Equivariant Networks

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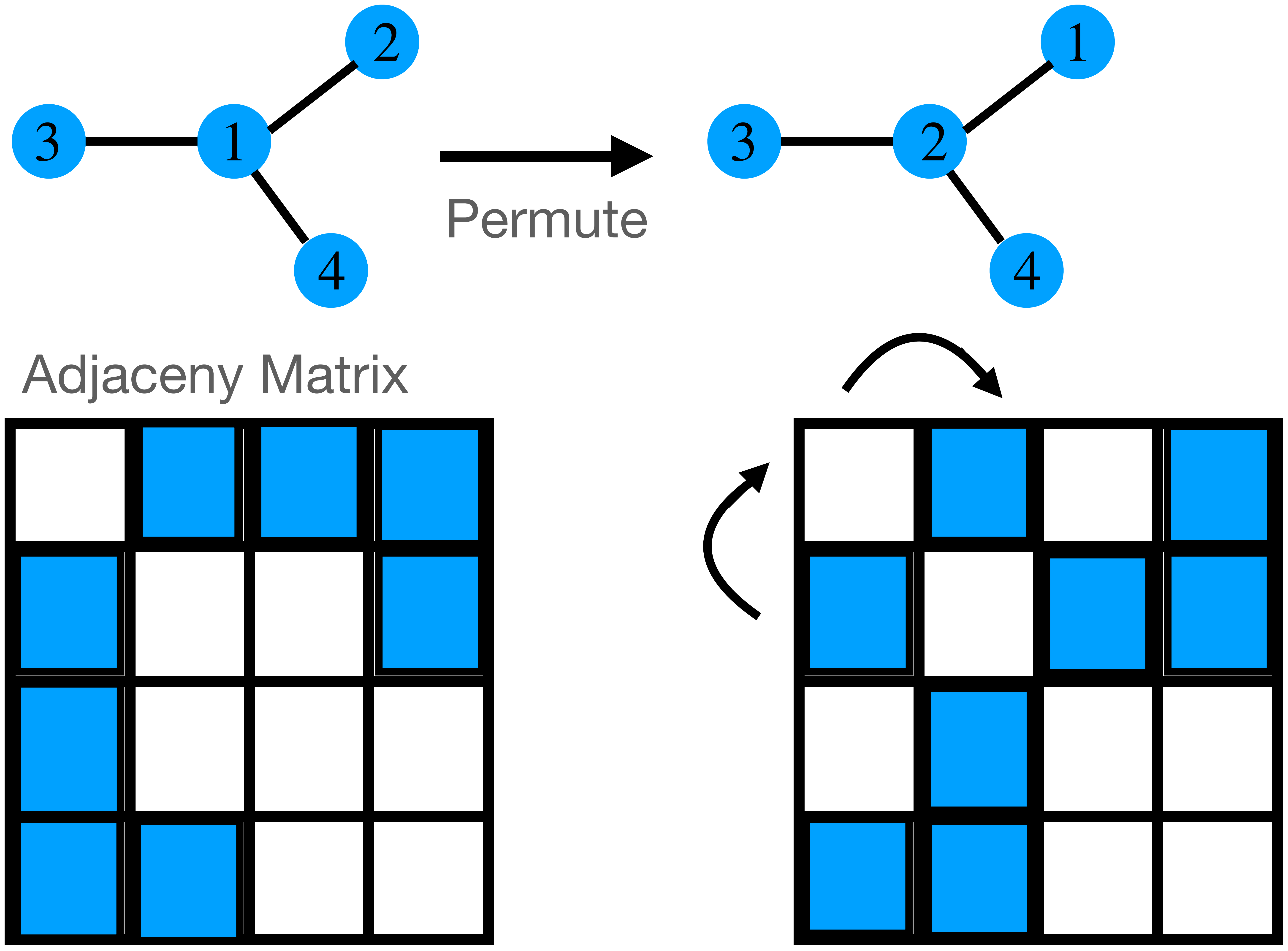
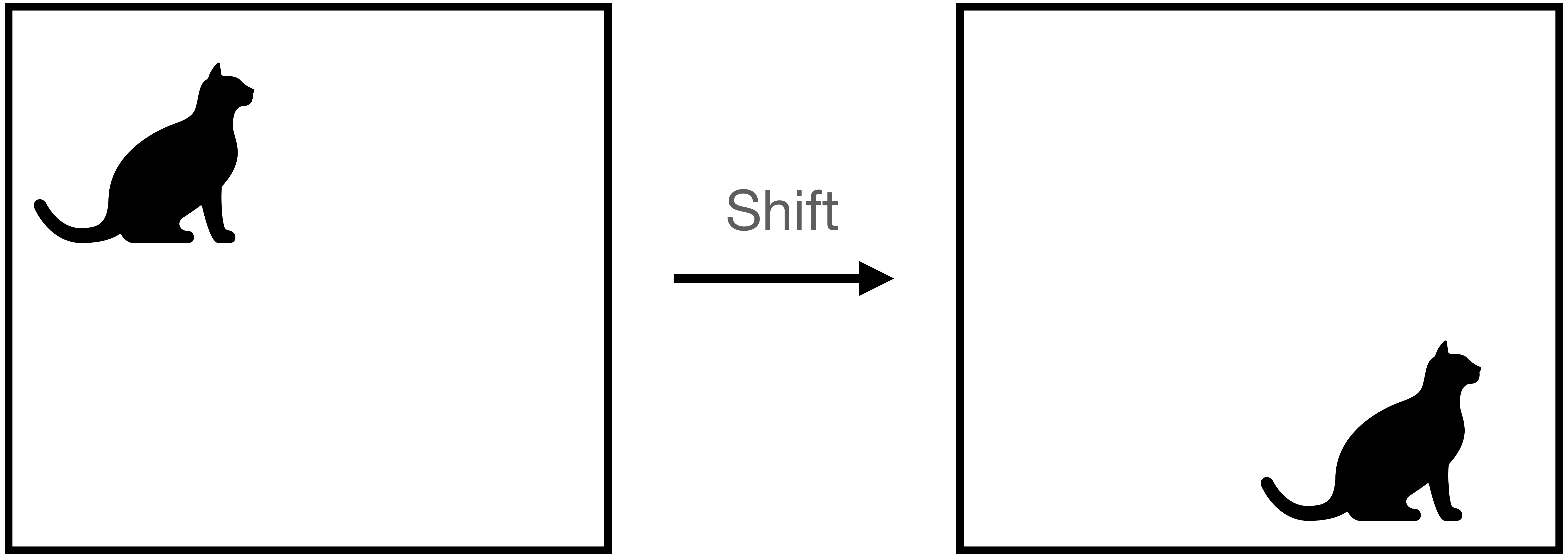
Symmetries in ML



