Qualcomm

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From Equivariance to Naturality

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Why Equivariance?

- Symmetry transformations relate “equivalent” descriptions of an object
- Equivariant maps respect symmetries, i.e. process equivalent inputs in essentially the same way
  - Fundamental idea of GDL
    - Bronstein, Bruna, Cohen, Velickovic, *Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges*, 2021
- Symmetry groups have some particular properties:
  - Invertibility: no information is lost; transformations can be undone
  - Composability: *any* two symmetry transformations can be composed
- In many cases we may want to loosen these assumptions
  - → This leads us to Categories, Functors, and Natural Transformations
  - → Generalizations of Groups, Representations, and Equivariant Maps
  - → Potential for less restricted network architectures & new application areas

“This may be regarded as a continuation of the Klein Erlanger Program, in the sense that a geometrical space with its group of transformations is generalized to a category with its algebra of mappings.”

S. Eilenberg & S. Mac Lane *A General Theory of Natural Equivalences* (1945, first paper on categories)

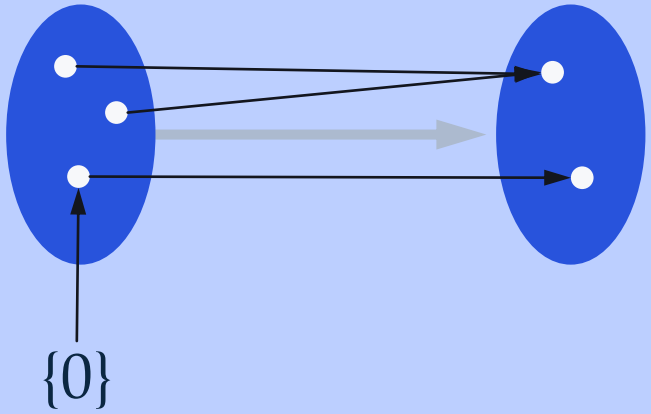
First example: the category of sets & mappings

- Categories consist of objects and arrows / maps / morphisms
- Arrows f : A → B with appropriate domain/codomain can be composed

The category only encodes how maps compose; doesn't care what objects/maps are "made of"

Set

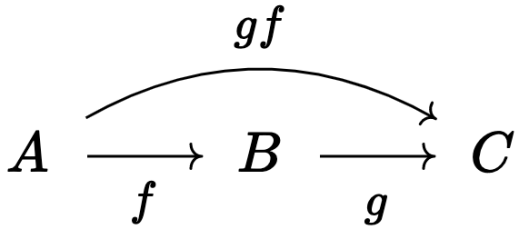
Ob(Set) = "all sets"
Hom(Set) = "all functions"



Lawvere, *Sets for Mathematics*

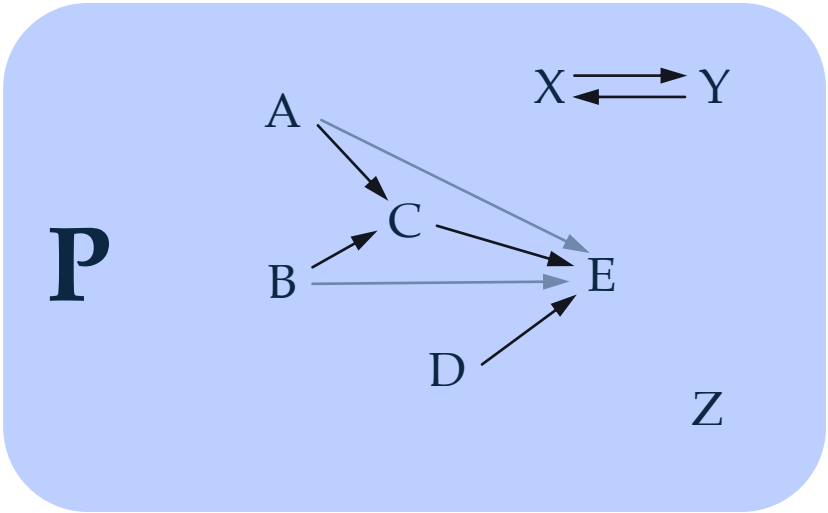
General Definition of Category

- A Category $\mathbb{C}$ consists of Objects and Arrows, such that:
  - For any object A there is an identity map $id_A : A \to A$
  - For any two arrows $f : A \to B$ and $g : B \to C$, there is a composite arrow $g\,f : A \to C$
    - A is called the domain of f, and B the codomain
  - Such that id acts as a unit: $f\,id_A = id_B\,f = f$ (for all f)
  - Composition is associative: $(f\,g)\,h = f\,(g\,h)$



- Examples:
  - Categories of mathematical gadgets: Set, Vect, Top, Grp
  - Mathematical gadgets as categories: Groups, Groupoids, Preorders,
  - Applied category theory: Resource theories, Markov Categories, Bayes Nets, Causal Theories, Monoidal Categories, Chemical Reaction Networks, …

Example: Preorders as Categories



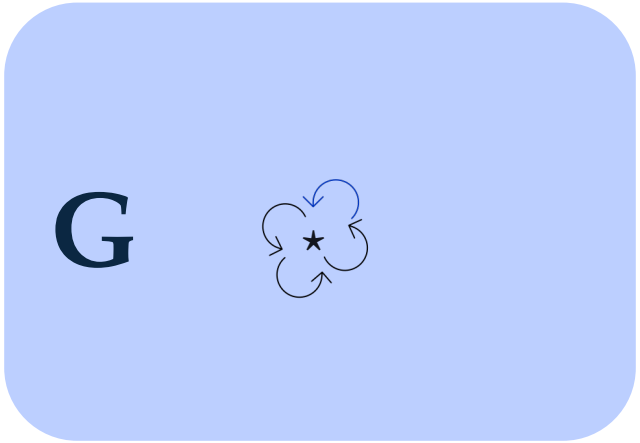
- Gadget as a category
- Classical definition: a relation A ≤ B that is:
  - Reflexive: A ≤ A
  - Transitive: A ≤ B and B ≤ C then A ≤ C
    - (Not necessarily antisymmetric as in a partial order; A ≤ B and B ≤ A then not necessarily A = B)
- Examples:
  - Reachability in graphs, ordering of numbers, ordering of subsets, …
- Categorical definition: a category with at most one arrow from any A to any B
  - Interpretation: we have A ≤ B if and only if there is an arrow A → B
  - ✅ Reflexive: in any category we have an identity arrow A → A
  - ✅ Transitive: the composition operation takes arrows A → B and B → C and produces an arrow A → C
    - Since a preorder category has at most one arrow A → C there is nothing to choose

Example: Groups as Categories

- Isomorphism: a map f : A → B in a category is called an isomorphism if there exists g : B → A s.t.

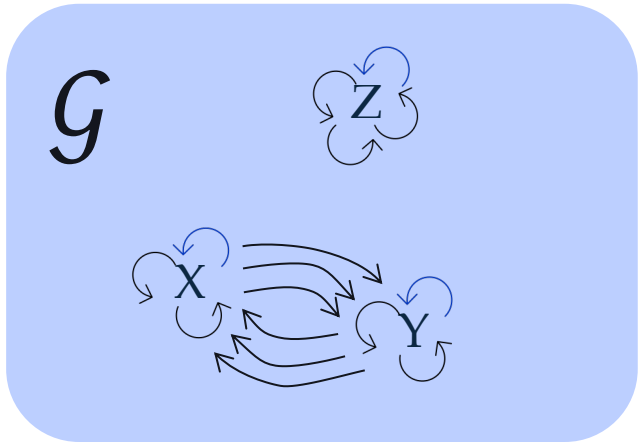
$$g\ f = id_A \quad \text{and} \quad f\ g = id_B$$

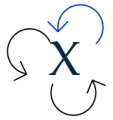
- Classical definition: a set with an associative binary relation, identity maps, and inverses (…)
- Categorical definition: a category with one object $\star$, where each morphism $g: \star \to \star$ is an isomorphism
  - ✅ All arows $g: \star \to \star$ and $\mathrm{h}: \star \to \star$ can be composed and composition is associative
  - ✅ G has an identity $\mathrm{id}_\star: \star \to \star$
  - ✅ Since all arrows are iso, we have inverses



Groupoids

- A Groupoid $\mathcal{G}$ is a category where every morphism is an isomorphism
  - A group is a groupoid with one object
- Example: the category of graphs, restricted to only contain graph isomorphisms
- A groupoid has two kinds of maps: general isomorphisms A → B and automorphisms A → A
- Automorphisms are symmetries. The automorphisms of an object X form a group
- Isomorphism classes are connected by isomorphisms: $\{\{X, Y\}, \{Z\}\}$



$Aut_{\mathcal{G}}(X) =$ 

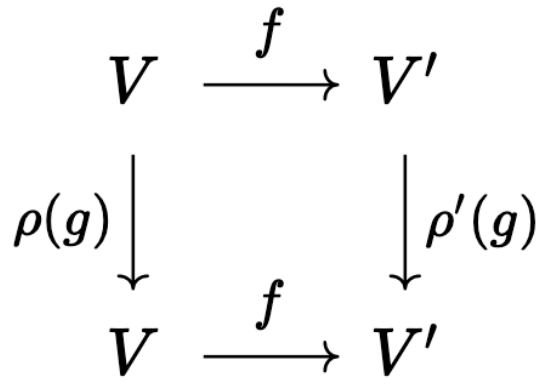
Group Actions & Representations as Functors

- A group action F of a group G on a set X,
  - Has for each element $g \in G$, a bijection $F(g): X \to X$
  - Respecting group multiplication: $F(g\ g') = F(g) \circ F(g')$
- A group representation ρ of a group G is a linear action on a vector space V
- A functor $F: C \to D$ between categories is:
  - A mapping on objects $F: Ob(C) \to Ob(D)$
  - A mapping on morphisms that takes $f: A \to B \in C$ to $F(f): F(A) \to F(B) \in D$
  - Such that $F(\mathrm{id}_X) = \mathrm{id}_{F(X)}, \mathrm{F}(f \circ g) = F(f) \circ F(g)$
- Examples:
  - A functor between groups is a group homomorphism
  - A functor between preorders is a monotone map
  - A group action is a functor $\rho: G \to Set, \quad \rho(\star) = X, \ \rho(g): X \to X$
  - A group representation is a functor $\rho: G \to Vec, \ \rho(\star) = V, \ \rho(g): V \to V$

