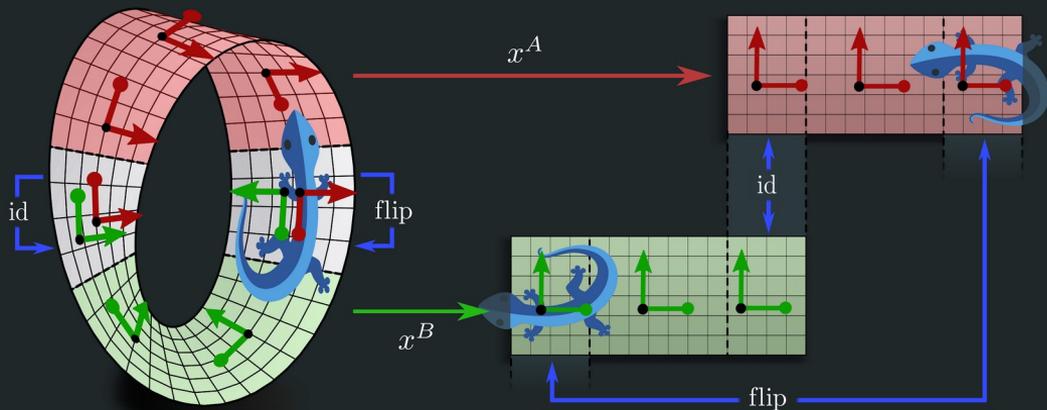


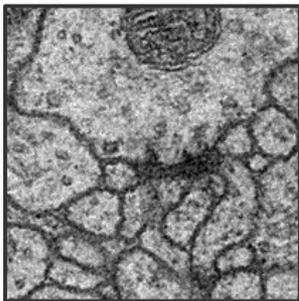
Equivariant & Coordinate Independent Convolutional Neural Networks

Maurice Weiler
AMLab, QUVA Lab
University of Amsterdam

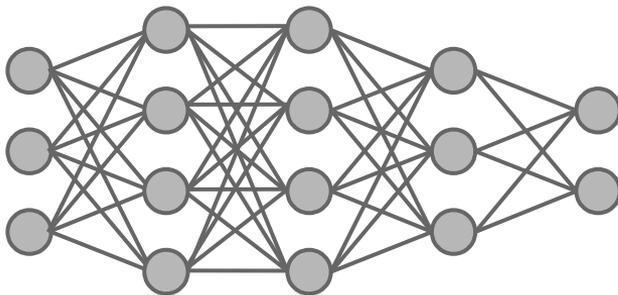
 @maurice_weiler



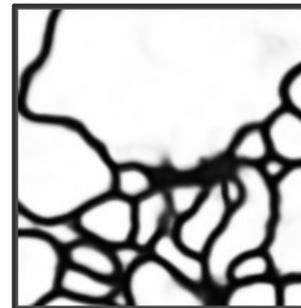
input



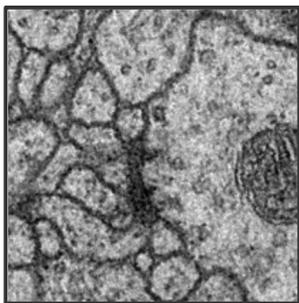
ML model f



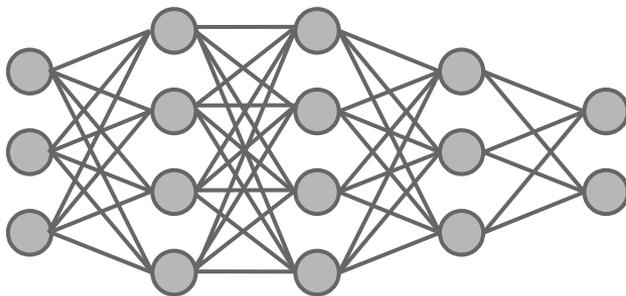
prediction



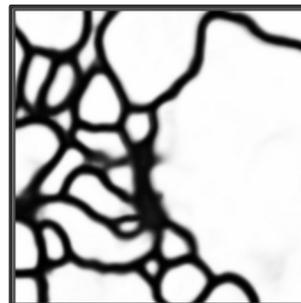
group
action



G -equivariance: $f \circ g = g \circ f \quad \forall g \in G$

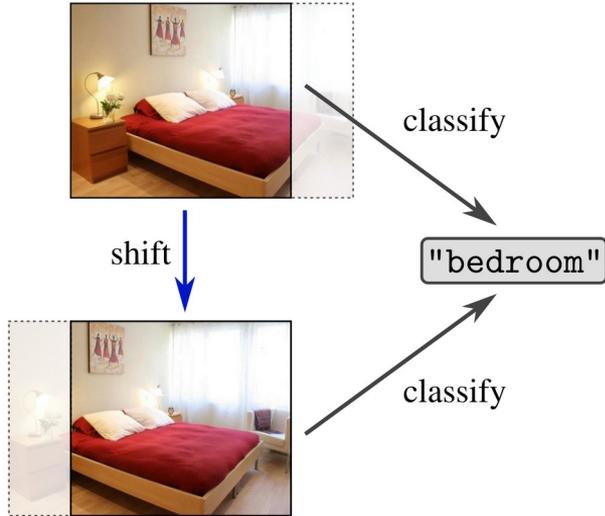


group
action

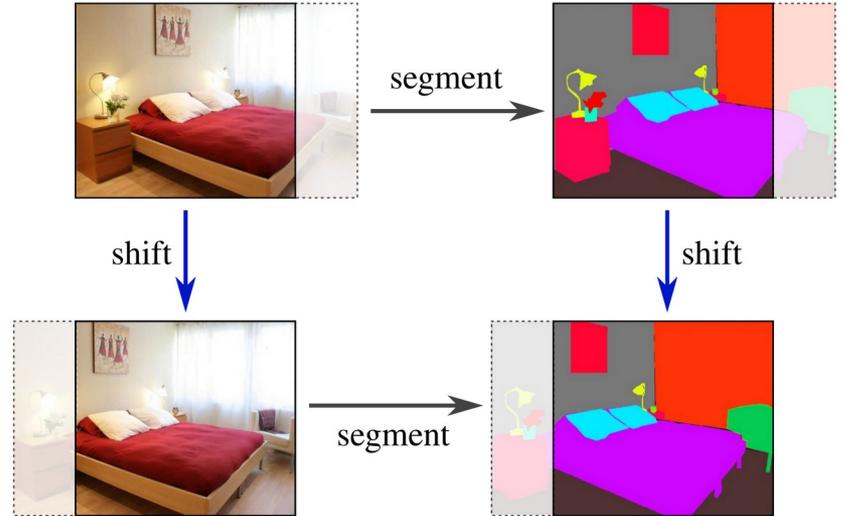


convolutional neural networks are **translation invariant / equivariant**

invariant image classification



equivariant image segmentation



research goals: generalize equivariant convolutions to...

...larger symmetry groups (of Euclidean spaces)

...more general manifolds

Outline

MLPs for image processing?

Translation equivariant CNNs

(Euclidean spaces)

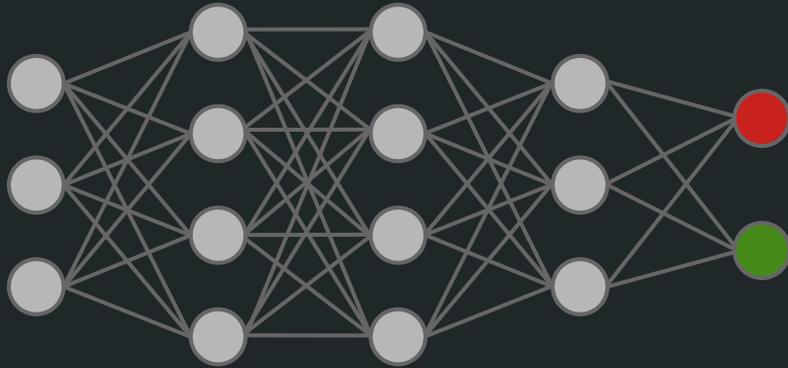
Affine equivariant CNNs

(Euclidean spaces)

Coordinate independent CNNs

(Riemannian manifolds)

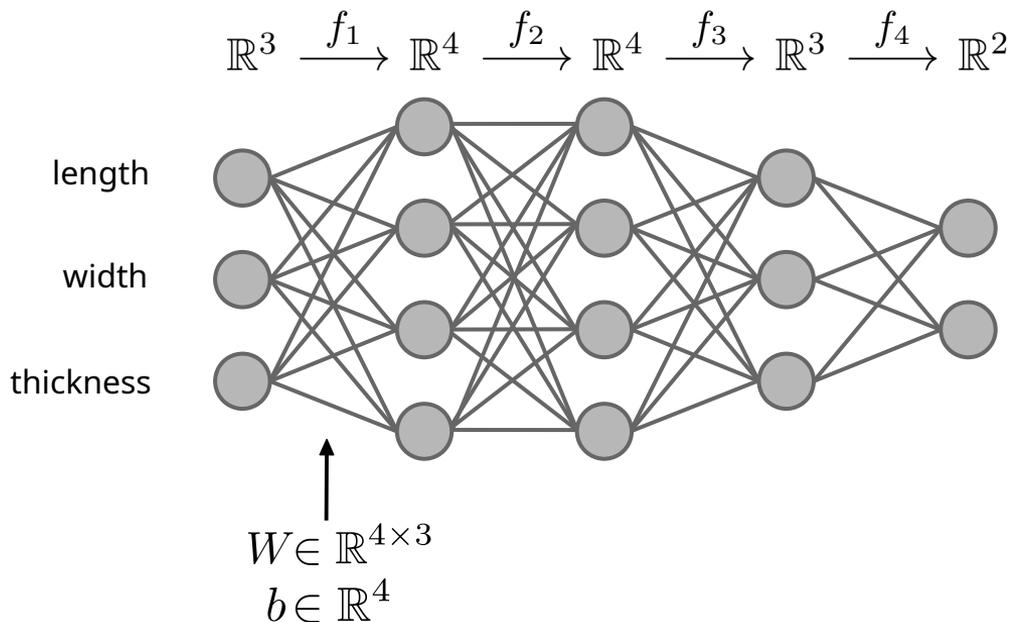
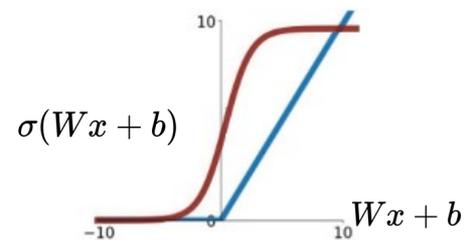
MLPs for image processing ?