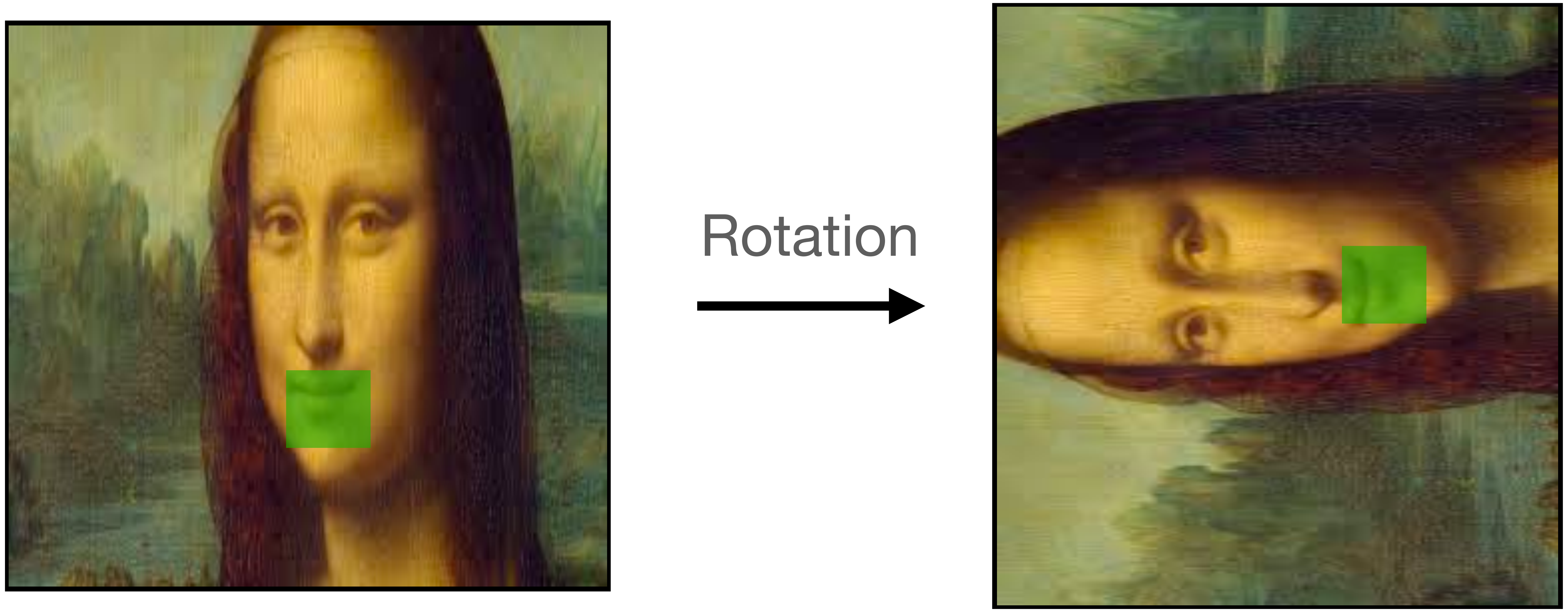
Permutation Invariance in Node Labels in a Graph

Symmetries in ML



Translation Invariance
in image labels

Symmetries in ML



Rotation Equivariance
in image features

Symmetries of the Label function

$g : \mathscr{X} \to \mathscr{Y}$ Symmetry Transformation

$L : \mathscr{X} \to \mathscr{Y}$ Label Function

Transformation is a symmetry of g

$$L \circ g = L$$

$$\begin{tikzcd}
\mathscr{X} \arrow[d, "g"'] \arrow[dr, "L"] & \\
\mathscr{X} \arrow[r, "L"'] & \mathscr{Y}
\end{tikzcd}$$

Group Actions

1. We have a set $\mathcal{X}$ and $f : \mathcal{X} \to \mathbb{C}$

2. Group G acts on $\mathcal{X}$

$$T_g : \mathcal{X} \to \mathcal{X} \quad \forall g \in G$$

$$\forall g1, g2 \in G,\ T_{g2g1} : T_{g2} \circ T_{g1}$$

If $\mathcal{X}$ is a (finite) Vector Space then $T_g \in GL(n)$

3. Extending the action to functions

$$\mathbb{T}_g : f \to f' \qquad f'(T_g(x)) = f(x)$$

<u>Groups</u>

1. $e \in G$

   Identity

2. $(a \circ b) \circ c = a \circ (b \circ c)$

   Associativity

3. $\forall a \in G \quad \exists b \in G$

   $a \circ b = e$

   Unique Inverses

Induced Actions: Example on $\mathbb{Z}^2$

$\mathscr{X} = \mathbb{Z}^2$

$G = \mathbb{Z}^2$ Group of integer translations, isomorphic to $\mathbb{Z}^2$

$$T(t_1, t_2)(x_1, x_2) = (x_1 + t_1, x_2 + t_2), \quad (t_1, t_2) \in \mathbb{Z}^2$$

Induced action on functions

$$\mathbb{T} : f \to f' \quad f'(x_1, x_2) = f(x_1 - t_1, x_2 - t_2)$$

Equivariance

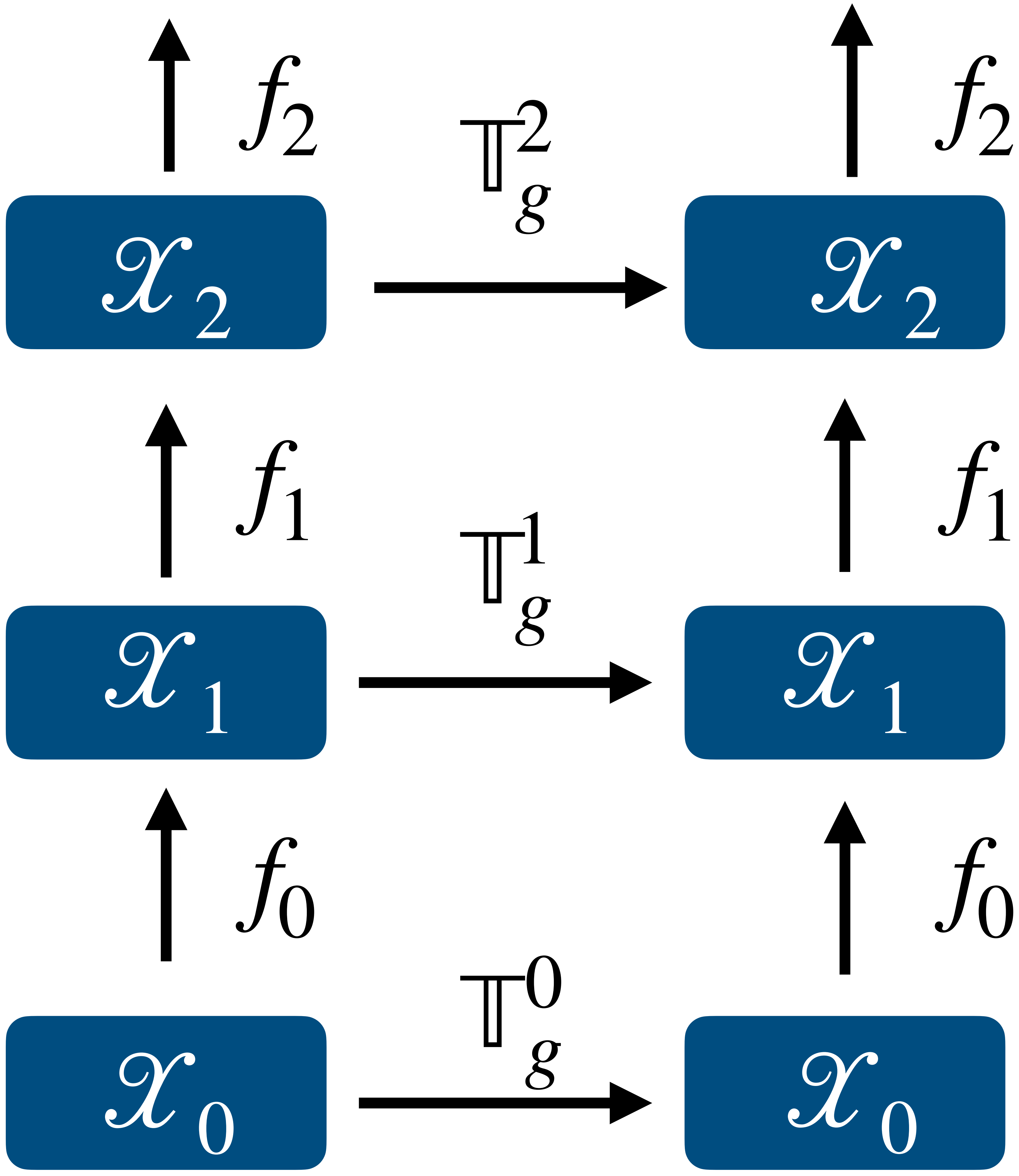
Definition: Let G be a group and $\mathscr{X}_1$ and $\mathscr{X}_2$ be two sets with corresponding G-actions and induced actions $\mathbb{T}$, $\mathbb{T}'$ on the space of linear transformations on each respective set ($-$i.e. $L_{(V_i)}(\mathscr{X}_i)$). Then a map $\phi : L_{(V_1)}(\mathscr{X}_1) \to L_{(V_2)}(\mathscr{X}_2)$ Is G-equivariant if:

$$\phi(\mathbb{T}_g(f)) = \mathbb{T}'_g(\phi(f)) \qquad \forall f \in L_{(V_1)}(\mathscr{X}_1)$$

Equivariance

$$\begin{tikzcd}
L_{(V_1)}(\mathscr{X}_1) \arrow[r, "\mathbb{T}_g"] \arrow[d, "\phi"'] & L_{(V_1)}(\mathscr{X}_1) \arrow[d, "\phi"] \\
L_{(V_2)}(\mathscr{X}_2) \arrow[r, "\mathbb{T}'_g"] & L_{(V_2)}(\mathscr{X}_2)
\end{tikzcd}$$

Equivariance Networks Recipe



Applying Equivariance: Equivariant Densities

Let p be an invariant density with representation T_g

Fact 1: $|\text{det}(T_g)| = 1$

$Proof:$

Applying Equivariance: Symmetric Densities

Theorem 1: Let $p(x)$ be density resulting from applying an invertible map F to $p(u)$. If T is G-equivariant and $p(u)$ is G-invariant density then $p(x)$ is also G-invariant.

Applying Equivariance: Symmetric Densities

Proof :

Planar Convolutions

Convolution of two function $f, g : \mathbb{R} \to \mathbb{R}$

$$(f * g)(x) = \int f(x - y)g(y)dy$$

We will study this convolution and its generalizations for the rest of the talk!

Group Convolutions

Convolution of two functions f, g on a compact group G

$$(f * g)(u) = \int f(uv^{-1})g(v)d\mu(v) \rightarrow$$

Haar measure μ unique for compact groups

$x - y$ is replaced by the group operation uv^{-1}

$$(x, y) \mapsto x + y, \qquad G = (\mathbb{R}, +)$$

Group Convolutions

If we model images and stacks of feature maps as $f : \mathbb{Z}^2 \to \mathbb{R}^k$. At each pixel location $(p, q) \in \mathbb{Z}^2$ the feature map is a K-dimensional vector. Feature maps transform under group representations as follows:

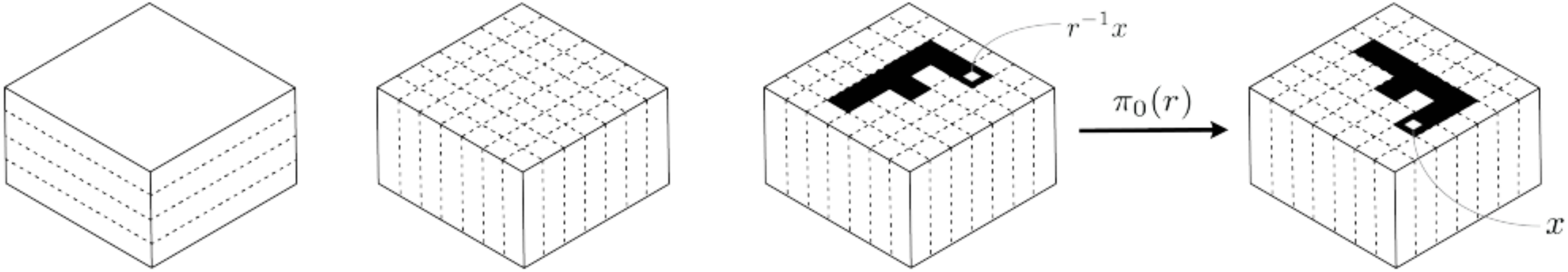
$$[T_g f](x) = [f \circ g^{-1}](x) = f(g^{-1}x) \longrightarrow$$

Group acts via what is known as the Regular Representation

Intermediate feature maps in a G-CNN are functions on G and **not** $\mathbb{Z}^2$**.** The first layer —i.e. input is a special case but every subsequent layer must have filters defined on the group

Steerable CNN’s

If we model images and stacks of feature maps as $f : \mathbb{Z}^2 \to \mathbb{R}^k$. At each pixel location $(p, q) \in \mathbb{Z}^2$ the feature map is a K-dimensional vector. The set of signals forms a linear space $\mathscr{F}$. We can also decompose $\mathscr{F}$ into *fibres.* The fiber F_x is attached to $\mathbb{Z}^2$ at all points x