Equivariant Maps as Natural Transformations

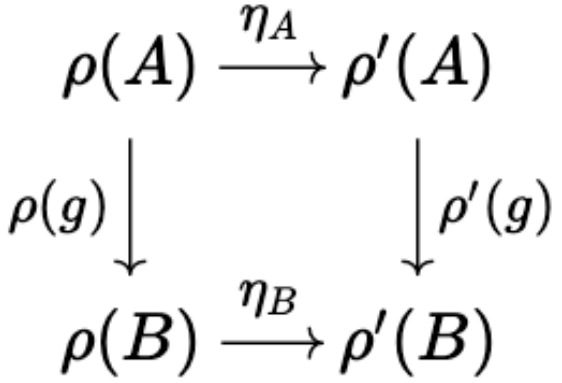
- An equivariant linear map $f: V \to V'$ between group representations $(\rho, V), (\rho', V')$ is a map satisfying for each $g \in G$:

$$f \circ \rho(g) = \rho'(g) \circ f$$



- A Natural Transformation η between Functors $\rho, \rho': C \to D$
  - Written $\eta: \rho \Rightarrow \rho'$
  - For each *object* A of C, a mapping $\eta_A: \rho(A) \to \rho'(A)$ such that for every *arrow* $g : A \to B$ in C:

$$\eta_B \circ \rho(g) = \rho'(g) \circ \eta_A$$



- Hence, an equivariant map is a natural transformation between functors $\rho, \rho': G \to Vec$:
  - For the one and only object $\star$, $\rho(\star) = V, \rho'(\star) = V'$
  - Single linear mapping $f = \eta_\star: \rho(\star) \to \rho'(\star)$, such that tor every $g: \star \to \star$ in G:

Natural Graph Networks

Team

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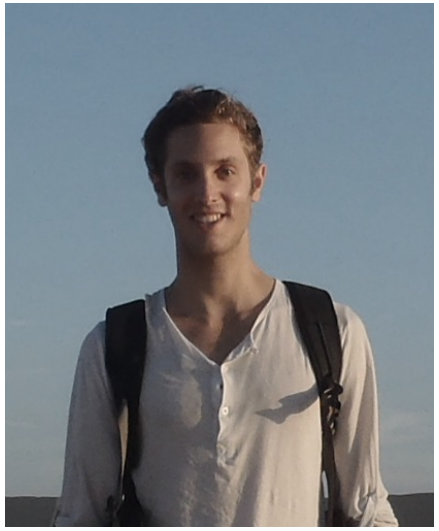

Taco Cohen
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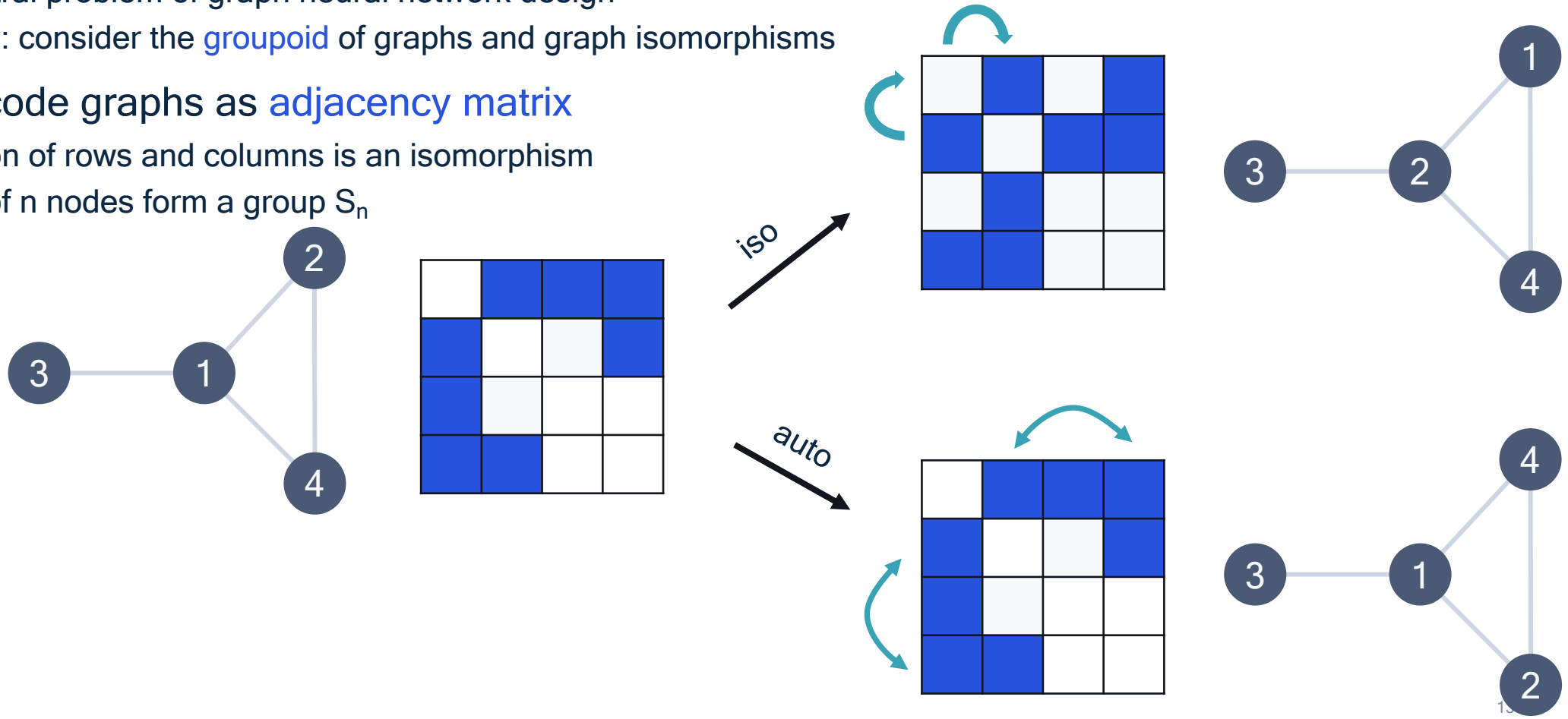
https://arxiv.org/abs/2007.08349

Graph Iso- and automorphisms

- There are many ways to encode the same graph!
  - All of these should be treated in an equivalent manner by the neural network
  - This is the central problem of graph neural network design
  - Mathematically: consider the groupoid of graphs and graph isomorphisms
- Example: encode graphs as adjacency matrix
  - Any permutation of rows and columns is an isomorphism
  - Permutations of n nodes form a group S_n



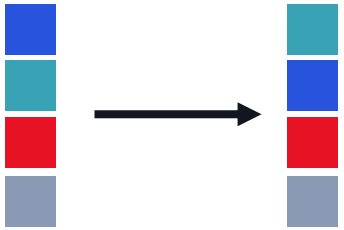
Graph Features

Group / groupoid representations

- Graph feature == representation of S_n
  - S_n is the group of permutations of n nodes

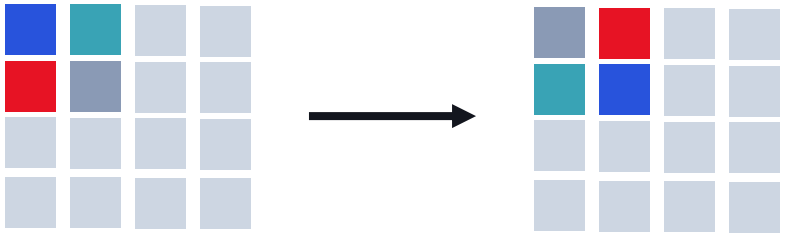
$$\rho_0(P_{12})s = 1 \cdot s$$

Scalar feature
e.g network output in graph classification



$$\rho_1(P_{12})v = P_{12}v$$

Vector feature
e.g. one feature per node



$$\rho_2(P_{12})M = P_{12}MP_{12}^T$$

Tensor feature
e.g. one feature per edge or node pair

Equivariant Graph Networks

- Common approach[1,2,3]: interpret adjacency matrix as a 2nd order graph feature, stack with other features along channel dim, and use this as input to the network:

$$\Phi([G, f]) = f'$$

- Network should be equivariant:

$$\Phi(\rho_{\text{in}}(P)[G, f]) = \rho_{\text{out}}(P)\Phi([G, f])$$

- For linear maps:
  - Order 1 -> 0 (Invariant Deep Sets): 1 parameter
  - Order 1 -> 1 (Equivariant Deep Sets): 2 parameters
  - Order 2 -> 2 (PPGN [1]): 15 parameters
- Not a lot of parameters!

[1] Provably Powerful Graph Networks, Haggai Maron*, Heli Ben-Hamu*, Hadar Serviansky*, Yaron Lipman (*equal contribution), *NeurIPS 2019*
[2] Invariant and Equivariant Graph Networks, Haggai Maron, Heli Ben-Hamu, Nadav Shamir and Yaron Lipman, *ICLR 2019*
[3] Incidence Networks for Geometric Deep Learning, Albooyeh, Marjan, Bertolini, Daniele, and *Ravanbakhsh, ICML 2020*

Natural Graph Networks: global version

- Groupoid $Graph$

- Groupoid representation $\rho: Graph \to Vec$, e.g.
  - Node feature $\rho(G) = \mathbb{R}^n$,
  - Permutation $\rho(g): \mathbb{R}^n \to \mathbb{R}^n$

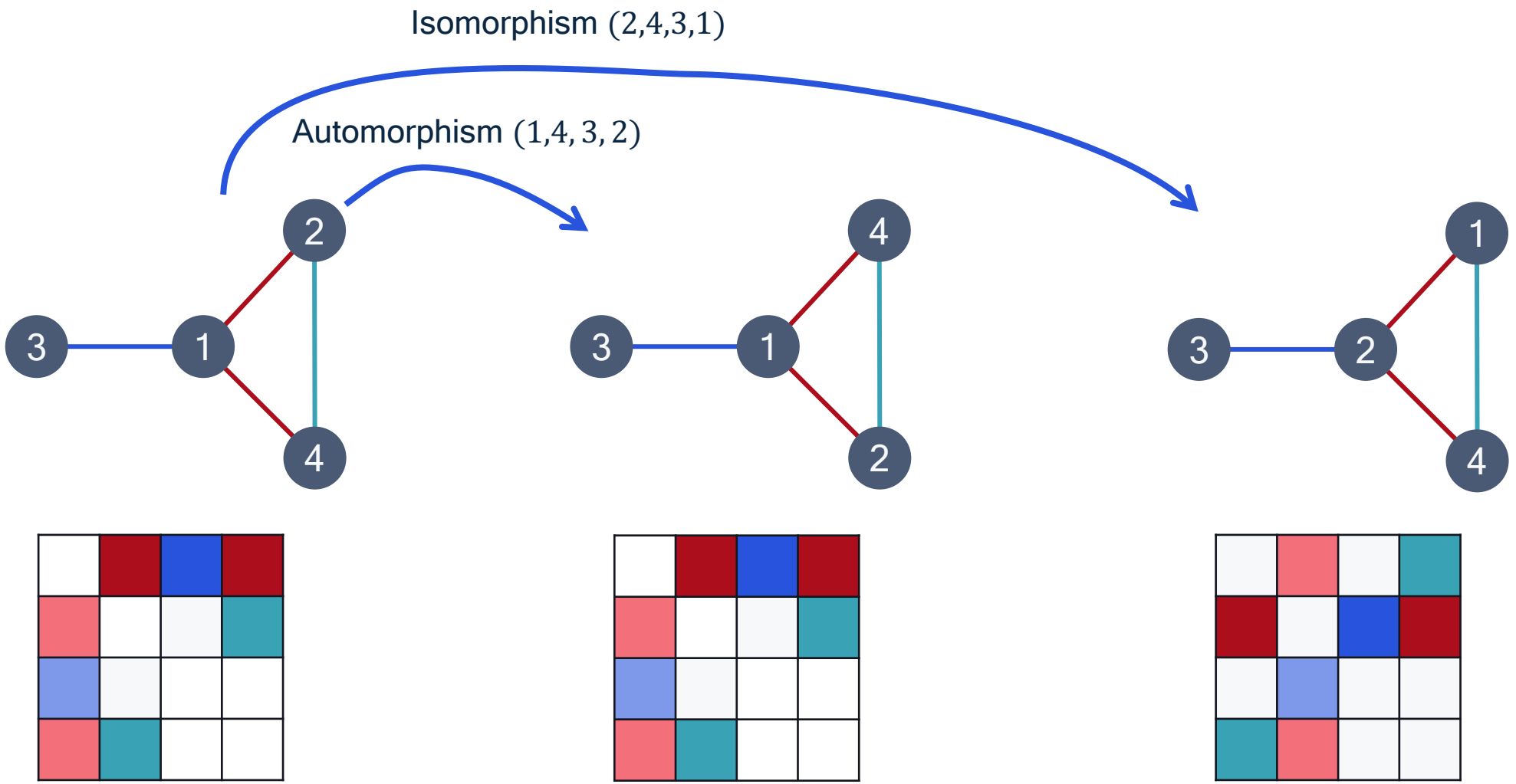
- Natural transformation $\eta: \rho_{\text{in}} \Rightarrow \rho_{\text{out}}$, contains
  - For each graph $G \in Ob(Graph)$, a map $\eta_G: \rho_{\text{in}}(G) \to \rho_{\text{out}}(G)$
  - Such that