Multilayer Perceptrons (MLPs)

universal function approximators $f: \mathbb{R}^N \rightarrow \mathbb{R}^M$

composed of affine maps + nonlinearities: $x_{i+1} = \sigma(Wx_i + b)$



length

width

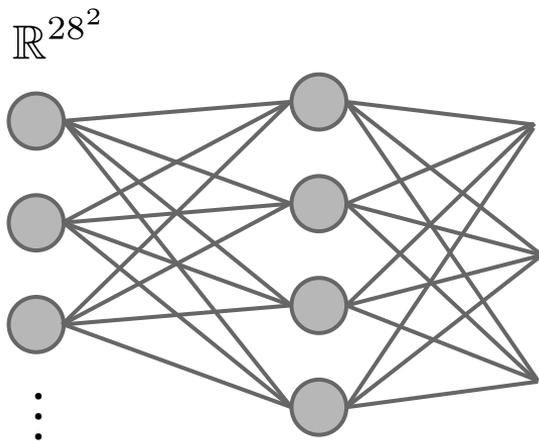
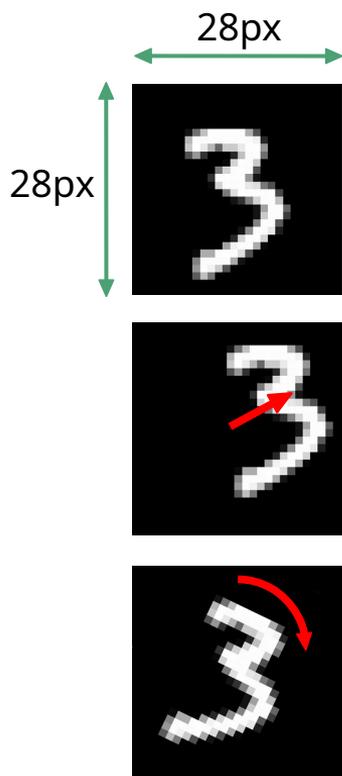
thickness

$p(\text{species A} \mid \text{iris})$

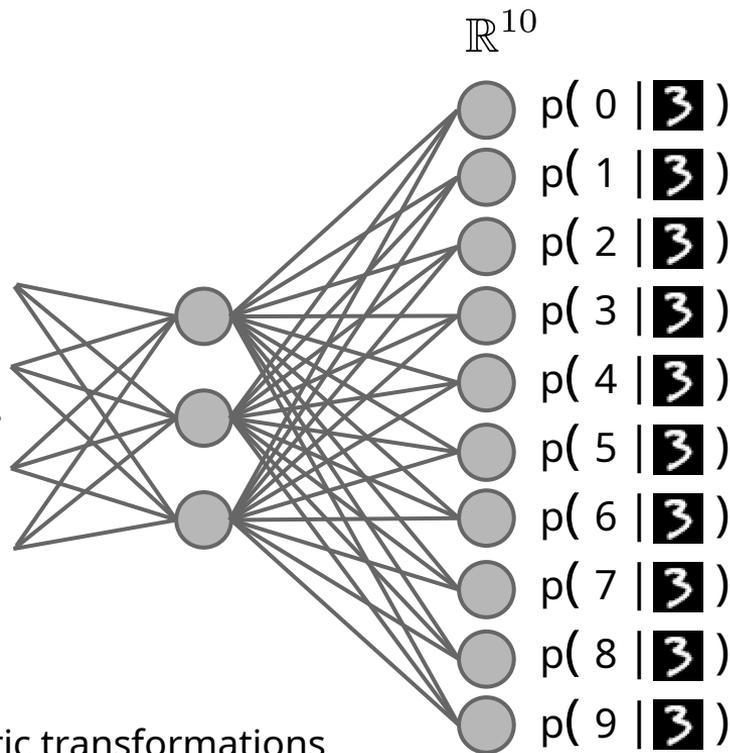
$p(\text{species B} \mid \text{iris})$

Multilayer Perceptrons (MLPs)

using MLPs for image processing



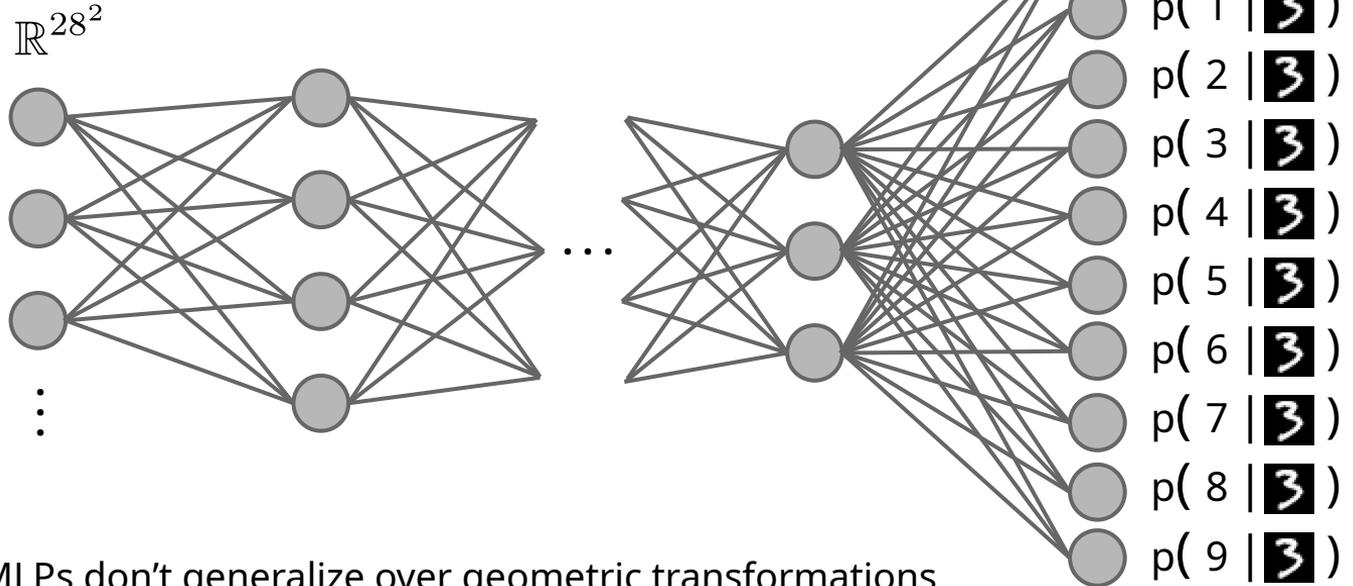
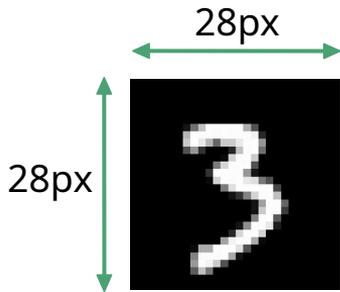
...



MLPs don't generalize over geometric transformations

Multilayer Perceptrons (MLPs)

using MLPs for image processing

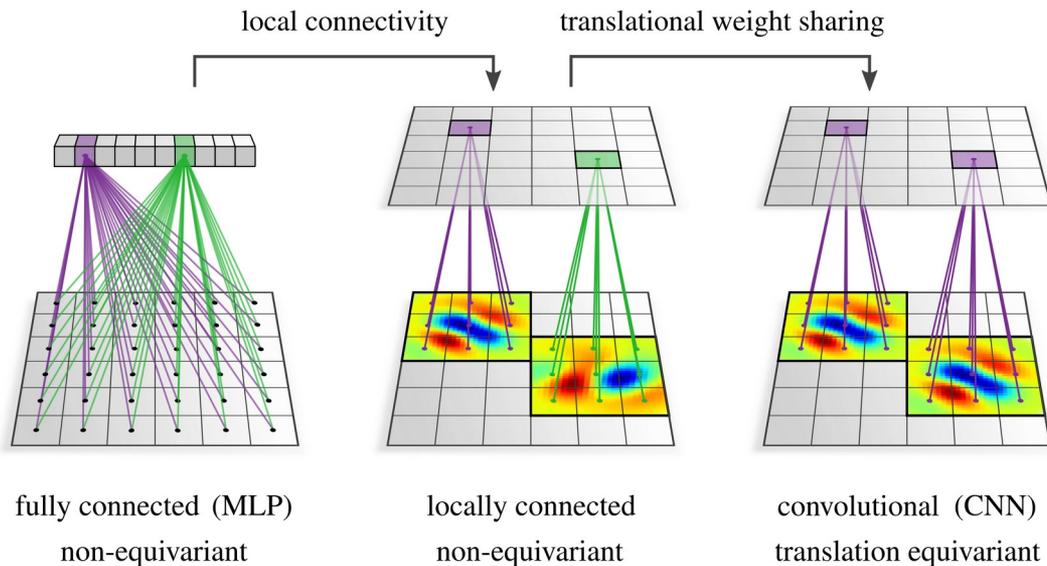


MLPs don't generalize over geometric transformations

MLPs are ignorant of the geometric arrangement of pixels
(any permutation of pixels would be equivalent)



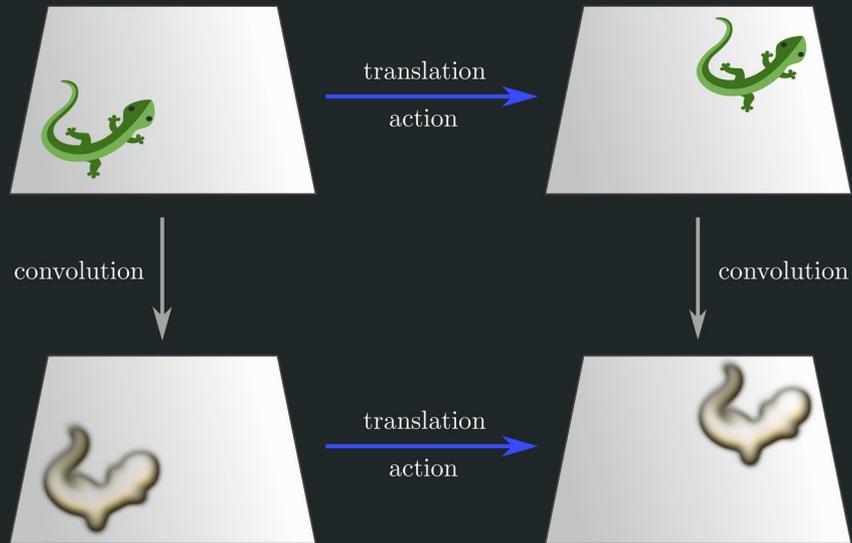
convolutional networks == MLPs + geometric inductive biases



usually: weight sharing \implies equivariance (sufficiency)

our approach: weight sharing \longleftarrow equivariance (necessity)

Translation equivariant CNNs on Euclidean spaces



Equivariant Neural Networks

(feed forward) neural networks are sequences of layers:

$$\mathcal{F}_0 \xrightarrow{L_1} \mathcal{F}_1 \xrightarrow{L_2} \mathcal{F}_2 \xrightarrow{L_3} \dots \xrightarrow{L_{N-1}} \mathcal{F}_{N-1} \xrightarrow{L_N} \mathcal{F}_N$$

equivariant NNs are sequences of equivariant layers:

$$\begin{array}{ccccccccccc} \mathcal{F}_0 & \xrightarrow{L_1} & \mathcal{F}_1 & \xrightarrow{L_2} & \mathcal{F}_2 & \xrightarrow{L_3} & \dots & \xrightarrow{L_{N-1}} & \mathcal{F}_{N-1} & \xrightarrow{L_N} & \mathcal{F}_N \\ \downarrow g \triangleright_0 & & \downarrow g \triangleright_1 & & \downarrow g \triangleright_2 & & & & \downarrow g \triangleright_{N-1} & & \downarrow g \triangleright_N \\ \mathcal{F}_0 & \xrightarrow{L_1} & \mathcal{F}_1 & \xrightarrow{L_2} & \mathcal{F}_2 & \xrightarrow{L_3} & \dots & \xrightarrow{L_{N-1}} & \mathcal{F}_{N-1} & \xrightarrow{L_N} & \mathcal{F}_N \end{array}$$

to design an equivariant network, we need to ...

