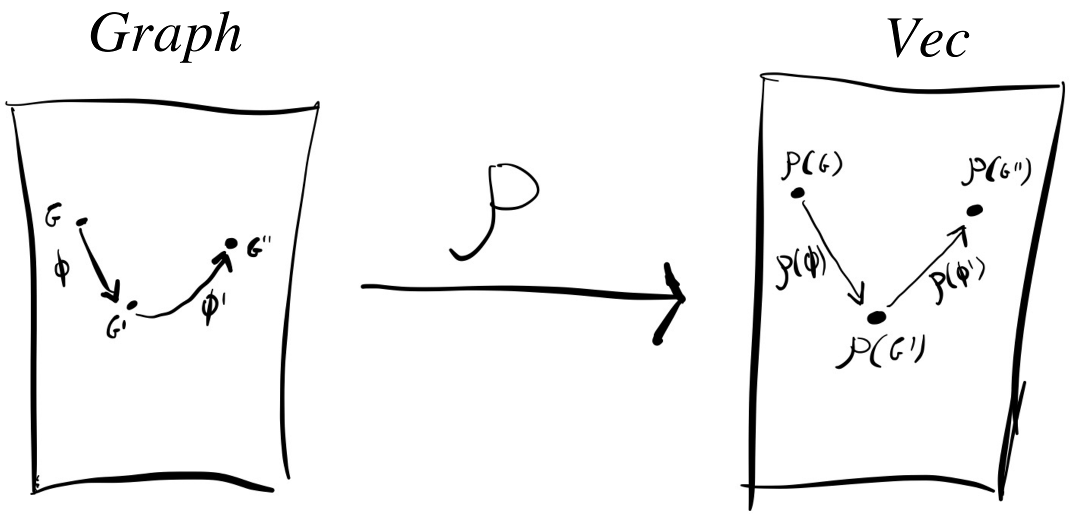
- An isomorphism $\phi : G \to G'$ is a mapping $\phi : V(G) \to V(G')$ that satisfies:
  - $(i, j) \in E(G) \iff (\phi(i), \phi(j)) \in E(G')$
  - Preserves edges!
- An isomorphism from a graph to itself: automorphism or symmetry!



Graph feature space ρ

- Associates:
  - To each graph G a vector space $V_G = \rho(G)$
  - To each graph isomorphism $\phi : G \to G'$ an invertible linear map $\rho(\phi) : V_G \to V_{G'}$
- Such that composition is preserved:
  - $\rho(\phi \circ \phi') = \rho(\phi) \circ \rho(\phi')$

The graph feature space is a functor: $\rho : Graph \longrightarrow Vec$



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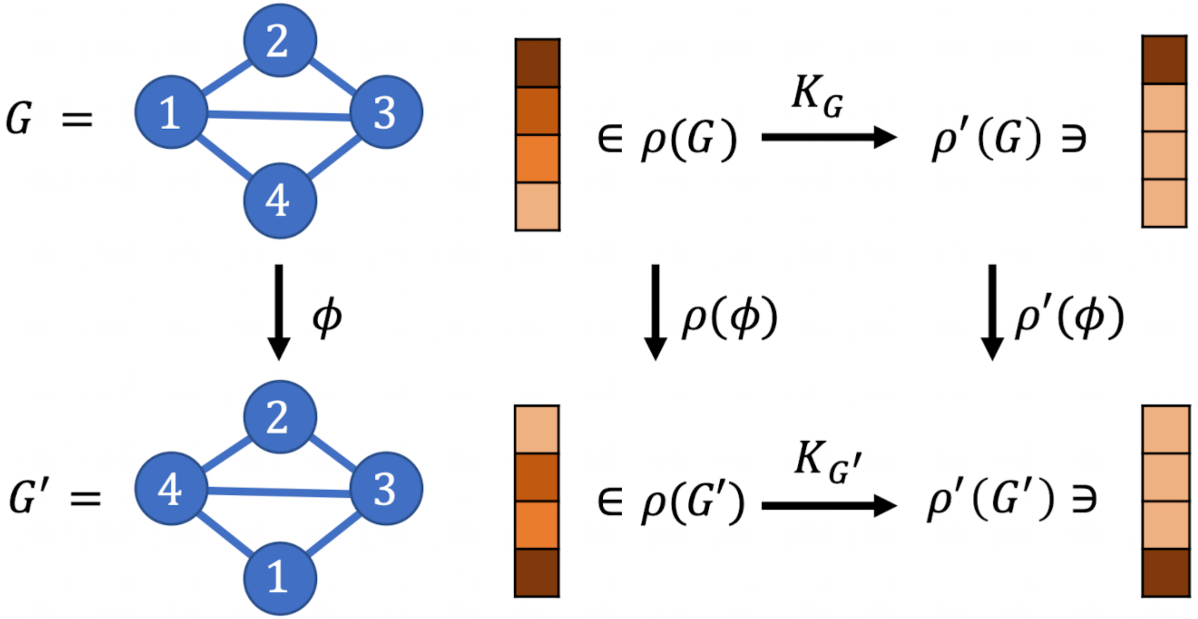
Global Natural Network Layer

- Given two graph feature spaces $\rho, \rho' : Graph \to Vec$
- The GNN layer is a natural transformation between these two functors
  - Consisting of a different map K_G for each graph G

$$\boxed{K : \rho \implies \rho'}$$

$$\begin{tikzcd} \rho(G) \arrow[r, "K_G"] \arrow[d, "\rho(\phi)"] & \rho'(G) \arrow[d, "\rho'(\phi)"] \\ \rho(G') \arrow[r, "K_{G'}"] & \rho'(G') \end{tikzcd}$$