- Isomorphism gives weight sharing
  - Non-isomorphic graphs untied weights
- Automorphism gives constraint
  - Non-symmetric graph unconstrained

$$
\begin{array}{ccc}
\rho_{\text{in}}(G) & \xrightarrow{\eta_G} & \rho_{\text{out}}(G) \\
\text{auto}\uparrow & & \uparrow\text{auto} \\
\rho_{\text{in}}(G) & \xrightarrow{\eta_G} & \rho_{\text{out}}(G) \\
\text{iso}\downarrow & & \downarrow\text{iso} \\
\rho_{\text{in}}(G') & \xrightarrow{\eta_{G'}} & \rho_{\text{out}}(G') \\
\\
\rho_{\text{in}}(G'') & \xrightarrow{\eta_{G''}} & \rho_{\text{out}}(G'')
\end{array}
$$

Natural Graph Networks: example

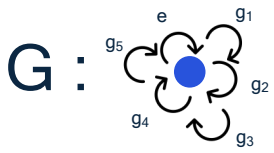
Message passing - 7 parameters



Equivariant vs Natural Networks

Equivariant Graph Networks

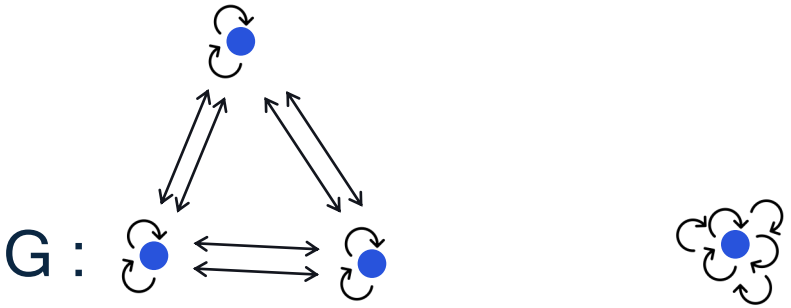
- Symmetry group G = S_n



- Feature space: Functor G → Vect
  - (Group representation)
- Network layer: natural transformation
  - (Equivariant map)
  - One constraint per permutation
  - The same map for every graph

Natural Graph Networks

- Symmetry groupoid G = {adjacency mats} // S_n
  - Called the action groupoid



- Feature space: Functor G → Vect
  - (Groupoid representation)
- Network layer: natural transformation
  - One constraint per *automorphism*
  - Different maps for non-isomorphic graphs

...

Going local

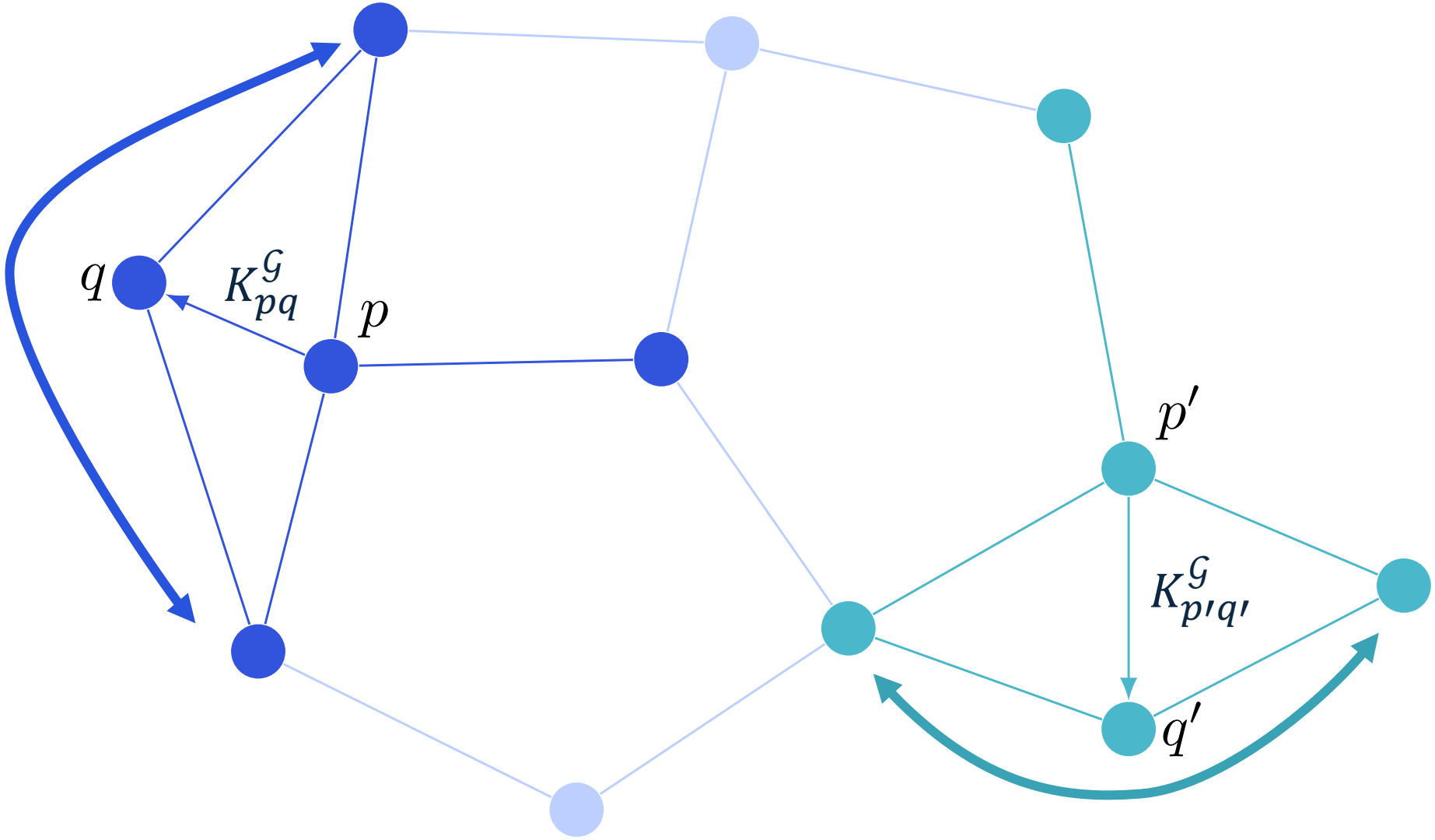
- Global methods are not scalable to large graphs
- Vanilla NGNs do not generalize across non-isomorphic graphs

Natural Graph Networks

Local version

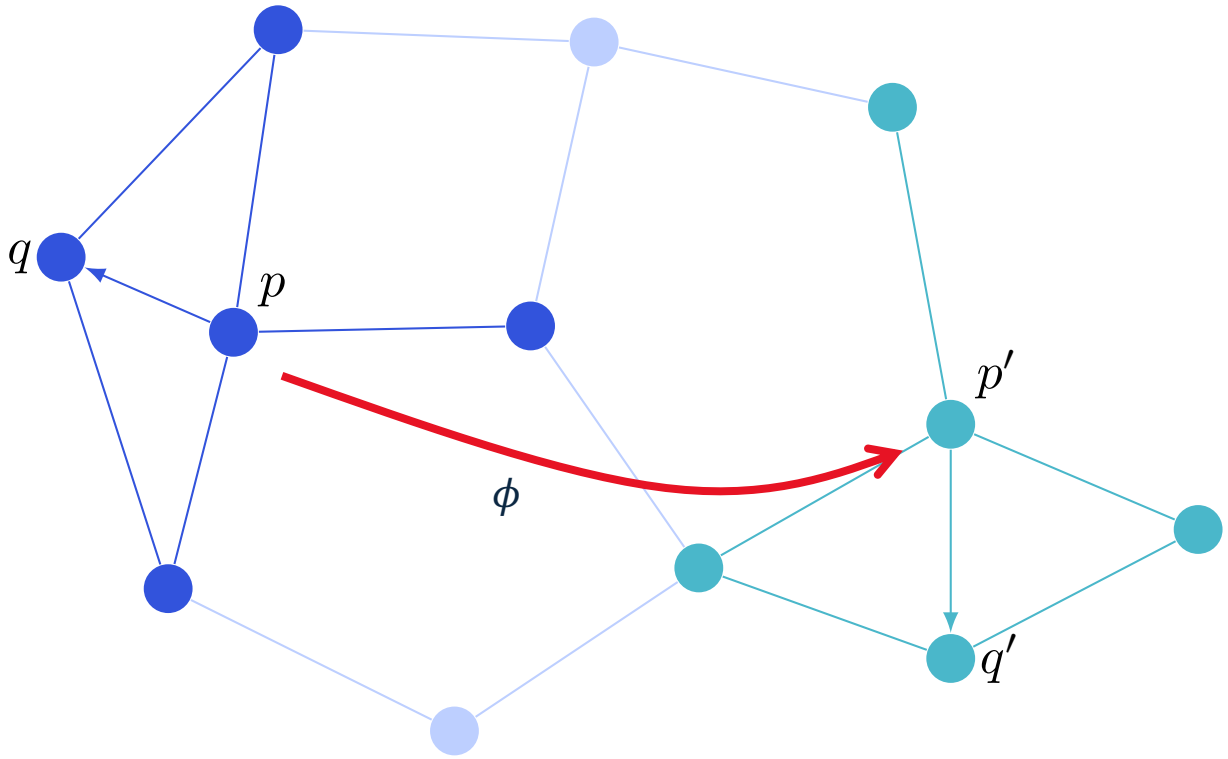
- For each node and edge, define a neighbourhood
  - Edge neigbourhoods should include the node neighbourhoods of the start and end node
  - E.g. one-hop neighbourhood
- Neighbourhood isomorphisms give node and graph isomorphisms
- To each node, attach a graph feature
  - I.e. a representation of S_n where n is the size of the node neighbourhood
  - Typically we use a vector feature (i.e. one number per neigbour)
- Constraints:
  - Weight matrix for an edge is constrained by the automorphisms of the edge neighbourhood
  - Weight matrices on isomorphic edges share weights