$\mathscr{F}$ as stack of maps

$\mathscr{F}$ as a bundle of fibres

Fig credit: https://arxiv.org/pdf/1612.08498.pdf

Steerable Representations

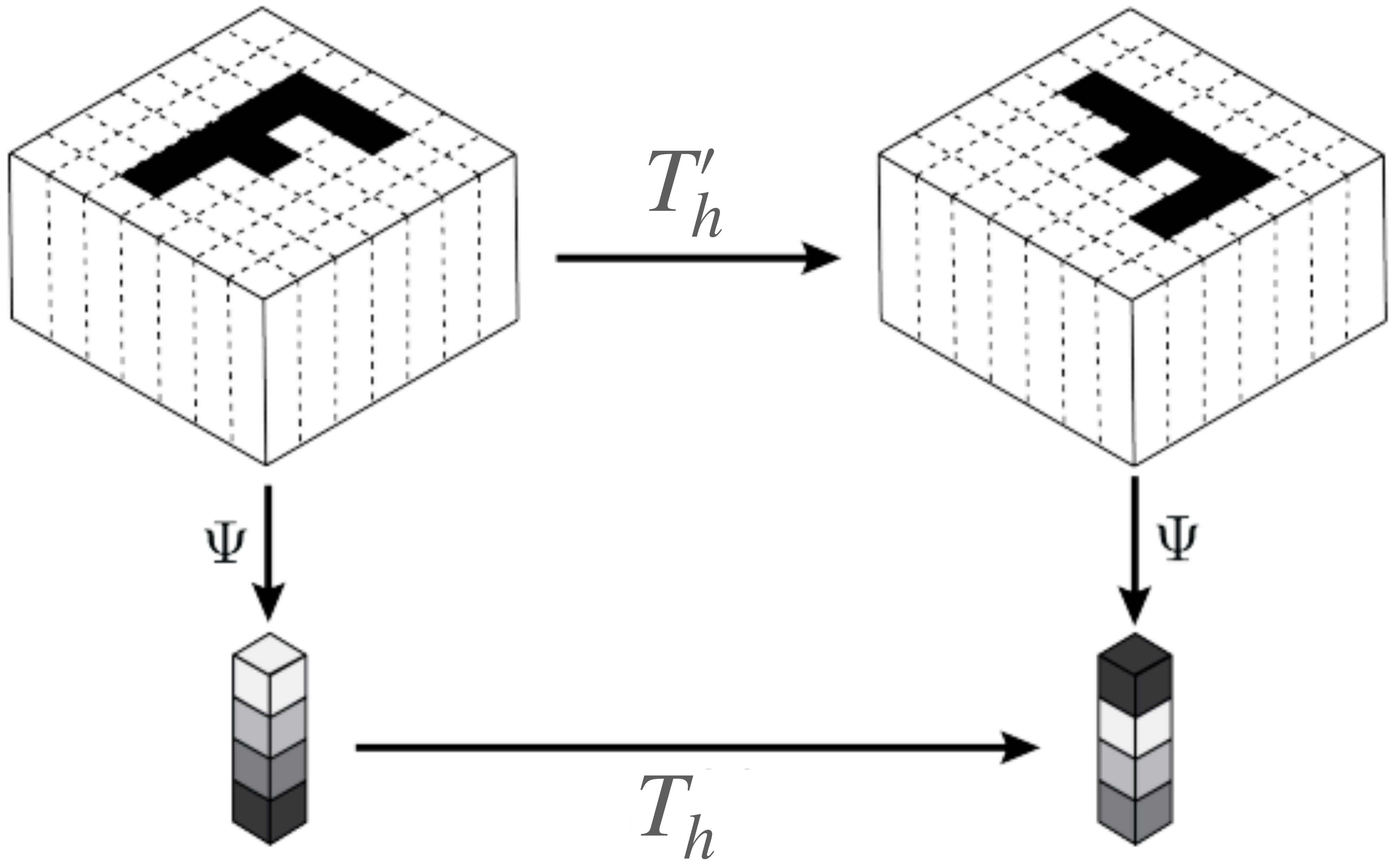
Definition: Let $(\mathcal{F}, T)$ be a feature space with a group rep. and $\Phi : \mathcal{F} \to \mathcal{F}'$. Then $\mathcal{F}'$ is said to be linearly steerable if:

$$\Phi T_g = T'_g \Phi$$

That is T'_g does not depend on any . Also T'_g must be a group rep

Equivariant Filter Banks

Filter bank (K', K, s, s) is an array with K', K input/output channels —i.e. a linear map $\Psi : \mathscr{F} \to \mathbb{R}^{K'}$ which is applied to translated copies of $f \in \mathscr{F}$ one fiber at a time. Let $H < G$ and T_h and T'_h be representations of H



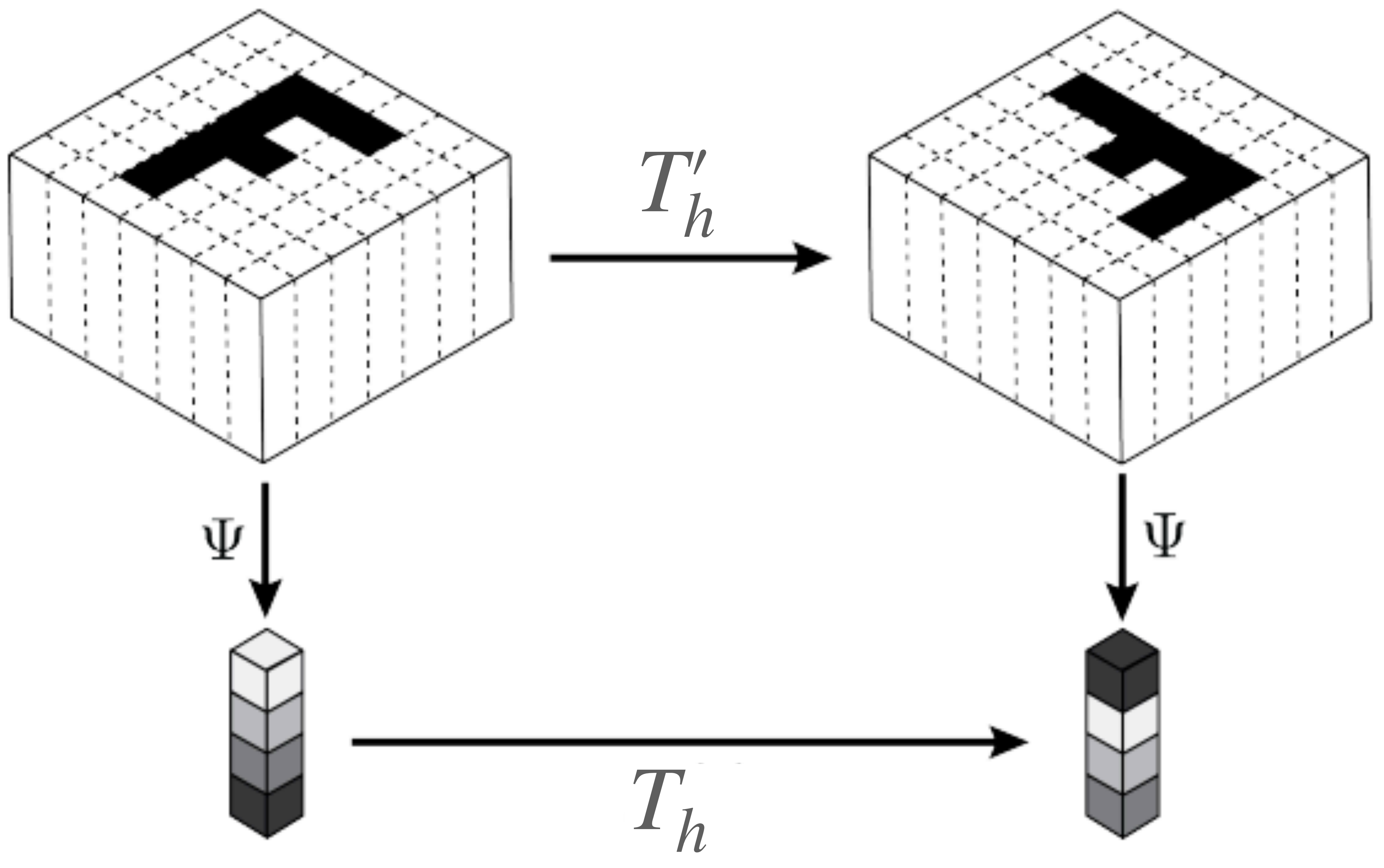
H-equivariant Condition:

$$T_h \Psi = \Psi T'_h \quad \forall h \in H$$

Fig credit: https://arxiv.org/pdf/1612.08498.pdf

Equivariant Filter Banks

Space of maps satisfying the equivariance condition is a vector space: $\mathrm{Hom}_H(T, T')$. Given T, T' we can compute a basis by solving the linear system. With a basis $\psi_1, \ldots \psi_n$ for $\mathrm{Hom}_H(T, T')$ any Equivariant filter bank is a linear combination.