... specify the *feature spaces* and *group actions* on them \rightarrow feature maps with translation action

... design *equivariant layers*, which commute with the group actions \rightarrow convolutions, bias summation, nonlinearities, etc.

Feature maps

discretized feature maps on \mathbb{R}^d are implemented as “tensors” of shape (X_1, \dots, X_d, C)

spatial / pixel dimensions feature channels

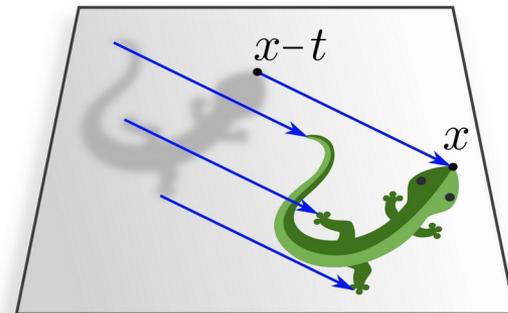
continuous feature maps are functions $f : \mathbb{R}^d \rightarrow \mathbb{R}^c$ that assign feature vectors $f(x) \in \mathbb{R}^c$ to points $x \in \mathbb{R}^d$

$$L^2(\mathbb{R}^d, \mathbb{R}^c) = \text{feature vector space}$$

linear

feature maps carry a translation **group action** $[t \triangleright f](x) := f(x - t)$

feature maps form the *regular* $(\mathbb{R}^d, +)$ -representation



Translation equivariant NNs

translation equivariant networks consist of layers $\mathcal{L} : L^2(\mathbb{R}^d, \mathbb{R}^{c_{\text{in}}}) \rightarrow L^2(\mathbb{R}^d, \mathbb{R}^{c_{\text{out}}})$ that ...

... map between c_{in} and c_{out} -dimensional input and output feature maps

... commute with the group action:

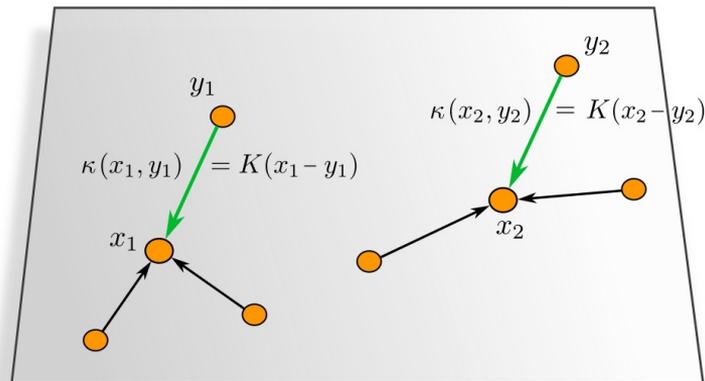
$$\begin{array}{ccc} L^2(\mathbb{R}^d, \mathbb{R}^{c_{\text{in}}}) & \xrightarrow{\mathcal{L}} & L^2(\mathbb{R}^d, \mathbb{R}^{c_{\text{out}}}) \\ \downarrow t \triangleright_{\text{in}} & & \downarrow t \triangleright_{\text{out}} \\ L^2(\mathbb{R}^d, \mathbb{R}^{c_{\text{in}}}) & \xrightarrow{\mathcal{L}} & L^2(\mathbb{R}^d, \mathbb{R}^{c_{\text{out}}}) \end{array}$$

Linear equivariant maps \Leftrightarrow convolutions

ansatz for linear map:

generic integral transform
$$\mathbb{I}_\kappa[f](x) := \int_{\mathbb{R}^d} dy \kappa(x, y) f(y)$$

parameterized by 2-point correlator
$$\kappa : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}$$



Theorem (linearity + translation equivariance \Rightarrow convolution)

The integral transform \mathbb{I}_κ is translation equivariant iff the 2-point correlator is *invariant*:

$$\kappa(x + t, y + t) = \kappa(x, y) \quad \forall x, y, t \in \mathbb{R}^d$$

It depends only on the *relative distance* $x - y$, that is,

$$\kappa(x, y) = K(x - y) \quad \text{for some } K : \mathbb{R}^d \rightarrow \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}$$

The integral transform is therefore given by a *convolution integral*:

$$\mathbb{I}_\kappa[f](x) = [K * f](x) = \int_{\mathbb{R}^d} dy K(x - y) f(y)$$

on pixel grids: tensors of shape

$$\underbrace{(X_1, \dots, X_d)}_{\mathbb{R}^d} \rightarrow \underbrace{(C_{\text{out}}, C_{\text{in}})}_{\mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}}$$

Translation equivariant bias summation

consider a general bias summation operation $f \mapsto f + \mathfrak{b}$

parameterized by a **bias field** $\mathfrak{b} : \mathbb{R}^d \rightarrow \mathbb{R}^c \implies$ allows to sum a *different bias* $\mathfrak{b}(x) \in \mathbb{R}^c$ at each $x \in \mathbb{R}^d$

Theorem (translation equivariant bias summation)

Bias summation is translation equivariant iff the bias field is *invariant*:

$$\mathfrak{b}(x) = b \quad \text{for some } b \in \mathbb{R}^c \text{ and any } x \in \mathbb{R}^d$$

similar *spatial invariance* results hold for other operations like nonlinearities, pooling, ...

Translation equivariant CNNs - Summary

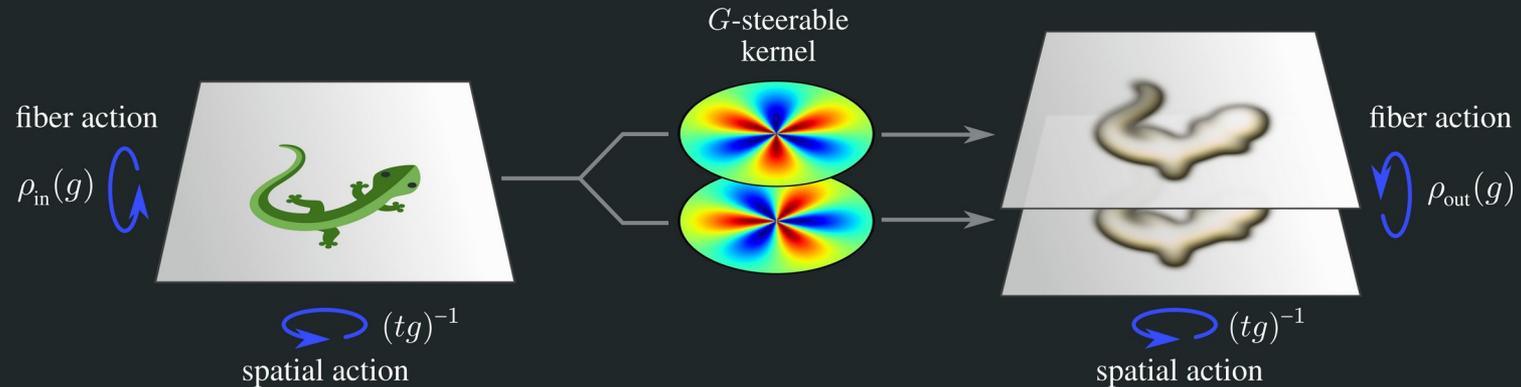
we defined **feature vector spaces** as spaces of feature maps
we defined a (linear) **translation group action** on feature maps } (regular) **translation group representation**

we derived **CNN operations** like convolutions / bias summation / etc by:

- 1) assuming a flexible **ansatz** (linear map, bias field summation)
- 2) demanding **translation equivariance** → resulting in **spatial invariance / relativity / weight sharing**

next we do the same with more general symmetries of Euclidean space

Steerable CNNs on Euclidean spaces

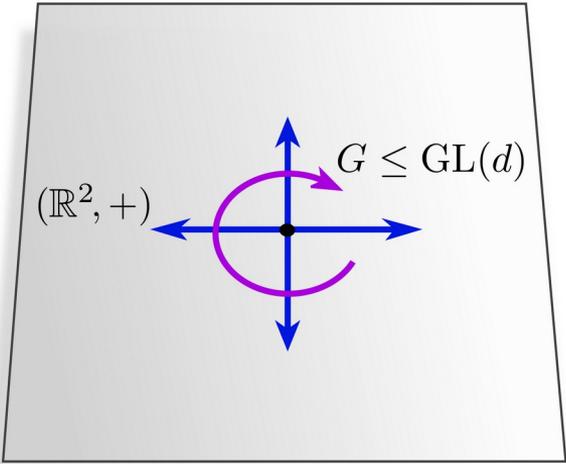
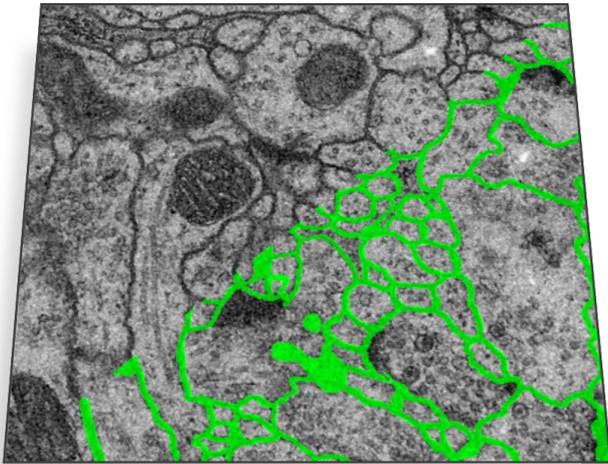


Affine group equivariant CNNs

affine groups: $\text{Aff}(G) := (\mathbb{R}^d, +) \rtimes G$ $G \leq \text{GL}(d)$

translations
stabilizer / local symmetries (rotations / reflections / scaling / shearing / ...)

action on \mathbb{R}^d : $(tg)x := gx + t$



Affine group equivariant CNNs

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action on feature spaces ?