Natural Message Passing - local version



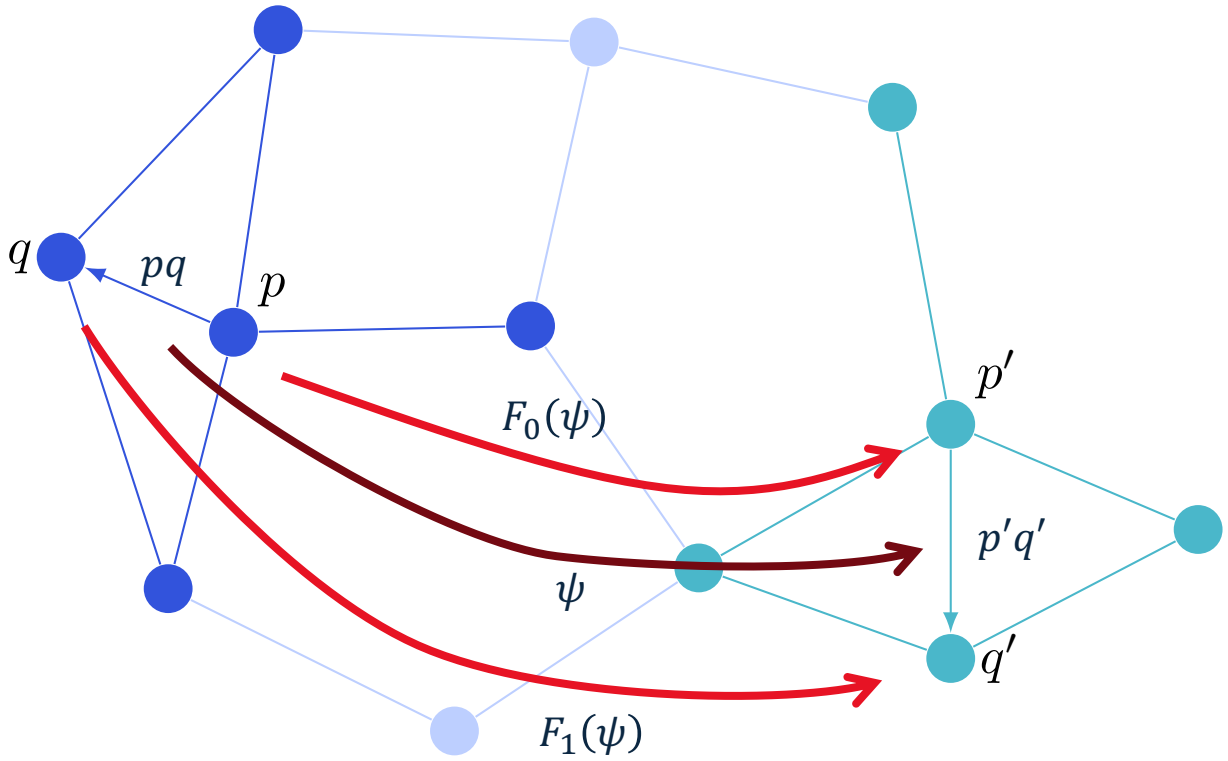
Node groupoid

- For each node p find neighbourhood N_p
- Graph isomorphism ϕ: $N_p \to N_{p'}$
- Node groupoid $\mathcal{N}$
  - Objects are nodes p
  - Morphisms are neighbourhood isomorphisms $\phi: p \to p'$



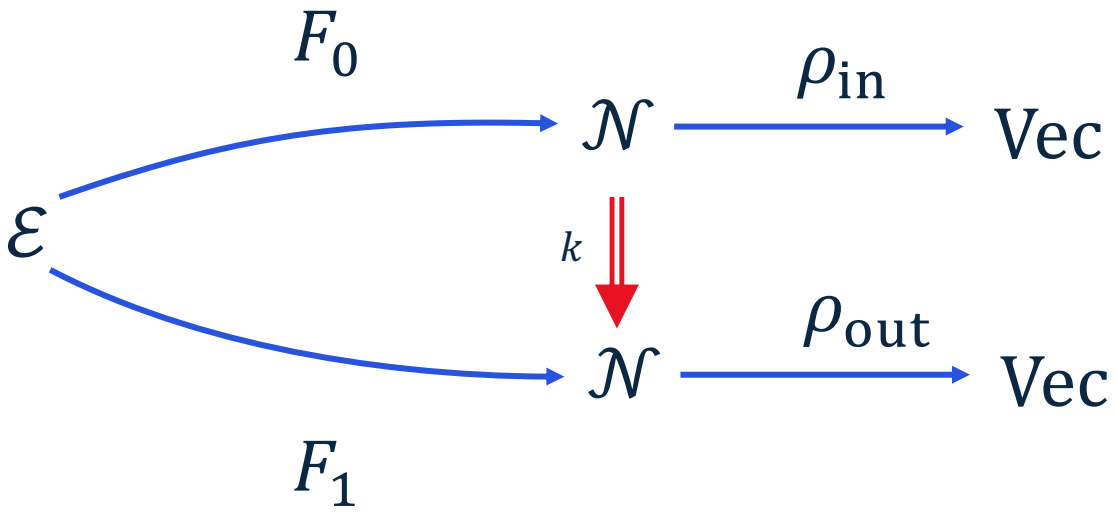
Edge groupoid

- For each edge pq find neighbourhood N_{pq}
- Graph isomorphism ψ: $N_{pq} \to N_{p'q'}$
- Edge groupoid $\mathcal{E}$
  - Objects are edge pq
  - Morphisms are neighbourhood isomorphisms $\psi: pq \to p'q'$
- Edge/node correspondence:
  - Edge pq has start node p
  - Edge isomorphism $\psi: pq \to p'q'$ has start node isomorphism $p \to p'$
- Functor $F_0: \mathcal{E} \to \mathcal{N}$
  - Maps $F_0(pq) = p$
  - Maps $F_0(\psi) = p \to p'$
- Similar for tail node: $F_1: \mathcal{E} \to \mathcal{N}$



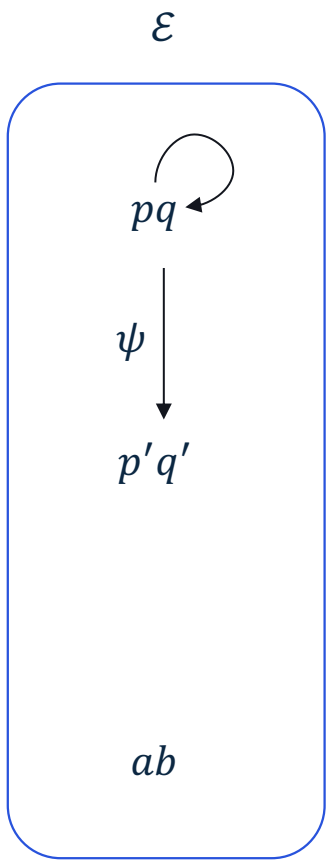
Natural Graph Network - abstractly

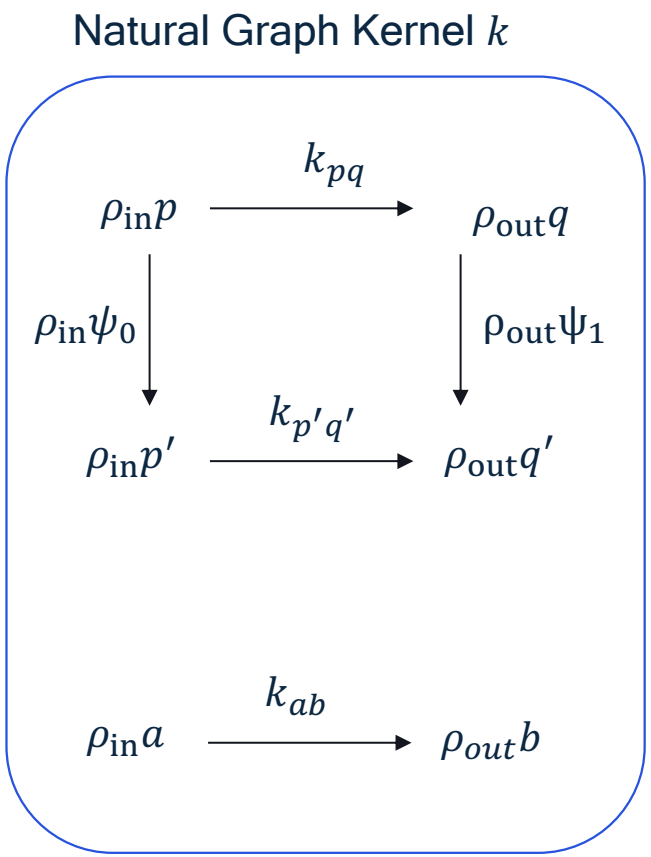
- Node features $\rho: \mathcal{N} \to Vec$
  - $\rho(p)$ is graph feature of neighbourhood N_p, e.g. $\mathbb{R}^{n_p}$
  - Node iso $\phi: p \to p'$ becomes linear transformation $\rho(\phi): \rho(p) \to \rho(p')$, e.g. permutation
- Compose functors



- Message passing kernel is natural transformation $k: \rho_{\text{in}} \circ F_0 \Rightarrow \rho_{\text{out}} \circ F_1$