$\boxed{H\text{-equivariant Condition:}}$

$$T_h \Psi = \Psi T'_h \quad \forall h \in H$$

Linear Constraint on Ψ

Fig credit: https://arxiv.org/pdf/1612.08498.pdf

Convolutions on Quotient Spaces

Major complication in NN's is that $\mathscr{X}_0, \ldots, \mathscr{X}_n$ are homogenous spaces of G rather than the group G itself.

We need a way to generalize convolutions from groups to their homogenous spaces!

General strategy: We will "lift" functions on homogenous spaces to groups when necessary and "project" back down after.

<u>Homogenous Spaces</u>

$\mathscr{X}$ is a homogenous space for G if $\forall x, y \in \mathscr{X}$ there exists $g \in G$ such that $g \circ x = y$

<u>Stabilizer subgroup</u>

$$H_x = \{g \in G \,|\, gx = x\}$$

Convolutions on Quotient Spaces

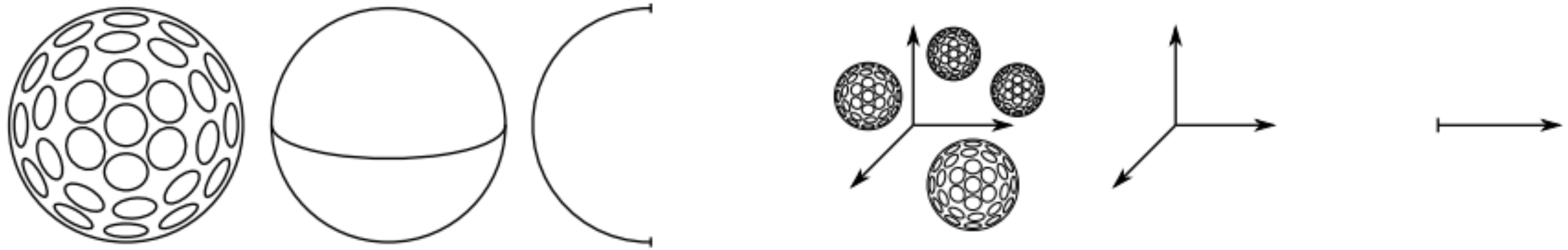
We can fix an origin $x_0 \in \mathscr{X}$ then by the definition of transitivity each $x = g(x_0)$ −i.e. we can “index” elements of $\mathscr{X}$ with elements of G denoted as $[g]_{\mathscr{X}} = g(x_0)$

Left Quotient Space

For a subgroup $H < G$ the left coset is $gH := \{gh \,|\, h \in H\}$. The set of all cosets partitions G/H

Lifting: Given $f : \mathscr{X} \to \mathbb{C}$ we can lift f to G

$$f \uparrow^G : G \to \mathbb{C} \qquad f \uparrow^G (g) = f([g]_{\mathscr{X}})$$



$\mathrm{SO}(3)$ $\quad$ $\mathrm{SO}(3)/\mathrm{SO}(2)$ $\quad$ $\mathrm{SO}(2)\backslash\mathrm{SO}(3)/\mathrm{SO}(2)$ $\quad$ $\mathrm{SE}(3)$ $\quad$ $\mathrm{SE}(3)/\mathrm{SO}(3)$ $\quad$ $\mathrm{SO}(3)\backslash\mathrm{SE}(3)/\mathrm{SO}(3)$

Fig credit: https://arxiv.org/pdf/1811.02017.pdf

Convolutions on Quotient Spaces

For each coset we can pick a coset representative $g' \in gH$ and denote $\bar{x}$ the representative of group elements that map $x_0 \to x$

Projection: Given $f : G \to \mathbb{C}$ we can project to $\mathcal{X} = G/H$

$$f \downarrow_{\mathcal{X}} : \mathcal{X} \to \mathbb{C} \quad f \downarrow_{\mathcal{X}} (x) = \frac{1}{|H|} \sum_{g \in \bar{x}H} f(g)$$

Convolutions on Quotient Spaces

$$(f * g)(u) = \int f(uv^{-1})g(v)d\mu(v)$$

Group Convolution

$$(f * g)(u) = \int f \uparrow^G (uv^{-1}) g \uparrow^G (v)d\mu(v)$$

Generalized
Group Convolution

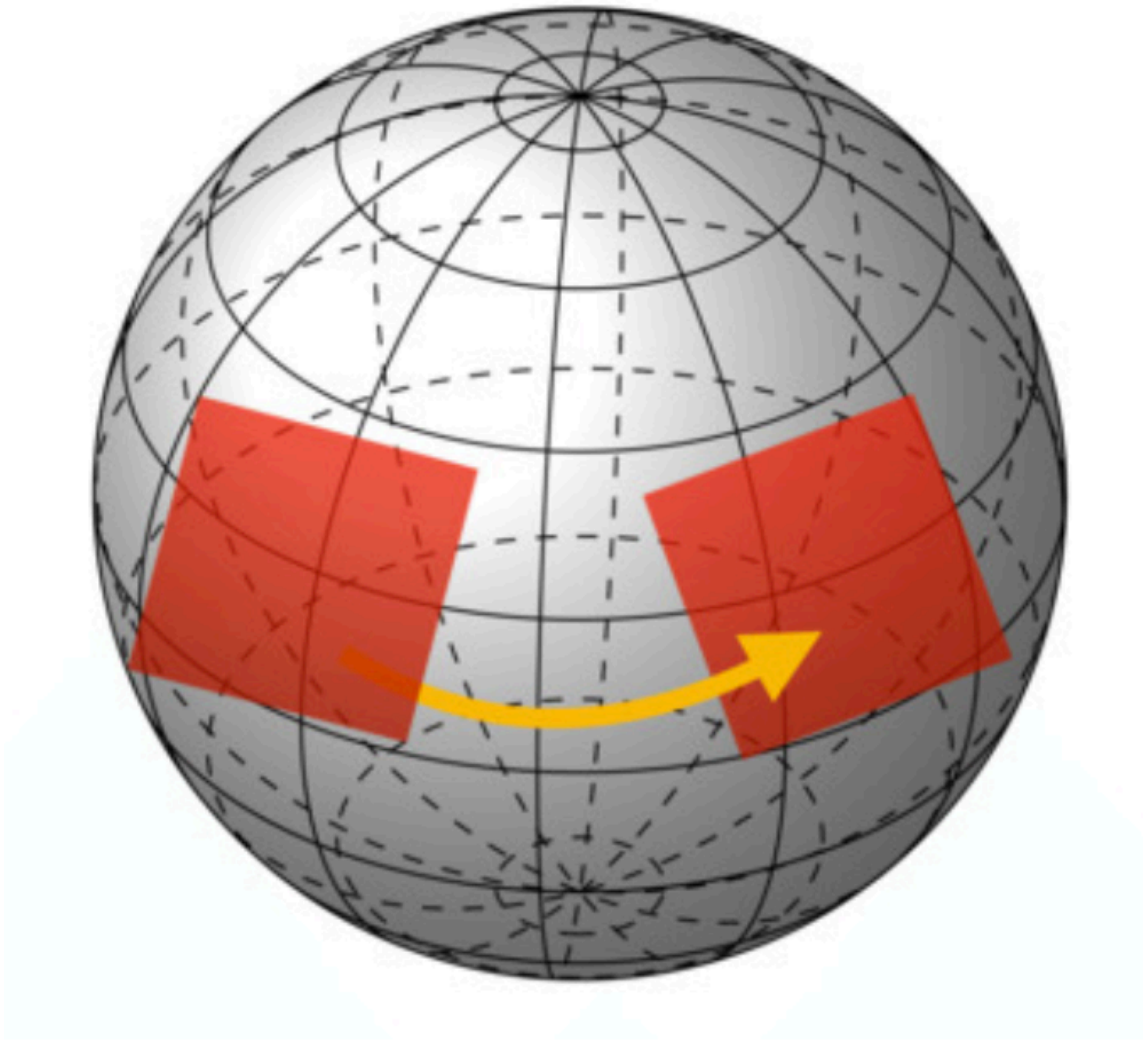


Fig Credit: https://slideslive.com/38943570/equivariant-networks

Convolutions is all you need!