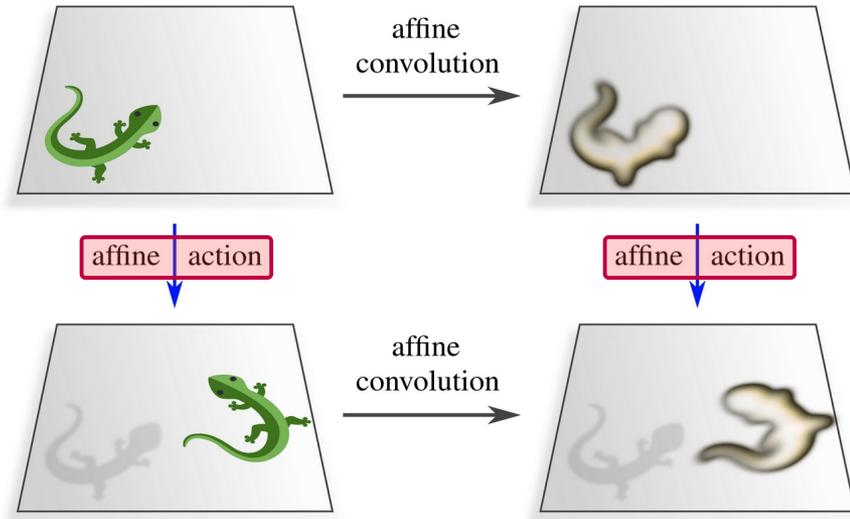


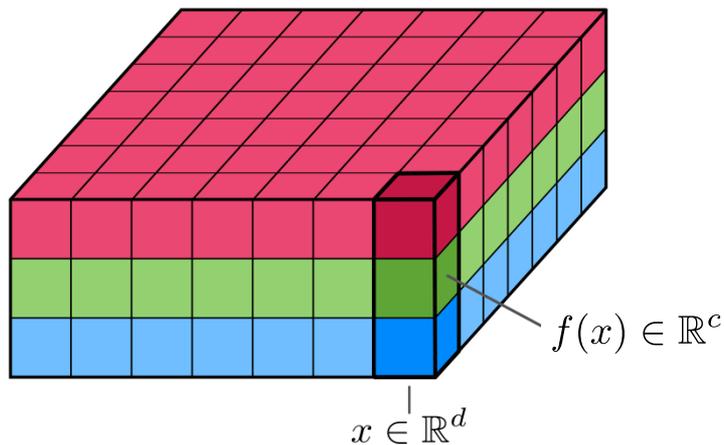
Image from ISBI 2012 EM segmentation challenge

Feature vector fields

feature vector fields on Euclidean spaces ...

... are functions $f : \mathbb{R}^d \rightarrow \mathbb{R}^c$ that assign feature vectors $f(x) \in \mathbb{R}^c$ to points $x \in \mathbb{R}^d$ (like feature maps)

... carry an $\text{Aff}(G)$ -action (the details depend on their *field type* ρ)



Feature vector fields

feature vector fields on Euclidean spaces ...

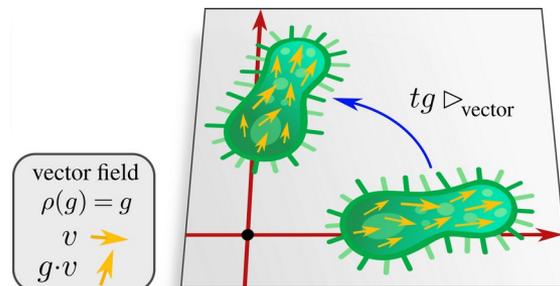
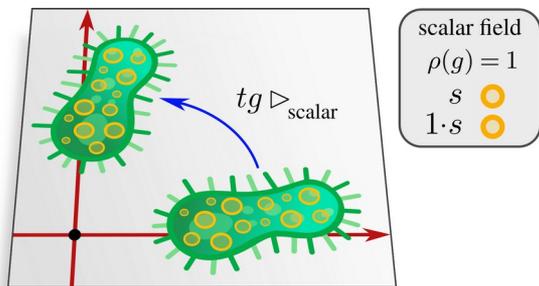
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... carry an $\text{Aff}(G)$ -action (the details depend on their *field type* ρ)

examples: scalar fields $s : \mathbb{R}^d \rightarrow \mathbb{R}^1$ transform like: $[(tg) \triangleright s](x) = 1 \cdot s((tg)^{-1}x)$

tangent vector fields $v : \mathbb{R}^d \rightarrow \mathbb{R}^d$ transform like: $[(tg) \triangleright v](x) = g \cdot v((tg)^{-1}x)$

$\text{Aff}(G)$ acts here by...
1) moving feature vectors on \mathbb{R}^d
2) G -transforming feature vectors in \mathbb{R}^c



Feature vector fields

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$\text{Aff}(G)$ acts here by...
1) moving feature vectors on \mathbb{R}^d
2) G -transforming feature vectors in \mathbb{R}^c

ρ -feature fields $f : \mathbb{R}^d \rightarrow \mathbb{R}^c$ transform like: $[(tg) \triangleright f](x) = \rho(g) f((tg)^{-1}x)$

where $\rho : G \rightarrow \text{GL}(c)$ is a G -representation acting on individual feature vectors in \mathbb{R}^c

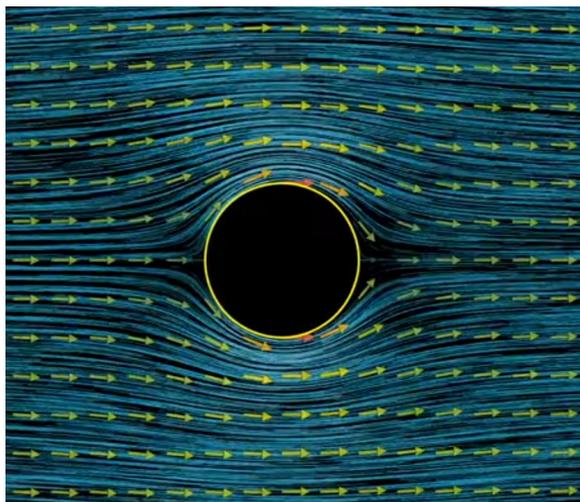
ρ -feature fields form an $\text{Aff}(G)$ -representation, denoted as **induced representation** $\text{Ind}_G^{\text{Aff}(G)} \rho$

Feature vector fields - examples

fluid flow

(vector)

$$\rho(g) = g$$



optical flow

(vector)

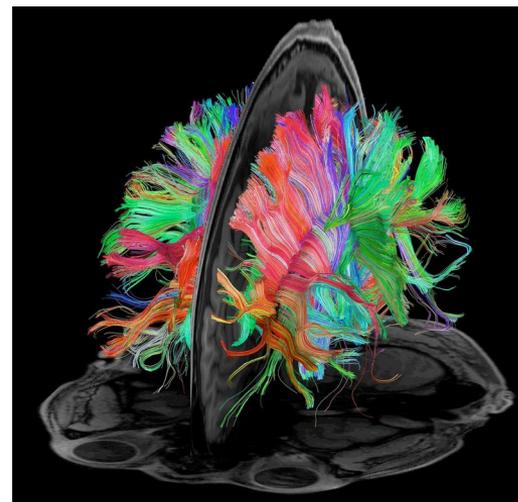
$$\rho(g) = g$$



diffusion tensor image

(symmetric pos. def. (1,1)-tensor)

(subspace of) $\rho(g) = g \otimes g^{-T}$



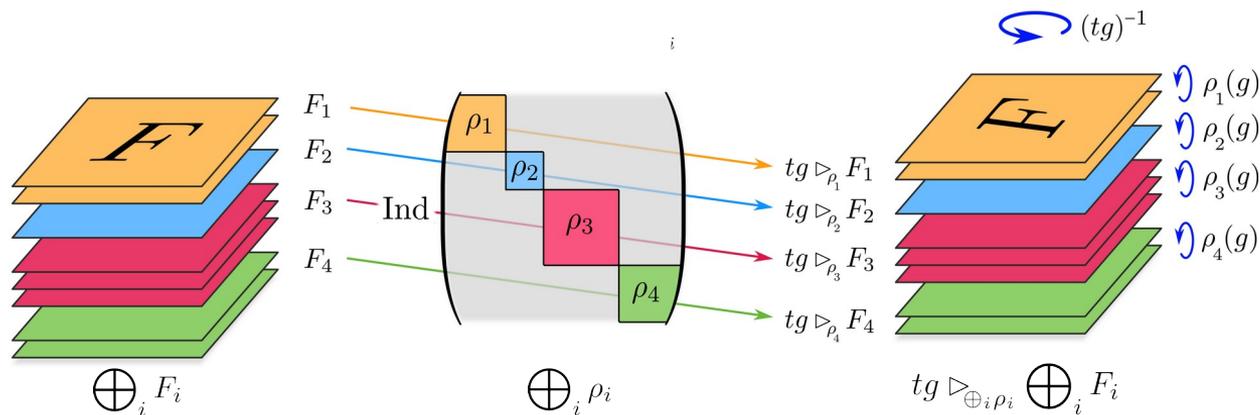
Feature vector fields – direct sum

conventional CNNs operate on a “stack” of multiple independent feature map channels

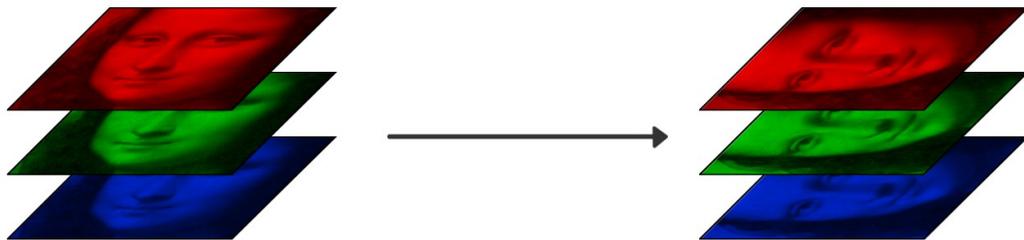
⇒ #channels as hyperparameter

steerable CNNs operate on “stacks” $\bigoplus_i f_i$ of multiple independent feature fields