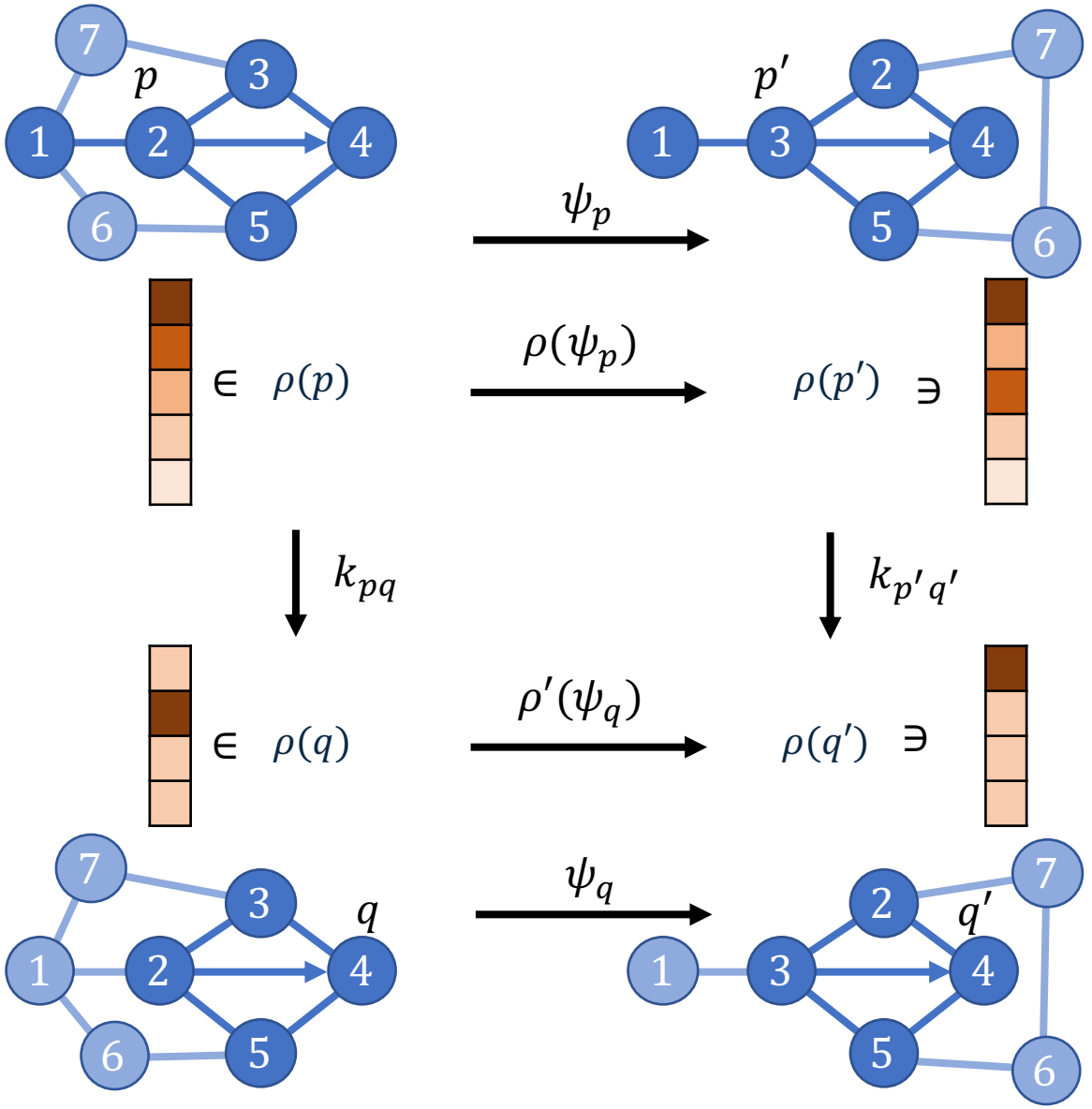
Natural Graph Networks





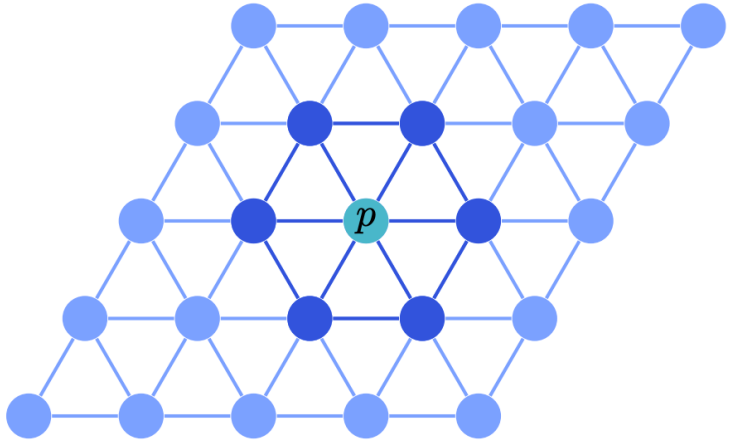
- Isomorphism = weight sharing
- Automorphism = constraints
- Linear kernel: solve linear constraints
- Layer: $v'_q = \sum_{e=(p,q)} k_{pq}(v_p)$

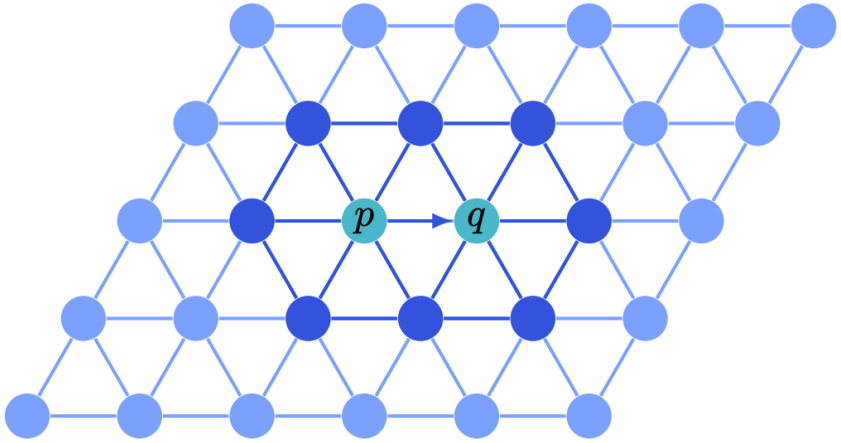
Local Natural Graph Network



Reduction to Group / Manifold Equivariance

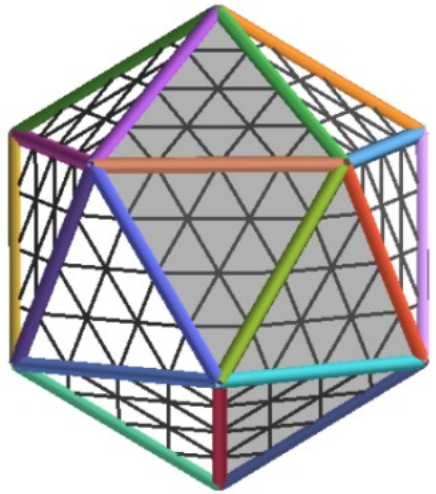
- If graph is a grid
- Node category $\mathcal{N}$
  - Objects are elements of grid
  - Automorphisms are D_4
    - Rotations
    - Mirrors
- Representation $\rho: \mathcal{N} \to Vec$, equivalent to D_4 representation
  - E.g. regular representation $\mathbb{R}^4$
- Edge automorphisms: mirror
- Equivalent to D_4-CNN
  - Cohen & Welling (2016): Group Equivariant CNNs





Equivalent to coordinate free CNN

- Graph = grid on manifold
- Equivalent to Icosahedral CNN
  - Cohen, Weiler, Kicanaoglu, Welling et al (2019): Gauge Equivariant CNNs
- Except at corners: these should have different weights



Basic Algorithm

- Precompute:

1. Define node and edge neighbourhoods
2. Classify edge neighbourhood isomorphism classes
3. Compute edge automorphisms
4. Solve kernel constraint, initialise params

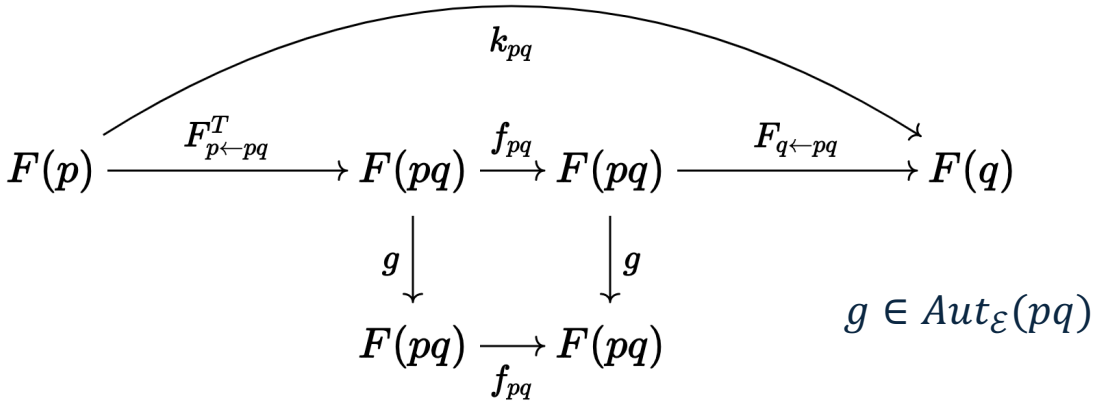
- During training:

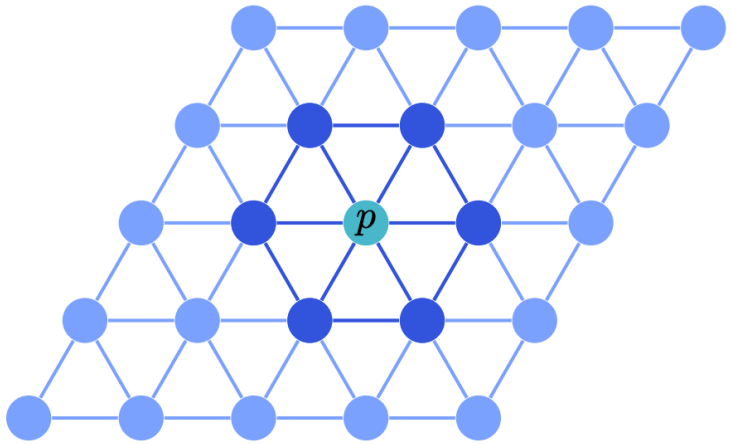
1. Linearly combine kernel solutions using parameters
2. Transport kernels by isomorphisms
3. Compute convolution

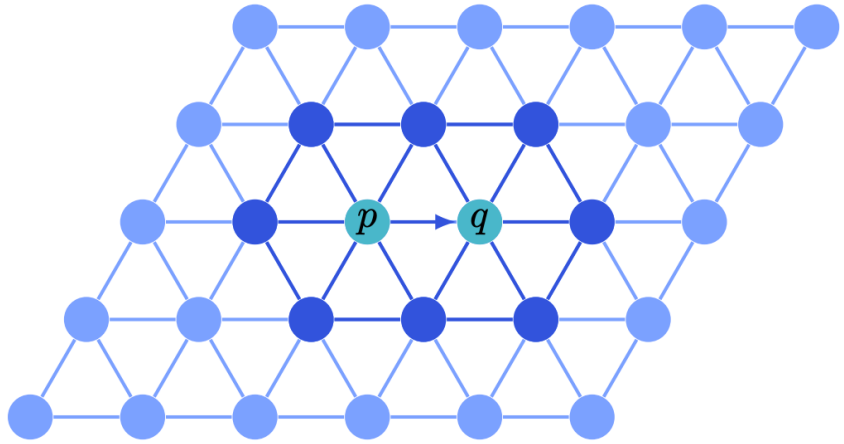
- Cost linear in number of edges, expensive in neighbourhood size

Connection to sheafs?