Theorem 2: Let G be a compact group and $\mathcal{N}$ be a feed forward neural network in which all intermediate feature spaces are of the form $\mathcal{X}_l = G/H_l$. Then $\mathcal{N}$ is Equivariant to the action of G iff it is a G-CNN where each linear map ϕ_l is a generalized convolution.

Convolutions is all you need!

$Proof:$ (forward direction)

Relationship to Fourier Analysis Teasor

$$\hat{f}(k) = \int f(x)e^{-ikk}dx$$

$$\hat{f}(\rho_i) = \int f(x)\rho_i(x)d\mu$$

Irreps. Of G

Convolution Theorem

Nasty Integral over G

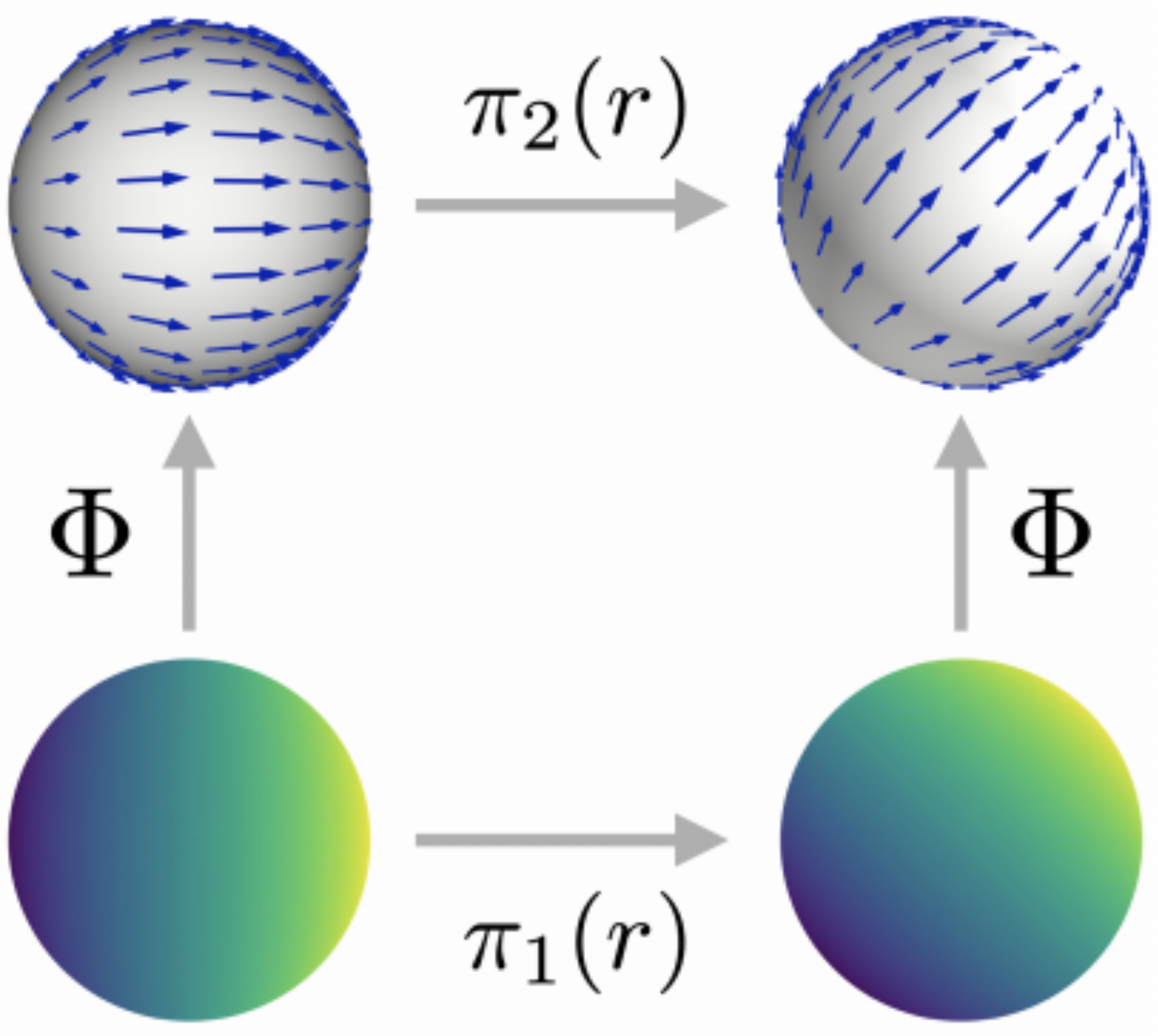
$$\widehat{f * g}(k) = \hat{f}(k)\hat{g}(k)$$

$$\widehat{f * g}(\rho_i) = \hat{f}(\rho_i)\hat{g}(\rho_i)$$

Matrix Product

Generalizing Convolutions to Feature Fields

Currently the generalized convolutions work with *scalar fields* but features can be vector fields or even tensor fields.

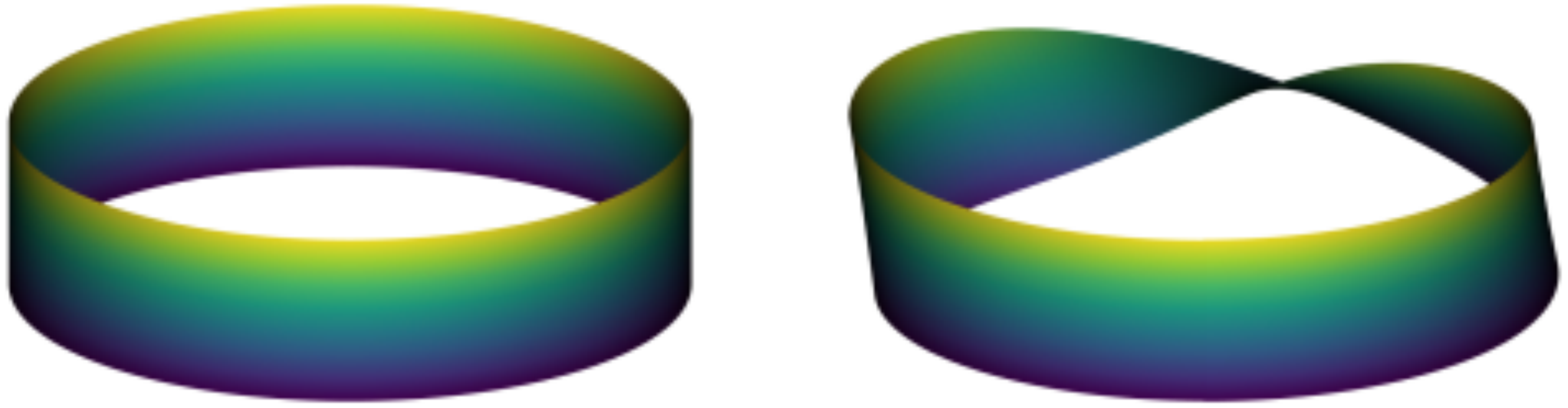


Vector Fields

Scalar fields

Fig credit: https://arxiv.org/pdf/1811.02017.pdf

Feature Fields: General Theory



Cylinder

Mobius Strip

Locally $S^1 \times [0,1]$

$S^1 \times [0,1]$ Locally

Sections s of a fiber bundle is an assignment to each $x \in B$ of an element $s(x) \in F_x$