⇒ field types ρ_i and multiplicities as hyperparameters

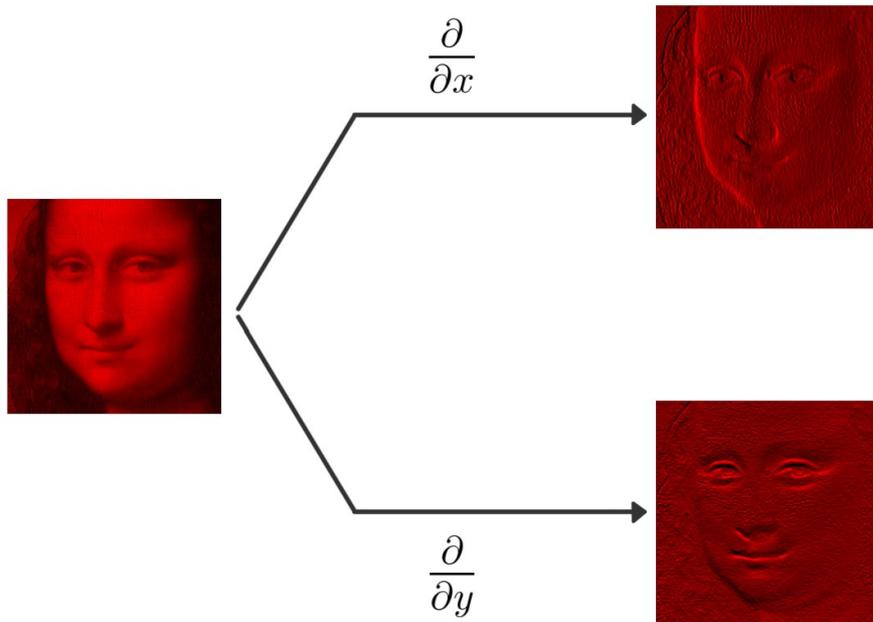


Feature vector fields - examples

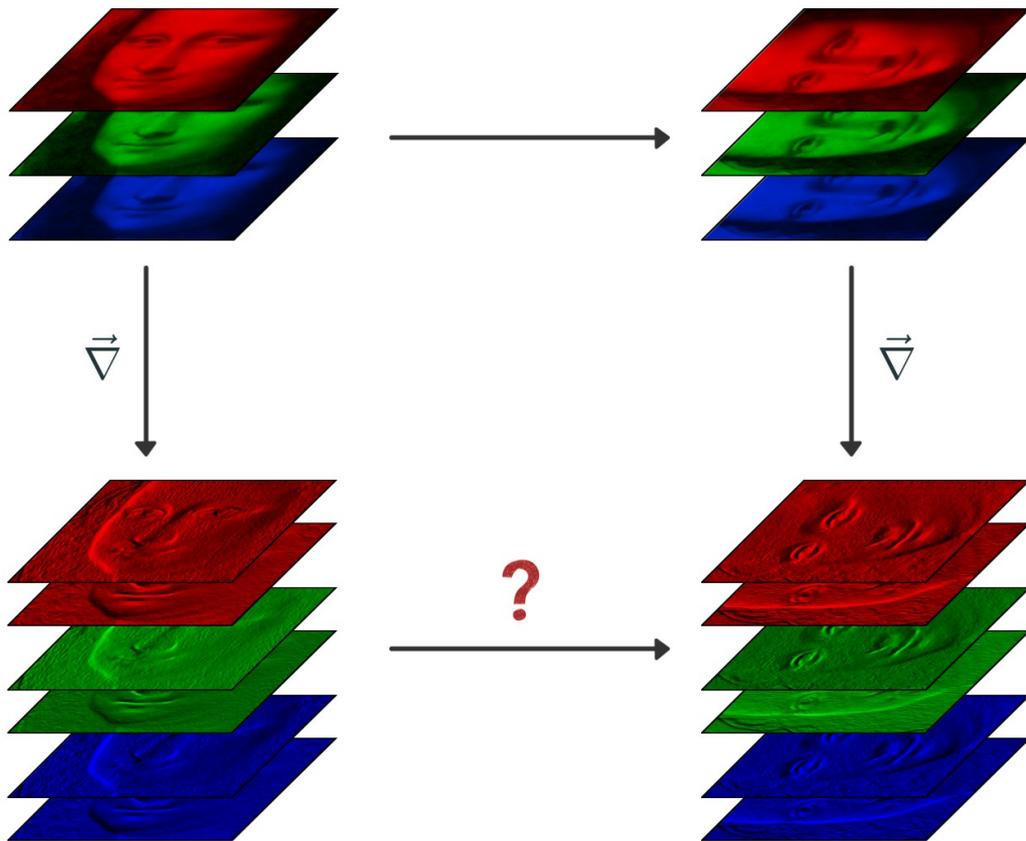


$$\begin{pmatrix} r \\ g \\ b \end{pmatrix} \rightarrow \underbrace{\begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}}_{\rho(g) = \bigoplus_{i=1}^3 (1)} \cdot \begin{pmatrix} r \\ g \\ b \end{pmatrix}$$

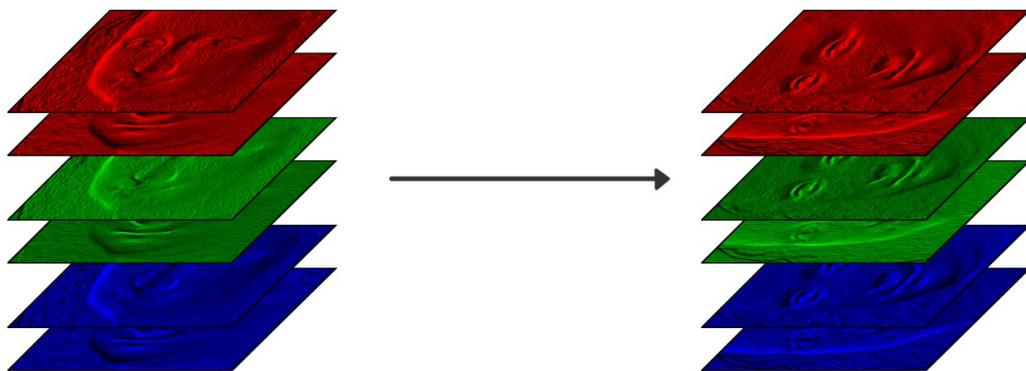
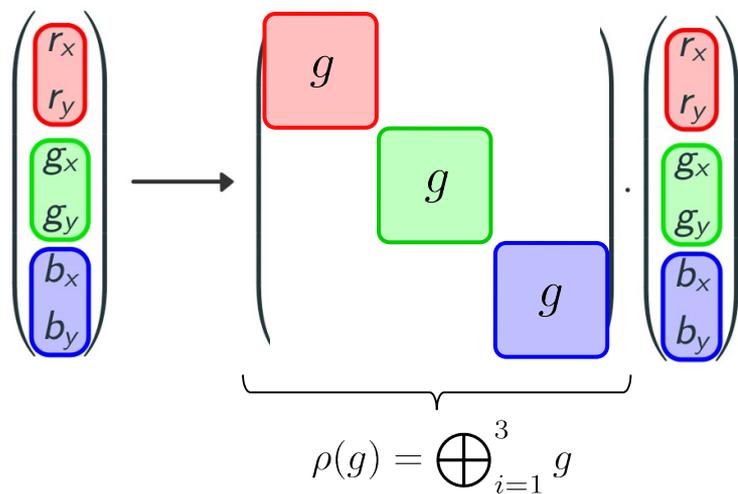
Feature vector fields - examples



Feature vector fields - examples



Feature vector fields - examples



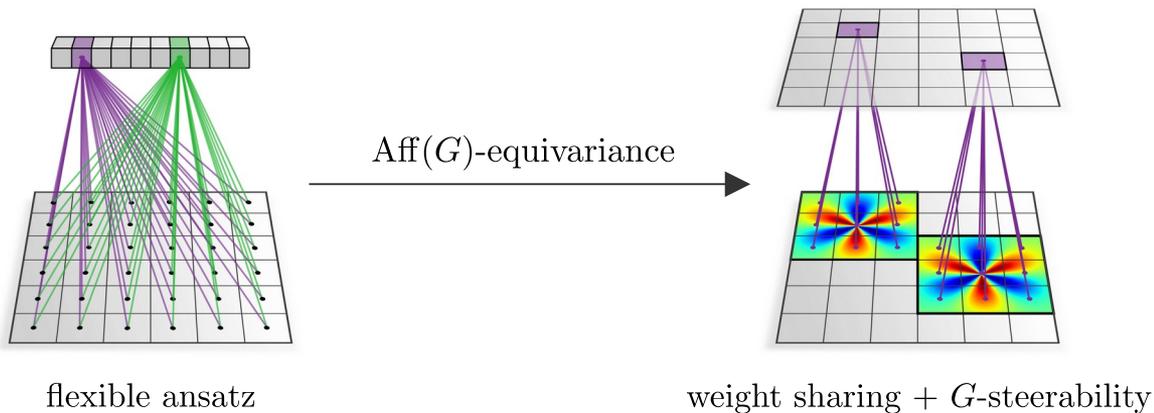
Steerable CNNs

Steerable CNN layers map between feature fields of types ρ_{in} and ρ_{out}

$$\begin{array}{ccc} \mathcal{L}^2(\mathbb{R}^d, \mathbb{R}^{c_{\text{in}}}) & \xrightarrow{L} & \mathcal{L}^2(\mathbb{R}^d, \mathbb{R}^{c_{\text{out}}}) \\ \text{Ind } \rho_{\text{in}}(tg) \downarrow & & \downarrow \text{Ind } \rho_{\text{out}}(tg) \\ \mathcal{L}^2(\mathbb{R}^d, \mathbb{R}^{c_{\text{in}}}) & \xrightarrow{L} & \mathcal{L}^2(\mathbb{R}^d, \mathbb{R}^{c_{\text{out}}}) \end{array}$$

Steerable CNNs

Steerable CNN layers map between feature fields of types ρ_{in} and ρ_{out}



approach: - start with flexible ansatz for layers

- demand $\text{Aff}(G)$ -equivariance, resulting in...

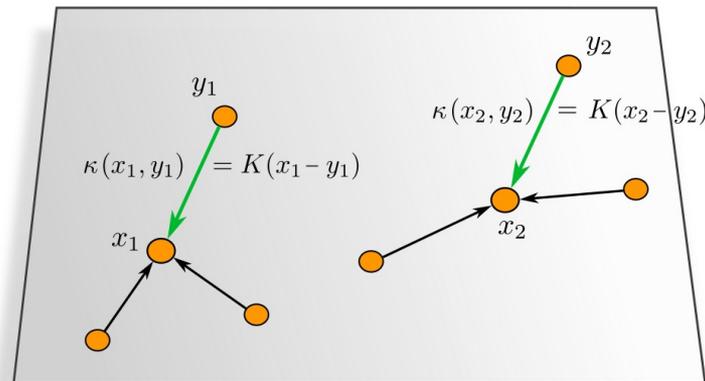
- 1) spatial weight sharing ————— $(\mathbb{R}^d, +) \rtimes G =: \text{Aff}(G)$
- 2) G -steerability —————

Linear equivariant maps $\Leftrightarrow G$ -steerable convolutions

ansatz for linear map:

generic integral transform
$$\mathbb{I}_\kappa[f](x) := \int_{\mathbb{R}^d} dy \kappa(x, y) f(y)$$

parameterized by 2-point correlator
$$\kappa : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}$$



demanding $\text{Aff}(G)$ -equivariance:

Theorem. *The integral transform \mathbb{I}_κ is $\text{Aff}(G)$ equivariant iff:*

1) *it is a convolution integral*

$$\mathbb{I}_\kappa[f](x) = [K * f](x) = \int_{\mathbb{R}^d} dy K(x - y) f(y).$$

with a matrix valued kernel $K : \mathbb{R}^d \rightarrow \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}$ defined by translation relativity $\kappa(x, y) = K(x - y)$

2) *the kernel is G -steerable: $K(gx) = \frac{1}{|\det g|} \rho_{\text{out}}(g) K(x) \rho_{\text{in}}(g)^{-1} \quad \forall g \in G, x \in \mathbb{R}^d$*

Linear equivariant maps $\Leftrightarrow G$ -steerable convolutions

ansatz for linear map:

generic integral transform $\mathbb{I}_\kappa[f](x) := \int_{\mathbb{R}^d} dy \kappa(x, y) f(y)$

parameterized by 2-point correlator $\kappa : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}$

$$\begin{array}{ccc} \mathbb{R}^d & \xrightarrow{K} & \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}} \\ \downarrow g \cdot & & \downarrow \frac{\rho_{\text{in}}^* \otimes \rho_{\text{out}}}{|\det|}(g) \\ \mathbb{R}^d & \xrightarrow{K} & \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}} \end{array}$$

demanding $\text{Aff}(G)$ -equivariance:

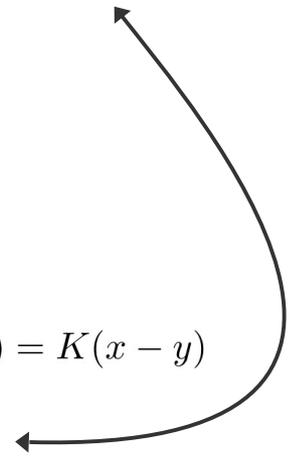
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Linear equivariant maps $\Leftrightarrow G$ -steerable convolutions

ansatz for linear map:

$$\text{general form: } f \mapsto [c](f) = \int_{\mathbb{R}^d} \tau_x(f) \cdot c(x) \, dx \quad \mathbb{R}^d \xrightarrow{K} \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}$$

takeaway:

linearity + translation equivariance \Leftrightarrow convolution

linearity + $\text{Aff}(G)$ equivariance \Leftrightarrow convolution with G -steerable kernel

$$\frac{\rho_{\text{in}}^* \otimes \rho_{\text{out}}(g)}{|\det|} \quad c_{\text{in}}$$

demanding $\text{Aff}(G)$ equivariance:

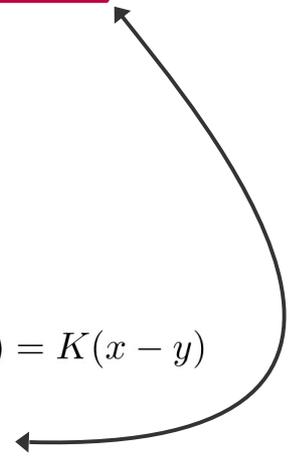
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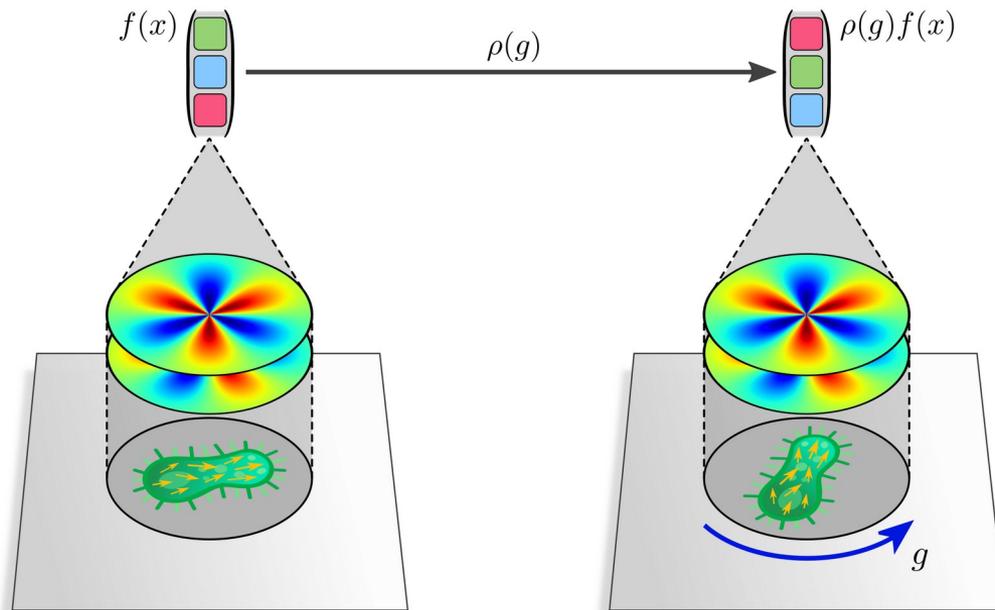
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G -steerable kernels

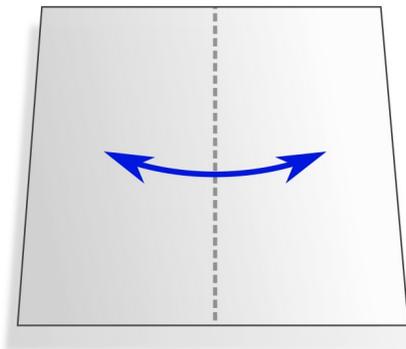
convolution kernels summarize their field of view around $x \in \mathbb{R}^d$ into a feature vector $f(x) \in \mathbb{R}^{c_{out}}$

G -steerable kernels guarantee: G -trafo of their input field of view \Rightarrow G -trafo of the output feature vector



G -steerable kernels – reflection group example

example: *reflection* steerable kernels $G = \{e, s\}, \quad s^2 = e$



G -steerable kernels – reflection group example

example: *reflection* steerable kernels $G = \{e, s\}, \quad s^2 = e$

field type ρ	$\rho(e)$	$\rho(s)$	original field	transformed field
trivial / scalar	(1)	(1)		
sign-flip / pseudo-scalar	(1)	(-1)		
regular	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$		

G -steerable kernels – reflection group example

example: *reflection* steerable kernels $G = \{e, s\}$, $s^2 = e$

general steerability constraint: $K(gx) = \frac{1}{|\det g|} \rho_{\text{out}}(g) K(x) \rho_{\text{in}}(g) \quad \forall g \in G, x \in \mathbb{R}^2$

$|\det g| = 1$ $g = g^{-1}$ constraint for $g = e$ trivial, only $g = s$ left

\Rightarrow specific reflection steerably constraint: $K(sx) = \rho_{\text{out}}(s) K(x) \rho_{\text{in}}(s) \quad \forall x \in \mathbb{R}^2$

spatially
reflected
kernel

channel-
transformed
kernel

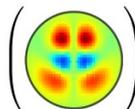
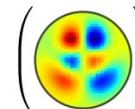
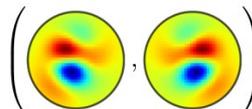
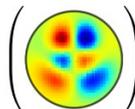
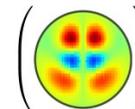
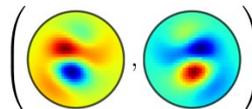
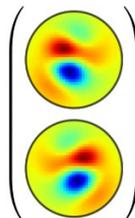
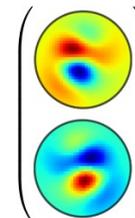
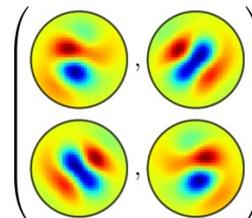
G -steerable kernels – reflection group examples

example: *reflection* steerable kernels

• **regular** \rightarrow **regular**: $K : \mathbb{R}^2 \rightarrow \mathbb{R}^{2 \times 2}$

$$\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix}(s \cdot x) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix}(x) \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} K_{22} & K_{21} \\ K_{12} & K_{11} \end{bmatrix}(x)$$

representation ρ	group elements	
	identity e	reflection s
trivial / scalar	(1)	(1)
sign-flip / pseudo-scalar	(1)	(-1)
regular	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\rho_{\text{out}} \backslash \rho_{\text{in}}$	trivial	sign-flip	regular
trivial	$K_{11}(sx) = K_{11}(x)$ 	$K_{11}(sx) = -K_{11}(x)$ 	$K_{11}(sx) = K_{12}(x)$ 
sign-flip	$K_{11}(sx) = -K_{11}(x)$ 	$K_{11}(sx) = K_{11}(x)$ 	$K_{11}(sx) = -K_{12}(x)$ 
regular	$K_{11}(sx) = K_{21}(x)$ 	$K_{11}(sx) = -K_{21}(x)$ 	$K_{11}(sx) = K_{22}(x)$ $K_{12}(sx) = K_{21}(x)$ 

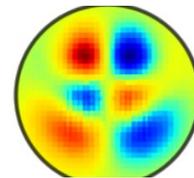
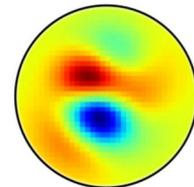
G -steerable kernels – expansion in linear basis

to solve the G -steerability kernel constraint in general, observe that:

- the set $\{K : \mathbb{R}^d \rightarrow \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}\}$ of *unconstrained* convolution kernels forms a *vector space*

- the constraint $K(gx) = \frac{1}{|\det g|} \rho_{\text{out}}(g) K(x) \rho_{\text{in}}(g)^{-1} \quad \forall g \in G, x \in \mathbb{R}^d$ is *linear*

\implies G -steerable kernels form a *linear (vector) subspace* !



to parameterize steerable convolutions:

1) solve for a *basis* $\{K_1, \dots, K_N\}$ of G -steerable kernels (precomputation step)

2) expand kernel in this basis with trainable weights: $K = \sum_{i=1}^N w_i K_i$ (during forward pass)

G -steerable kernels – Wigner-Eckart theorem

analytical solution for compact G

(including in particular any $G \leq O(d)$)

based on an analogy: G -steerable kernels \Leftrightarrow tensor operators in QM

A WIGNER-ECKART THEOREM FOR GROUP EQUIVARIANT CONVOLUTION KERNELS

Leon Lang*
AMLab, CSL
University of Amsterdam
l.lang@uva.nl

Maurice Weiler
AMLab, QUVA Lab
University of Amsterdam
m.weiler.ml@gmail.com

A PROGRAM TO BUILD $E(n)$ -EQUIVARIANT STEERABLE CNNs

Gabriele Cesa
Qualcomm AI Research*
University of Amsterdam
gcesa@qti.qualcomm.com

Leon Lang
University of Amsterdam
l.lang@uva.nl

Maurice Weiler
University of Amsterdam
m.weiler.ml@gmail.com



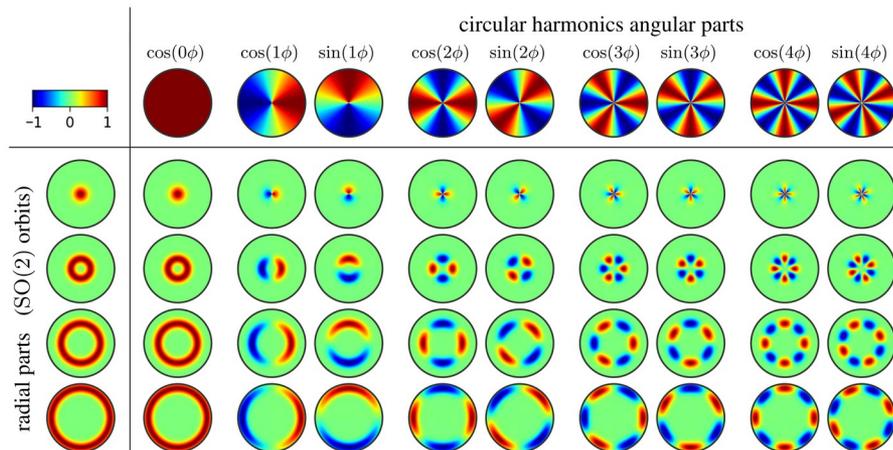
Leon Lang



Gabriele Cesa

the solution decomposes steerable kernels into:

- harmonics on G -orbits (Peter-Weyl)
- Clebsch-Gordan coefficients
- irrep endomorphisms (reduced matrix elements)