- Sheaf F
  - Node p, $F(p) =$ graph feature for N_p e.g. $\mathbb{R}^{n_p}$
    - $F(p) = \rho(p)$
  - Edge pq, $F(pq) =$ graph feature for N_{pq} e.g. $\mathbb{R}^{n_{pq}}$
  - $F_{p \leftarrow pq} : F(pq) \to F(p)$ projection
- $f_{pq} : F(pq) \to F(pq)$ graph network







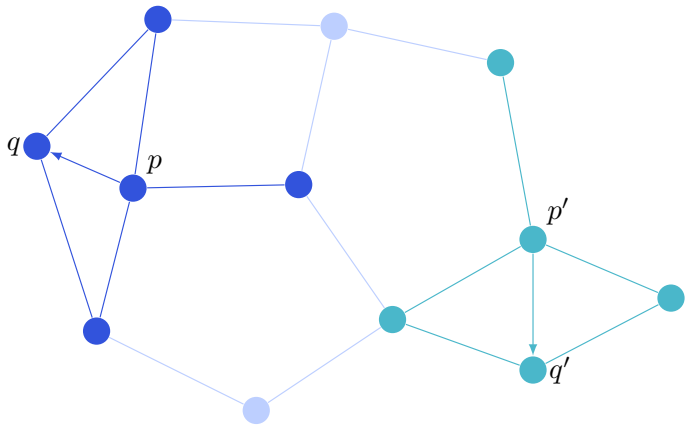
- f_{pq} “global” natural graph network ⇒ k_{pq} natural message passing

Challenges

- 1000s of edge iso classes
- How to find common parametrization for f_{pq}?
- Only treat common edges as non-trivial
- Canonization
  - Unique order for each graph – up to auto
  - One common $f: \mathbb{R}^n \to \mathbb{R}^n$
  - Symmetrize with automorphism group
- Make $f_{pq}(v)$ a graph neural net $\Phi(N_{pq}, v)$ - hypernetwork
  - E.g. graph CNN
- Only consider subgraphs with nice automorphism groups
  - Chains, cycles
  - Thiede et al, “Autobahn: Automorphism-based Graph Neural Nets” (2021)

Natural Graph Networks: Summary

- Graph networks must respect graph symmetries, & treat isomorphic graphs equivalently
- Graph symmetries = autmomorphisms ≠ permutation of nodes
- Network layer = natural transformation between functors
- Global NGN = natural transformation between graph symmetries
- Local NGN = natural transformation between edge symmetries
  - Induces Global NGN
  - More expressive message passing
- Exploiting local symmetries yields efficient and powerful graph networks

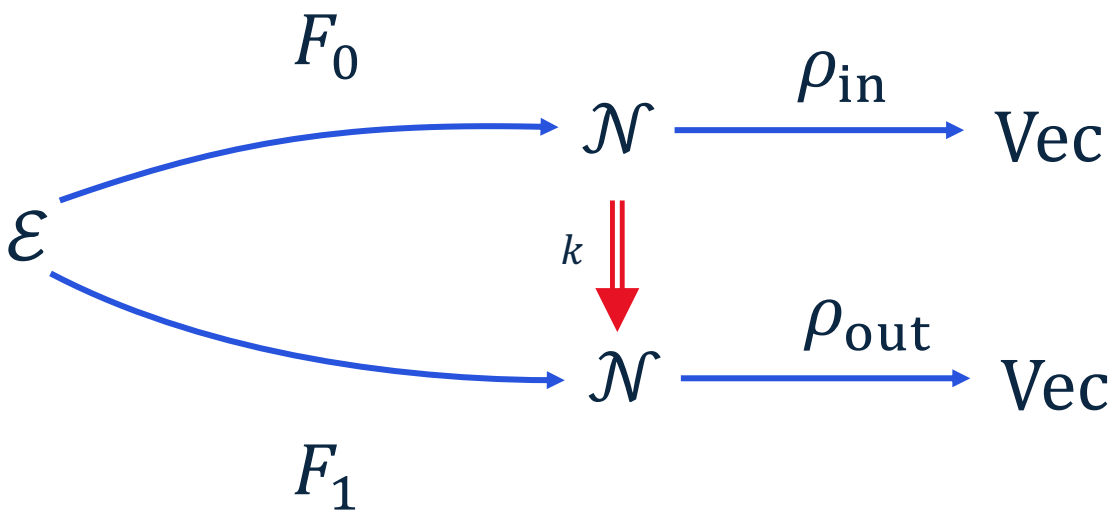


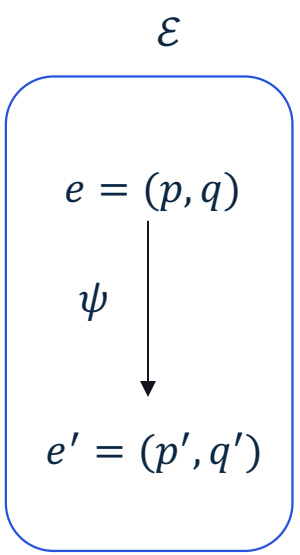
Euclidean Natural Message Passing

Applications to point clouds and meshes

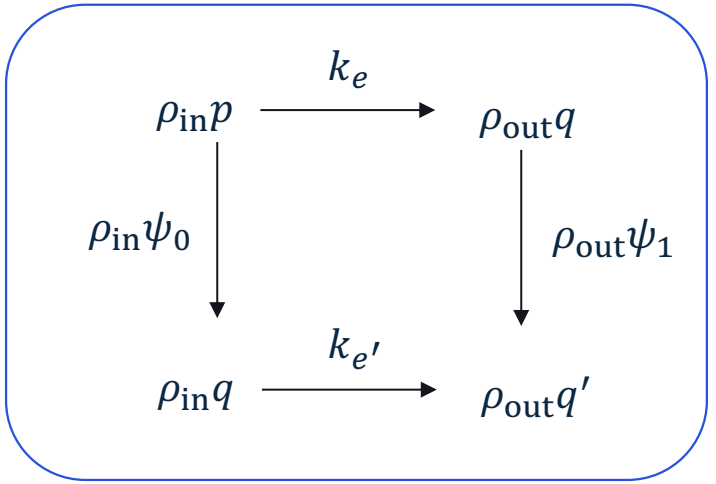
Work in progress

General Natural Message Passing



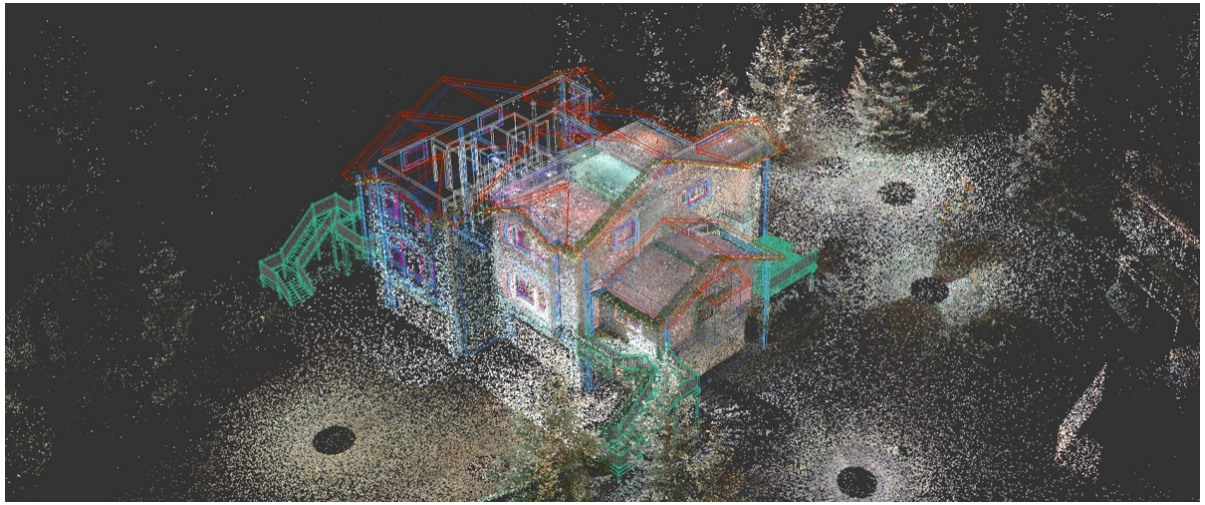


Natural Message Passing Kernel k



Point Clouds

- Set of n points in $\mathbb{R}^3$, data of shape $\mathbb{R}^{n \times 3}$
- Neural network $f: \mathbb{R}^{n \times 3} \to \mathbb{R}^{n \times d}$
- If cloud oriented arbitrarily, equivariant to
  - Translations
  - Permutations
  - Rotations
  - For all $g \in SE(3) \times S_n$, $f(gv) = gf(v)$
- Examples:
  - Molecule
  - Car pose
- Translation equivariance via differences
- Permutation equivariance via message passing
- Rotation equivariance: $R \in SO(3), f(Rv) = Rf(v)$