<u>Fiber-bundle</u>

A fiber bundle (E, B, π) denoted $E \xrightarrow{\pi} B$ with

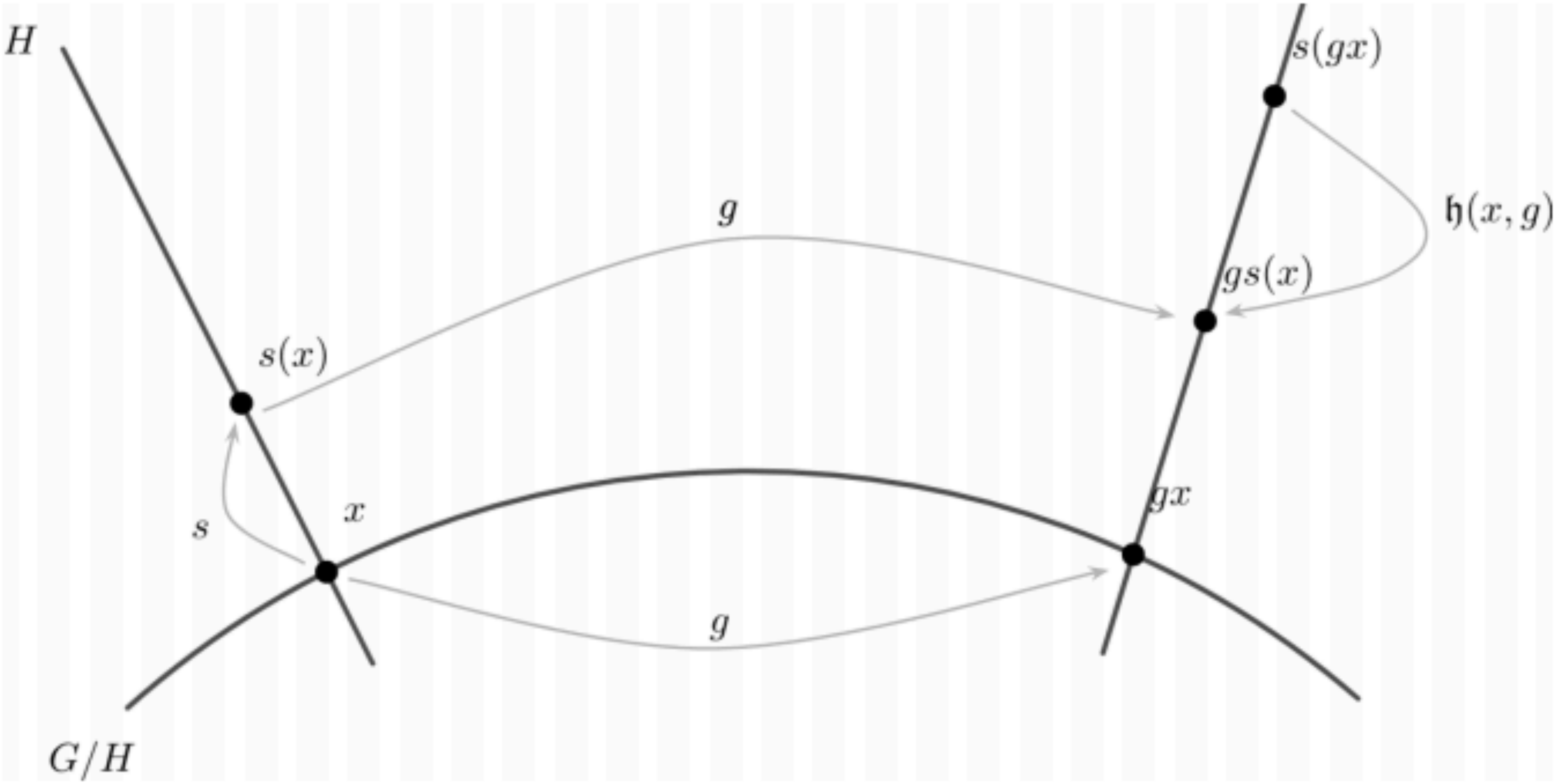
$\pi^{-1}(x)$ is isomorphic to a manifold F for every $x \in B$. The inverse map also locally trivializes the space over an open neighborhood $U \subset B$.

$$\pi^{-1}(U_i) \to B \times F$$

Fig credit: https://arxiv.org/pdf/1811.02017.pdf

Feature Fields: Principal Fiber Bundles

Group G and stabilizer subgroup H turns G into a "principal H-bundle"



Principal Fiber-bundle

A fiber bundle (E, B, π):

(i) G admits a right action on E.