Global Natural Network Layer



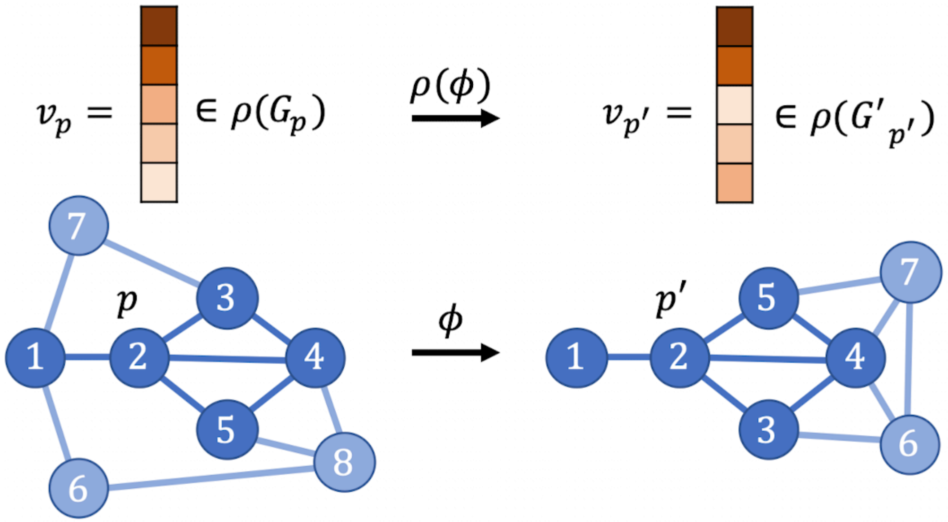
- $\rho(G) = \rho(G') = \mathbb{R}^4$
- $\rho'(\phi) \circ K_G = K_{G'} \circ \rho(\phi) \implies K_{G'} = \rho'(\phi) \circ K_G \circ \rho(\phi)^{-1} \implies$ weight sharing for isomorphisms
- $\rho'(\phi) \circ K_G = K_G \circ \rho(\phi) \implies$ linear constraint for automorphisms

Limitations of Global Natural Networks

Global computations on entire graph is intractable!

Local Natural Networks

Category of node neighbourhoods



- Define a category $\mathbf{C}$ of node neighbourhood:
  - $Ob(\mathbf{C}) = V$
  - For each node $p \in V$ associate a neighbourhood G_p
  - Morphisms of this category are isomorphisms between node neighbourhoods

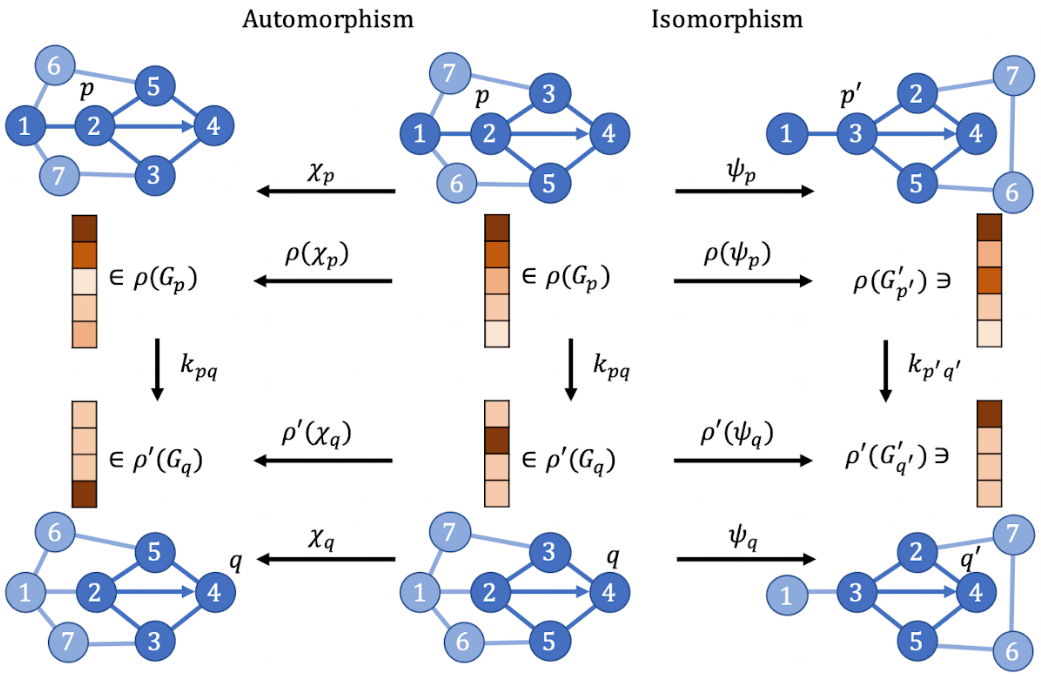
The local feature space $\rho : \mathbf{C} \longrightarrow Vec$ is a functor

Local Natural Network Layer

- Given two graph feature spaces $\rho, \rho' : \mathbf{C} \to Vec$
- The LNN layer is a natural transformation between
  - $\rho, \rho' : \mathbf{C} \to Vec$
  - Consisting of a different map for each node neighbourhood G_p
    - $k_p : \rho(G_p) \to \rho'(G_p)$

$$\rho \Longrightarrow \rho'$$

Local Natural Network Layer



Conclusions

- Invariance limits expressivity
- Equivariance let us learn a broader class of functions

- Treating the graph as a monolithic structure leads to intractable computations
- Restriction to the graph local structure solves the issue

Category theory paves the way towards a mathematical formulation of neural networks

Thank you for your attention!