f

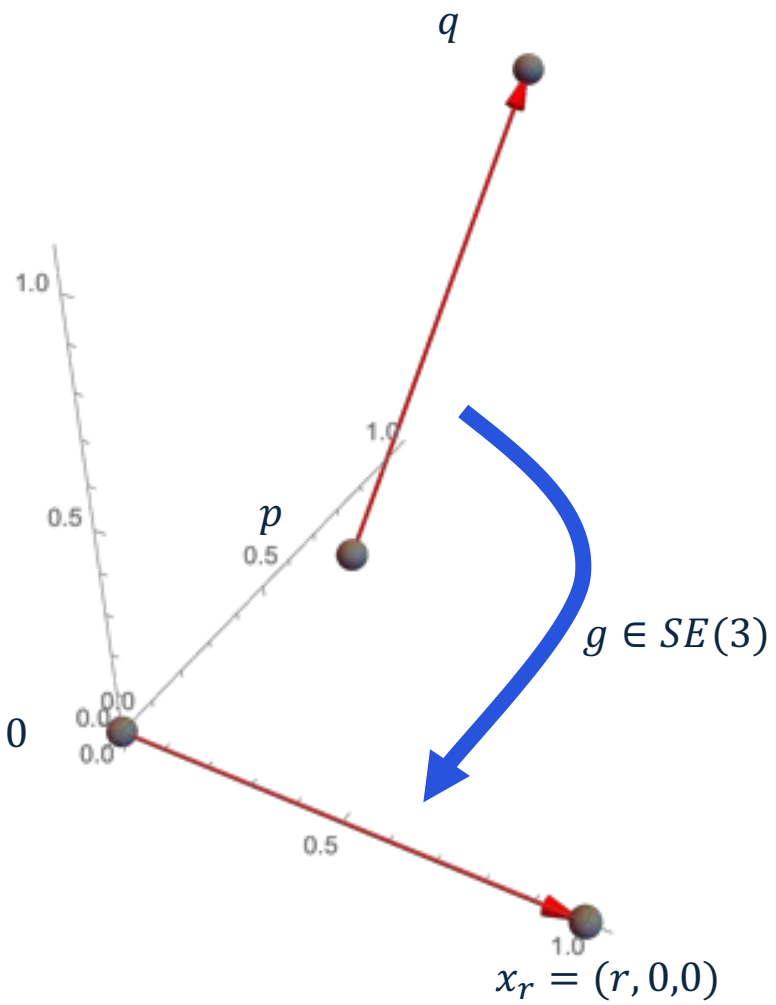
$\mathbb{R}^{n \times d}$

$SO(3)$ equivariant message passing

- Node features SO(3) representations $(\rho_{\text{in}}, \mathbb{R}^d)$, $(\rho_{\text{out}}, \mathbb{R}^{d'})$
  - Examples: $\mathbb{R}^1$ invariant; $\mathbb{R}^3$ 3-vector; $\mathbb{R}^9$ 3x3 matrix
- Message Network: $K: \mathbb{R}^3 \times \mathbb{R}^d \to \mathbb{R}^{d'}$
- Layer: $v'_q = \sum_{pq} K(x_q - x_p, v_p)$
- Equivariance constraint: $K(R(x_q - x_p), Rv_p) = RK(x_q - x_p, v_p)$
- Difficulties:
  - $SO(3)$ representation theory involves varying dimensions and Clebsch-Gordan coefficients. Difficult to implement cleanly and efficiently
  - The network is conditional on the direction, making it different for all edges. Additional computational cost

Natural Message Passing

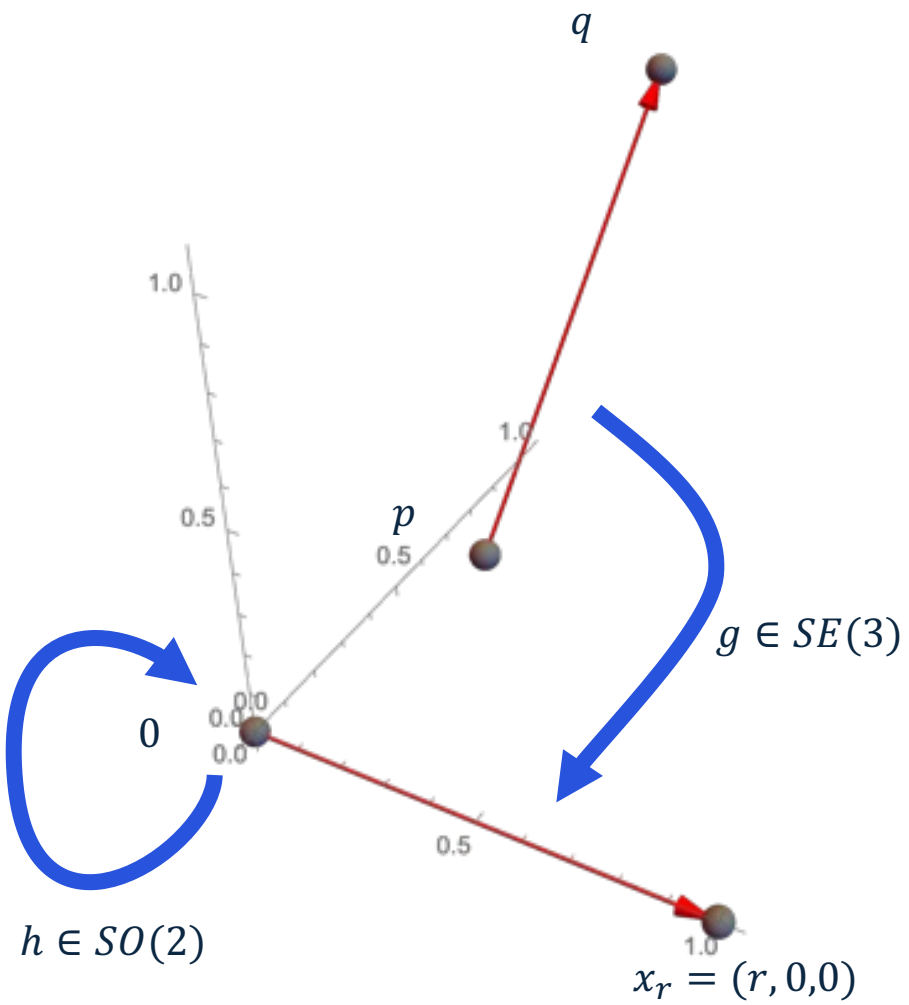
reduction of 3D symmetry to 2D symmetry of edges



- Node groupoid $\mathcal{N} = \mathbb{R}^3 \,//SE(3)$
  - Objects are points $p \in \mathbb{R}^3$
  - Isomorphisms $g_p: p \to p',\ g \in SE(3), g(p) = p'$
  - All points isomorphic
- Edge groupoid $\mathcal{E} = (\mathbb{R}^3 \times \mathbb{R}^3)//SE(3)$
  - Objects are pairs of points $p, q \in \mathbb{R}^3$
  - Isomorphisms $g_{pq}: pq \to p'q',\ g \in SE(3), g(p) = p', g(q) = q'$
  - Edges of same length isomorphic
- Node features $\rho: \mathcal{N} \to Vec$ is $SO(3)$ representation
  - $\rho(p) = \mathbb{R}^d$
  - $\rho(g_p) = \rho(g)$
- Natural Message Passing $k: \rho_{\text{in}} \circ F_0 \Rightarrow \rho_{\text{out}} \circ F_1$

Natural Message Passing

reduction of 3D symmetry to 2D symmetry of edges



- Automorphisms: $SO(2)$ aroud x axis

Natural Graph Kernel k

$$\begin{array}{ccc} \mathbb{R}^d & \xrightarrow{k_{pq}} & \mathbb{R}^{d'} \\ \downarrow \rho_{\text{in}} g & & \downarrow \rho_{\text{out}} g \\ \mathbb{R}^d & \xrightarrow{k_{0x_r}} & \mathbb{R}^{d'} \\ \downarrow \rho_{\text{in}} h & & \downarrow \rho_{\text{out}} h \\ \mathbb{R}^d & \xrightarrow{k_{0x_r}} & \rho_{out} b \end{array}$$

Algorithm

Precompute:

- For each edge (p, q) precompute $g \in SE(3)$ to move edge to $(0, (r, 0,0))$
- Construct $SO(2)$ radius-conditional network f_r: $\mathbb{R}^d \to \mathbb{R}^{d'}$

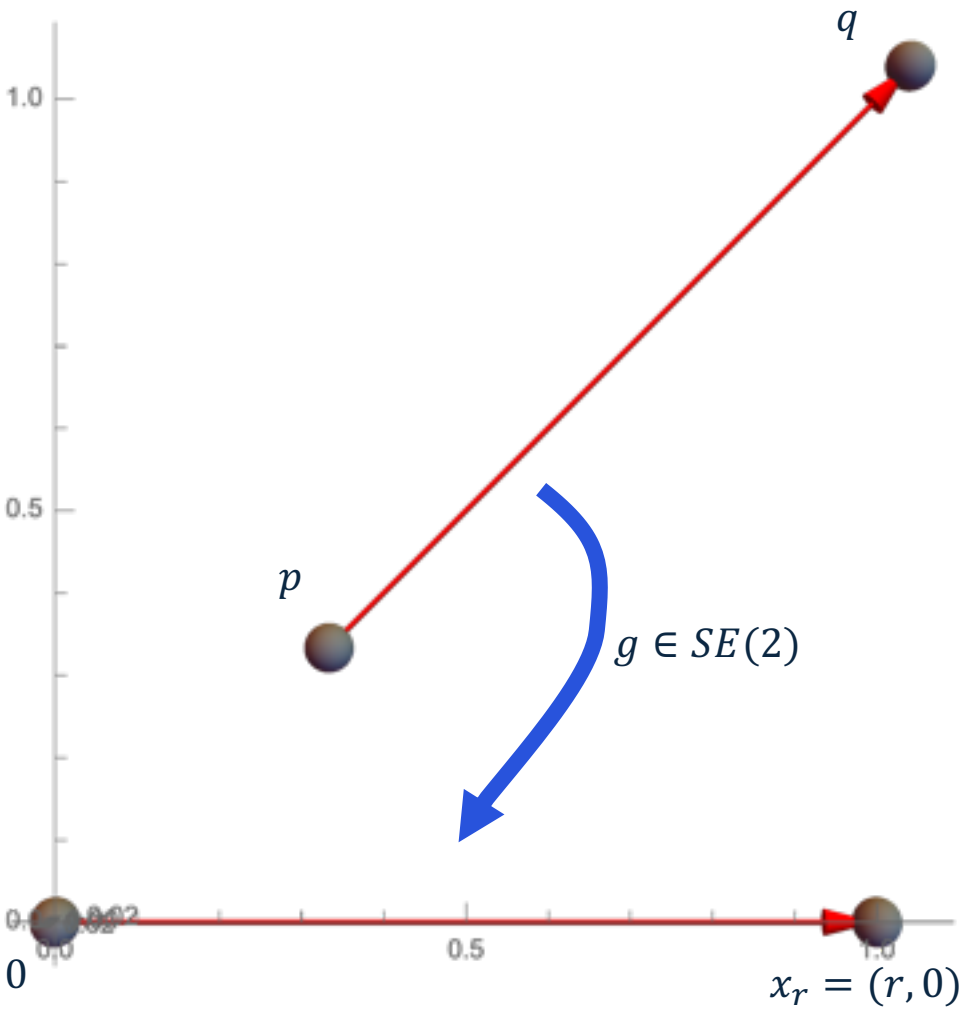
In network:

1. Move feature v from p to 0 with $SO(3)$ action g
2. Message pass from 0 to x_r with f_r
3. Move output feature from x_r to q with $SO(3)$ action g^{-1}
4. Sum over incomming messages

Used $SO(2)$ equivariance to make $SO(3)$ equivariant network!