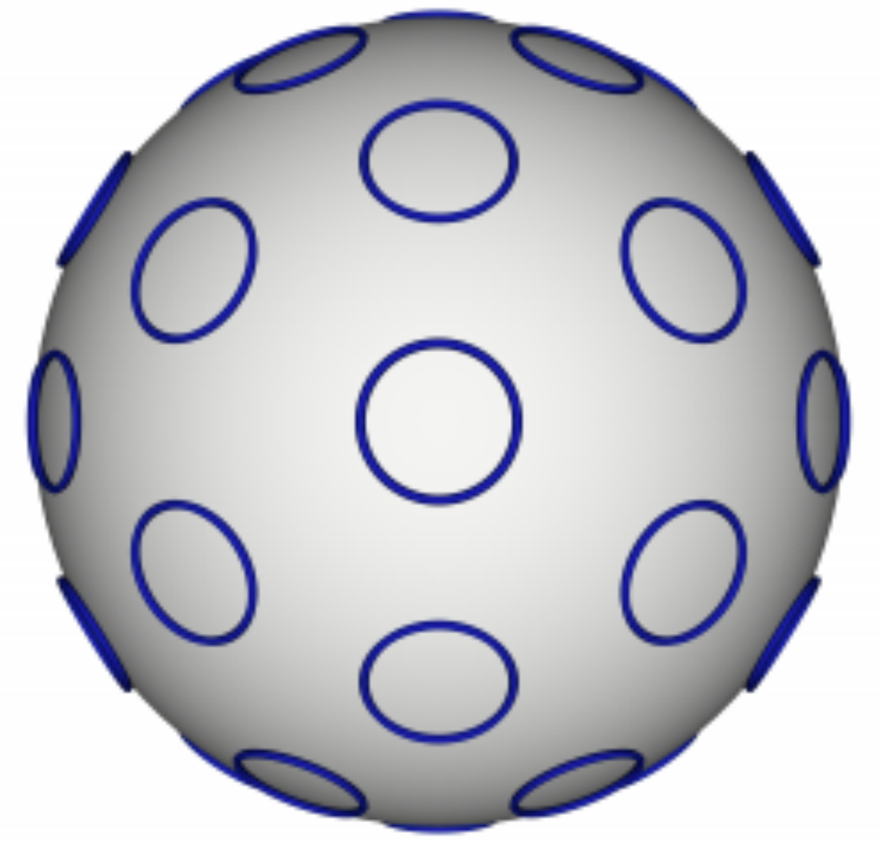
(ii) The Fiber F is home morphic to G

(iii) E/G is diffeomorphic to B

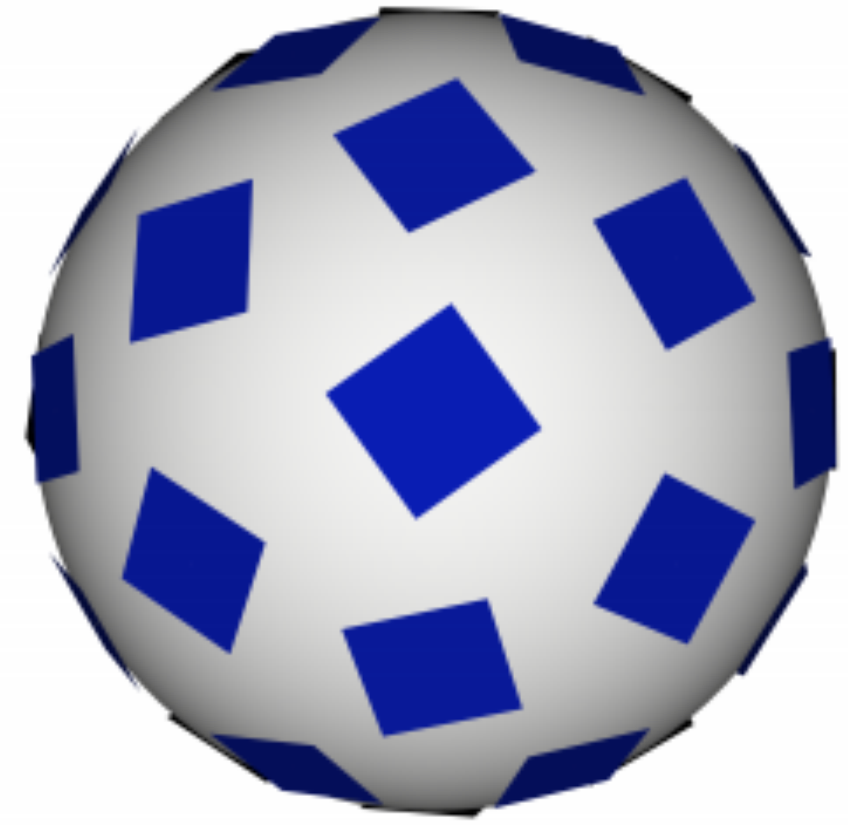
Fig credit: https://arxiv.org/pdf/2004.05154.pdf

Feature Fields: Associated Vector Bundles

Group G and stabilizer subgroup H turns G into a "principal H-bundle"



$S^2 \simeq SO(3)/SO(2)$

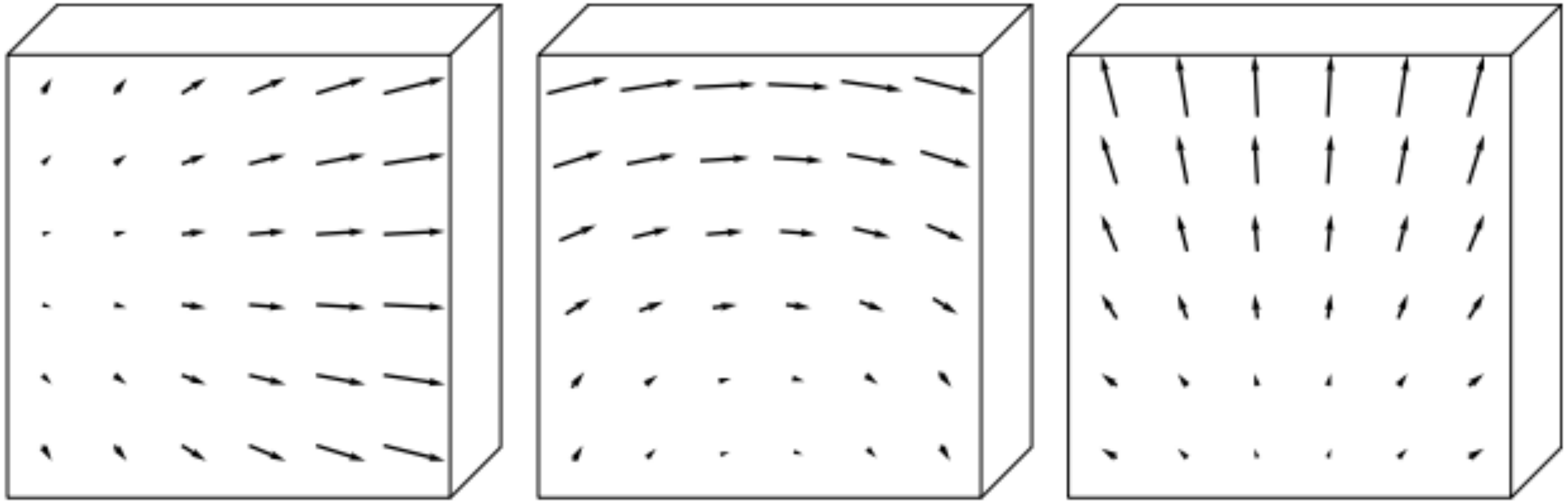


Attach a feature (vector) space $V_x \simeq V$ for each $x \in B$

V has a representation T of H

Fig credit: https://arxiv.org/pdf/1811.02017.pdf

Feature Fields: Transformations



$f(x)$ $\quad f(g^{-1}x)$ $\quad T_g f(g^{-1}x)$

$g \in SE(3)$

$g = tr,\ t \in \mathbb{R}^3,\ r \in SO(3)$

Induced representation of T of $SO(3)$

$\pi = \mathrm{Ind}_{SO(3)}^{SE(3)} T$

For scalar fields $T_g = I_n$

Fig credit: https://arxiv.org/pdf/1807.02547.pdf

Equivariant Maps and Convolutions

Each feature space in a G-CNN is defined as the space of sections of some associated vector bundle with $B = G/H$ and representation T of H that describes how the fibres transform.

The space of Equivariant linear maps between induced representations
$\mathscr{H} = \mathrm{Hom}_G(\mathscr{I}^1, \mathscr{I}^2) = \{\Phi \in \mathrm{Hom}_G(\mathscr{I}^1, \mathscr{I}^2) \,|\, \Phi T_{g1} = T_{g2}\Phi,\ \forall g \in G\}$

Convolution is all you need (revisited)

Theorem 3: An Equivariant map $\Phi \in \mathscr{H}$ can always be written as a convolution-like integral with two-argument linear operator-valued kernel $\kappa : G \times G \to \text{Hom}(V_1, V_2)$

Convolution is all you need (revisited)

$Proof:$

A word on Non-Linearities

Any point-wise Non-linearity will be Equivariant

Other option is a tensor product non-linearity ….