G -steerable kernels – Wigner-Eckart theorem

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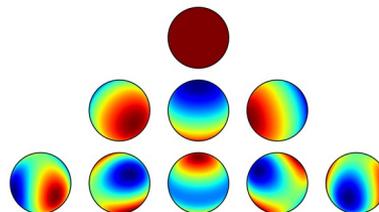
Leon Lang



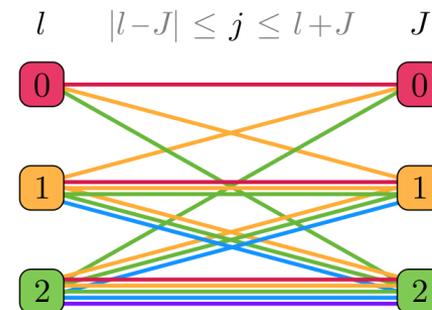
Gabriele Cesa

the solution decomposes steerable kernels into:

- harmonics on G -orbits (Peter-Weyl)
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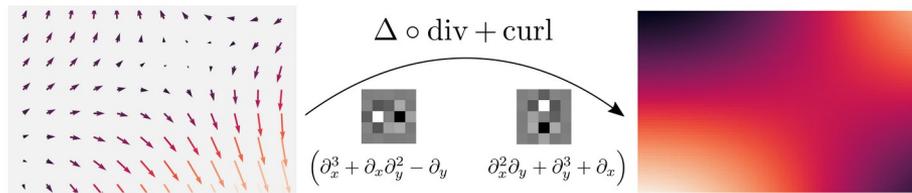


we get *transition rules* between irrep-fields (as in quantum mechanics)



transition rules for $SO(3)$

Linear equivariant maps $\Leftrightarrow G$ -steerable convolutions



STEERABLE PARTIAL DIFFERENTIAL OPERATORS FOR EQUIVARIANT NEURAL NETWORKS

Erik Jenner*
University of Amsterdam
erik@ejenner.com

Maurice Weiler
University of Amsterdam
m.weiler.ml@gmail.com



Erik Jenner

linear maps revisited:

our integral transform ansatz $\mathbb{I}_\kappa[f](x) := \int_{\mathbb{R}^d} dy \kappa(x, y) f(y)$ does not cover all possible linear maps

a stronger version of the theorem proves:

continuous, $\text{Aff}(G)$ -equivariant linear maps \Leftrightarrow convolutions with **G-steerable Schwartz distributions**

the distributional setting covers in particular **equivariant partial differential operators**

Aff(G)-equivariant bias summation

flexible ansatz:

consider a general bias summation operation $f \mapsto f + \mathfrak{b}$

parameterized by a **bias field** $\mathfrak{b} : \mathbb{R}^d \rightarrow \mathbb{R}^c \implies$ allows to sum a *different bias* $\mathfrak{b}(x) \in \mathbb{R}^c$ at each $x \in \mathbb{R}^d$

demanding equivariance, we get:

Theorem. *The bias field summation Aff(G)-equivariant iff the bias field is Aff(G)-invariant.
This requires in particular*

- 1) *a spatially constant bias field, i.e. $\mathfrak{b}(x) = b$ for some shared bias $b \in \mathbb{R}^c$, and*
- 2) *this shared bias needs to be G -invariant, that is, $b = \rho(g)b \quad \forall g \in G$.*

similar results for nonlinearities, pooling operations, etc.

PyTorch extension for $\text{Aff}(G)$ -steerable CNNs (for compact G)

General $E(2)$ - Equivariant Steerable CNNs

Maurice Weiler*
University of Amsterdam, QUVA Lab
m.weiler@uva.nl

Gabriele Cesa*†
University of Amsterdam
cesa.gabriele@gmail.com

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Gabriele Cesa
Qualcomm AI Research*
University of Amsterdam
gcesa@qti.qualcomm.com

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convolution in native PyTorch:

```
conv = nn.Conv2d(in_channels=3, out_channels=64, kernel_size=5)
```

convolution in e2cnn / escnn:

fix symmetry group $G = \mathbb{Z}_8$ + action on \mathbb{R}^2 →

```
r2_act = gspaces.Rot2dOnR2(N=8)
```

fix types + multiplicities of feature fields →

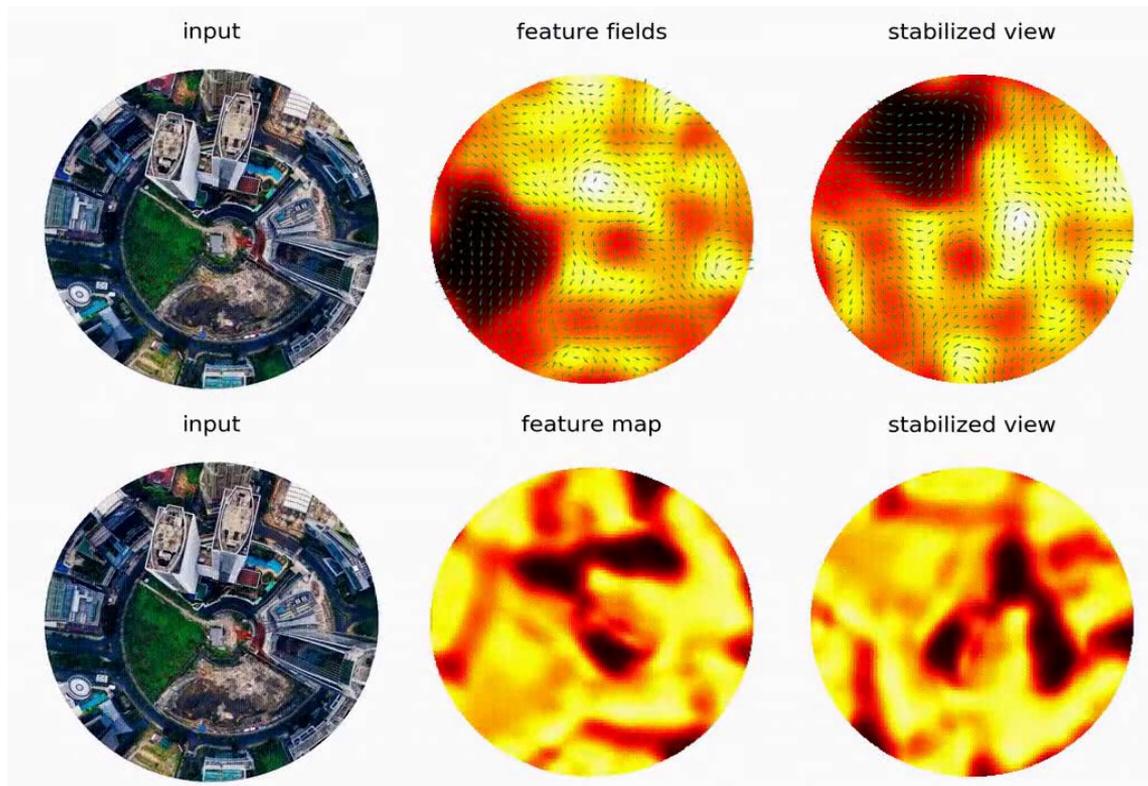
```
feat_type_in = nn.FieldType(r2_act, 3*[r2_act.trivial_repr])  
feat_type_out = nn.FieldType(r2_act, 10*[r2_act.regular_repr])
```

construct $\text{Aff}(G)$ -equivariant convolution →

```
conv = nn.R2Conv(feat_type_in, feat_type_out, kernel_size=5)
```

Equivariance demonstration

SE(2)-steerable CNN:



conventional CNN:

Emperical results – natural images

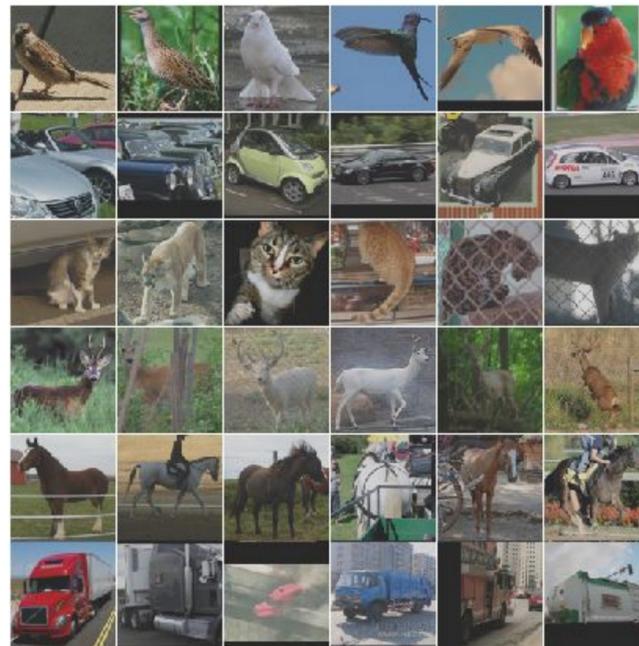
group convolutions as drop in replacement

- same number of parameters
- same training setup
- no hyperparameter tuning

model	CIFAR-10	CIFAR-100	STL-10
CNN baseline	2.6 ± 0.1	17.1 ± 0.3	12.74 ± 0.23
GCNN	2.05 ± 0.03	14.30 ± 0.09	9.80 ± 0.40

Test errors on natural image datasets

[12]



Emperical results - benchmarking

extensive benchmark of:

- groups $G \leq O(2)$
- G -representations / field types
- G -equivariant nonlinearities
- invariant maps

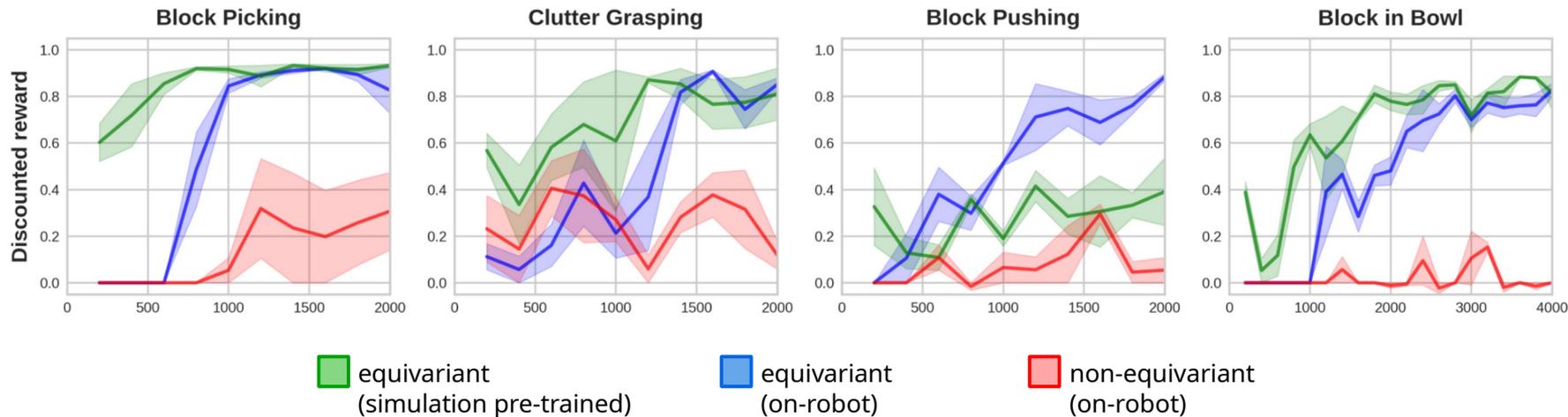
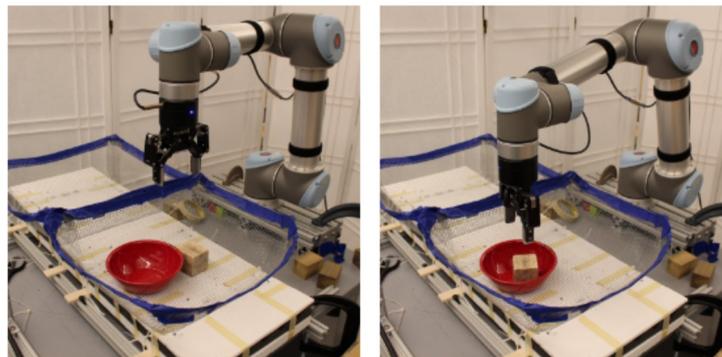
covering a wide range of related work and new models