- Simpler to construct
- More available non-linearities

Planar case: trivial automorphism



- Symmetry group $SE(2)$
  - Features are representations of $SO(2)$
- Edges have no automorphism constraints
- Message passing with unconstrained

$$f_r : \mathbb{R}^d \to \mathbb{R}^{d'}$$

  - ReLU non-linearities
- Also usable for Gauge Equivariant Mesh CNN

Conclusion

- Generalize groups to groupoids
- Generalize equivariance to natural transformations
- Message passing on graphs
  - Weight sharing if edges have isomorphic neighbourhoods
  - Local symmetries give constraints
  - More expressive
- Pointcloud equivariance via $SO(2)$ symmetry
  - Easier to implement
  - Better non-linearities
- Planar equivariance via unconstrained network
  - ReLU non-linearities
- Many more groups, groupoids, categories and representations to explore!
- Open question: link local – global naturality more formally

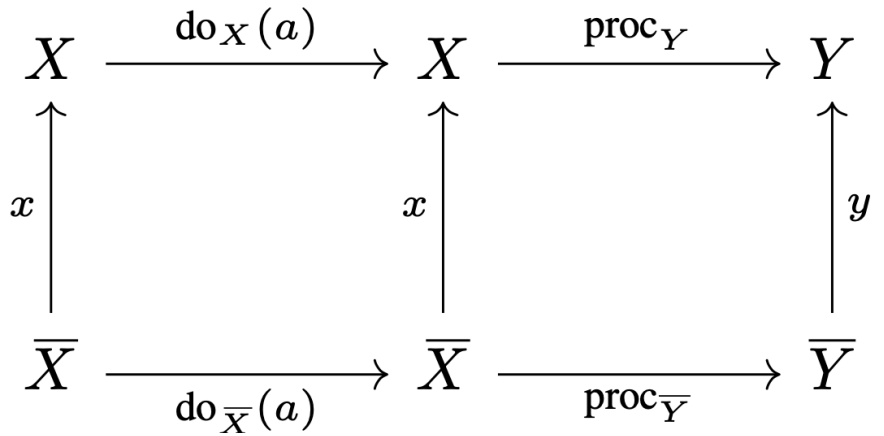
Categories & Causality

Postscriptum

Grounded Causal Models

Cohen 2022: Towards a Grounded Theory of Causation for Embodied AI

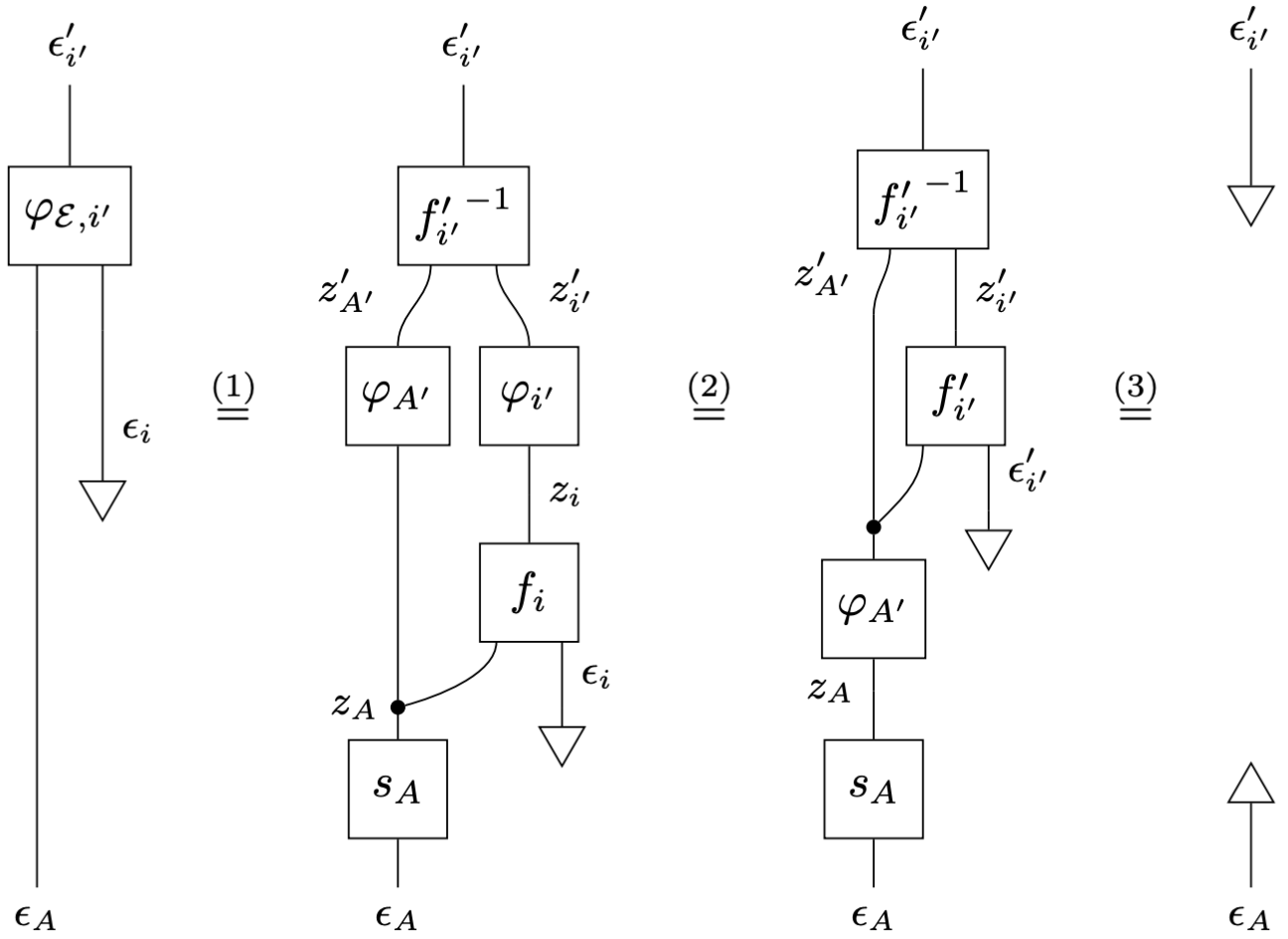
- Set of actions / interventions A
- Dynamics $\mathrm{do}(a)\colon X \to X$
- Effects $\mathrm{proc}\colon X \to Y$



A model is *grounded* if there is a natural transformation like this

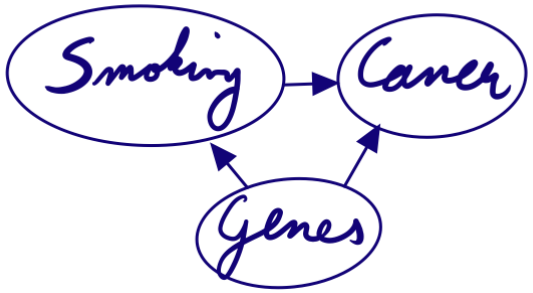
String diagrammatic proofs

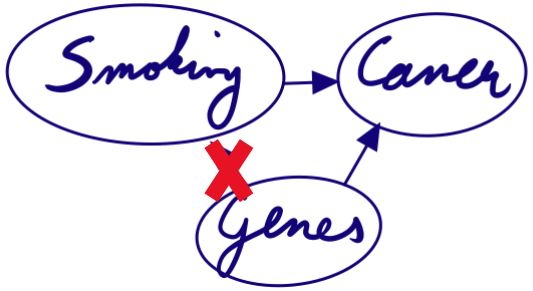
Brehmer, De Haan, Lippe, Cohen: Weakly supervised causal representation learning (2022)

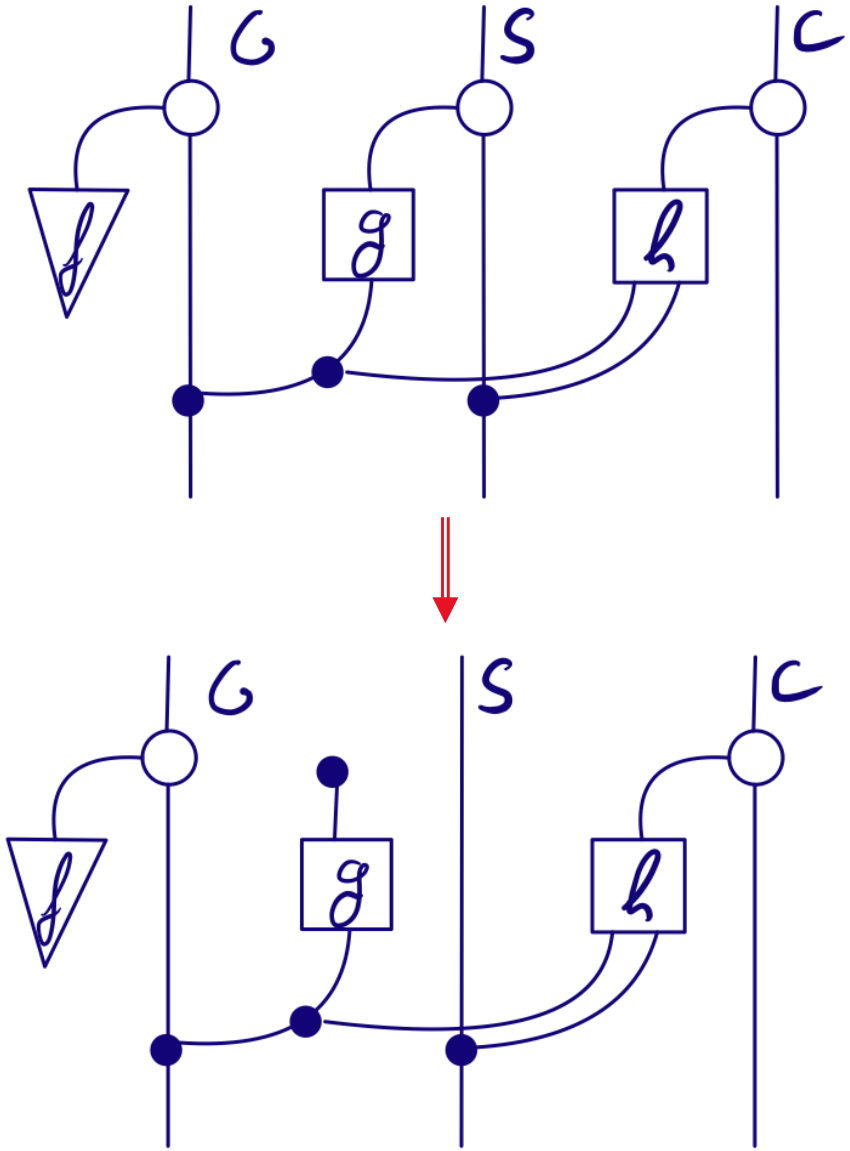


Causal Model – interventions as 2-cell

Bhat, Van Belle, De Haan, Lopez, Román (in progress)







Further reading

- Books:
  - Fong & Spivak, *Seven Sketches in Compositionality: an invitation to applied category theory*
  - Perrone, *Introduction to category theory*
  - Riehl, *Category Theory in Context*
  - Lawvere & Schanuel, *Conceptual Mathematics: a first introduction to categories*
- Papers:
  - De Haan, Cohen, Welling, Natural Graph Networks
  - Dudzik & Velickovic, Graph Neural Networks are Dynamic Programmers
  - Gavranovic, https://github.com/bgavran/Category_Theory_Machine_Learning

Thank you

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