group	representation	nonlinearity	invariant map	citation	MNIST O(2)	MNIST rot	MNIST 12k		
1	{e}	(conventional CNN)	ELU	-	5.53 ± 0.20	2.87 ± 0.09	0.91 ± 0.06		
2	C ₁			[7,9]	5.19 ± 0.08	2.48 ± 0.13	0.82 ± 0.01		
3	C ₂			[7,9]	3.29 ± 0.07	1.32 ± 0.02	0.87 ± 0.04		
4	C ₃			-	2.87 ± 0.04	1.19 ± 0.06	0.80 ± 0.03		
5	C ₄			[6,11,7,9,10]	2.40 ± 0.05	1.02 ± 0.03	0.99 ± 0.03		
6	C ₆	regular	ρ _{reg}	ELU	G-pooling	[8]	2.08 ± 0.03	0.89 ± 0.03	0.84 ± 0.02
7	C ₈			[7,9]	1.96 ± 0.04	0.84 ± 0.02	0.89 ± 0.03		
8	C ₁₂			[7]	1.95 ± 0.07	0.80 ± 0.03	0.89 ± 0.03		
9	C ₁₆			[7,9]	1.93 ± 0.04	0.82 ± 0.02	0.95 ± 0.04		
10	C ₂₀			[7]	1.95 ± 0.05	0.83 ± 0.05	0.94 ± 0.06		
11	C ₄			[11]	2.43 ± 0.05	1.03 ± 0.05	1.01 ± 0.03		
12	C ₈			-	2.03 ± 0.05	0.84 ± 0.05	0.91 ± 0.02		
13	C ₁₂	quotient		-	2.04 ± 0.04	0.81 ± 0.02	0.95 ± 0.02		
14	C ₁₆			-	2.00 ± 0.01	0.86 ± 0.04	0.98 ± 0.04		
15	C ₂₀			-	2.01 ± 0.05	0.83 ± 0.03	0.96 ± 0.04		
16	regular/scalar	$\psi_0 \xrightarrow{\text{conv}} \rho_{\text{reg}} \xrightarrow{\text{conv}} \psi_0$	ELU, G-pooling	[6,36]	2.02 ± 0.02	0.90 ± 0.03	0.93 ± 0.04		
17	regular/vector	$\psi_1 \xrightarrow{\text{conv}} \rho_{\text{reg}} \xrightarrow{\text{vector pool}} \psi_1$	vector field	[13,37]	2.12 ± 0.02	1.07 ± 0.03	0.78 ± 0.03		
18	mixed vector	$\rho_{\text{reg}} \oplus \psi_1 \xrightarrow{\text{conv}} \rho_{\text{reg}} \oplus \psi_1$	ELU, vector field	-	1.87 ± 0.03	0.83 ± 0.02	0.63 ± 0.02		
19	D ₁			-	3.40 ± 0.07	3.44 ± 0.10	0.98 ± 0.03		
20	D ₂			-	2.42 ± 0.07	2.39 ± 0.04	1.05 ± 0.03		
21	D ₃			-	2.17 ± 0.06	2.15 ± 0.05	0.94 ± 0.02		
22	D ₄			[6,11,38]	1.88 ± 0.04	1.87 ± 0.04	1.69 ± 0.03		
23	D ₆	regular	ρ _{reg}	ELU	G-pooling	[8]	1.77 ± 0.06	1.77 ± 0.04	1.00 ± 0.03
24	D ₈			-	1.68 ± 0.06	1.73 ± 0.03	1.64 ± 0.02		
25	D ₁₂			-	1.66 ± 0.05	1.65 ± 0.05	1.67 ± 0.01		
26	D ₁₆			-	1.62 ± 0.04	1.65 ± 0.02	1.68 ± 0.04		
27	D ₂₀			-	1.64 ± 0.06	1.62 ± 0.05	1.69 ± 0.03		
28	D ₁₆	regular/scalar	$\psi_{0,0} \xrightarrow{\text{conv}} \rho_{\text{reg}} \xrightarrow{G\text{-pool}} \psi_{0,0}$	ELU, G-pooling	-	1.92 ± 0.03	1.88 ± 0.07	1.74 ± 0.04	
29	ireps ≤ 1	$\bigoplus_{i=0}^1 \psi_i$		-	2.98 ± 0.04	1.38 ± 0.09	1.29 ± 0.05		
30	ireps ≤ 3	$\bigoplus_{i=0}^3 \psi_i$		-	3.02 ± 0.18	1.38 ± 0.09	1.27 ± 0.03		
31	ireps ≤ 5	$\bigoplus_{i=0}^5 \psi_i$		-	3.24 ± 0.05	1.44 ± 0.10	1.36 ± 0.04		
32	ireps ≤ 7	$\bigoplus_{i=0}^7 \psi_i$		-	3.30 ± 0.11	1.51 ± 0.10	1.40 ± 0.07		
33	C-ireps ≤ 1	$\bigoplus_{i=0}^1 \psi_i^c$	ELU, norm-ReLU	conv2triv	[12]	3.39 ± 0.10	1.47 ± 0.06	1.42 ± 0.04	
34	C-ireps ≤ 3	$\bigoplus_{i=0}^3 \psi_i^c$		-	3.48 ± 0.16	1.51 ± 0.05	1.53 ± 0.07		
35	C-ireps ≤ 5	$\bigoplus_{i=0}^5 \psi_i^c$		-	3.59 ± 0.08	1.59 ± 0.05	1.55 ± 0.06		
36	C-ireps ≤ 7	$\bigoplus_{i=0}^7 \psi_i^c$		-	3.64 ± 0.12	1.61 ± 0.06	1.62 ± 0.03		
37	SO(2)		ELU, squash	-	3.10 ± 0.09	1.41 ± 0.04	1.46 ± 0.05		
38			ELU, norm-ReLU	-	3.23 ± 0.08	1.38 ± 0.08	1.33 ± 0.03		
39			ELU, shared norm-ReLU	norm	-	2.88 ± 0.11	1.15 ± 0.06	1.18 ± 0.03	
40	ireps ≤ 3	$\bigoplus_{i=0}^3 \psi_i$	shared norm-ReLU	-	3.61 ± 0.09	1.57 ± 0.05	1.88 ± 0.05		
41			ELU, gate	conv2triv	-	2.37 ± 0.06	1.09 ± 0.03	1.10 ± 0.02	
42			ELU, shared gate	-	2.33 ± 0.06	1.11 ± 0.03	1.12 ± 0.04		
43			ELU, gate	norm	-	2.23 ± 0.09	1.04 ± 0.04	1.05 ± 0.06	
44			ELU, shared gate	-	2.20 ± 0.06	1.01 ± 0.03	1.03 ± 0.03		
45	ireps = 0	$\psi_{0,0}$	ELU	-	5.46 ± 0.46	5.21 ± 0.29	3.98 ± 0.04		
46	ireps ≤ 1	$\psi_{0,0} \oplus \psi_{1,0} \oplus 2\psi_{1,1}$		-	3.31 ± 0.17	3.37 ± 0.18	3.05 ± 0.09		
47	ireps ≤ 3	$\psi_{0,0} \oplus \psi_{1,0} \oplus \bigoplus_{i=1}^3 2\psi_{1,i}$		-	3.42 ± 0.03	3.41 ± 0.10	3.86 ± 0.09		
48	ireps ≤ 5	$\psi_{0,0} \oplus \psi_{1,0} \oplus \bigoplus_{i=1}^5 2\psi_{1,i}$	ELU, norm-ReLU	O(2)-conv2triv	-	3.59 ± 0.13	3.78 ± 0.31	4.17 ± 0.15	
49	ireps ≤ 7	$\psi_{0,0} \oplus \psi_{1,0} \oplus \bigoplus_{i=1}^7 2\psi_{1,i}$		-	3.84 ± 0.25	3.90 ± 0.18	4.57 ± 0.27		
50	Ind-ireps ≤ 1	$\text{Ind } \psi_0^{\text{SO}(2)} \oplus \text{Ind } \psi_1^{\text{SO}(2)}$		-	2.72 ± 0.05	2.70 ± 0.11	2.39 ± 0.07		
51	O(2)	Ind-ireps ≤ 3	$\text{Ind } \psi_0^{\text{SO}(2)} \oplus \bigoplus_{i=1}^3 \text{Ind } \psi_i^{\text{SO}(2)}$	ELU, Ind norm-ReLU	Ind-conv2triv	-	2.66 ± 0.07	2.65 ± 0.12	2.25 ± 0.06
52		Ind-ireps ≤ 5	$\text{Ind } \psi_0^{\text{SO}(2)} \oplus \bigoplus_{i=1}^5 \text{Ind } \psi_i^{\text{SO}(2)}$	-	-	2.71 ± 0.11	2.84 ± 0.10	2.39 ± 0.09	
53		Ind-ireps ≤ 7	$\text{Ind } \psi_0^{\text{SO}(2)} \oplus \bigoplus_{i=1}^7 \text{Ind } \psi_i^{\text{SO}(2)}$	-	-	2.80 ± 0.12	2.85 ± 0.06	2.25 ± 0.08	
54	ireps ≤ 3	$\psi_{0,0} \oplus \psi_{1,0} \oplus \bigoplus_{i=1}^3 2\psi_{1,i}$	ELU, gate	O(2)-conv2triv	-	2.39 ± 0.05	2.38 ± 0.07	2.28 ± 0.07	
55			norm	-	2.21 ± 0.09	2.24 ± 0.06	2.15 ± 0.03		
56	Ind-ireps ≤ 3	$\text{Ind } \psi_0^{\text{SO}(2)} \oplus \bigoplus_{i=1}^3 \text{Ind } \psi_i^{\text{SO}(2)}$	ELU, Ind gate	Ind-conv2triv	-	2.13 ± 0.04	2.09 ± 0.05	2.05 ± 0.05	
57			Ind-norm	-	1.96 ± 0.06	1.95 ± 0.05	1.85 ± 0.07		

Empirical results – reinforcement learning

On-Robot Learning With Equivariant Models

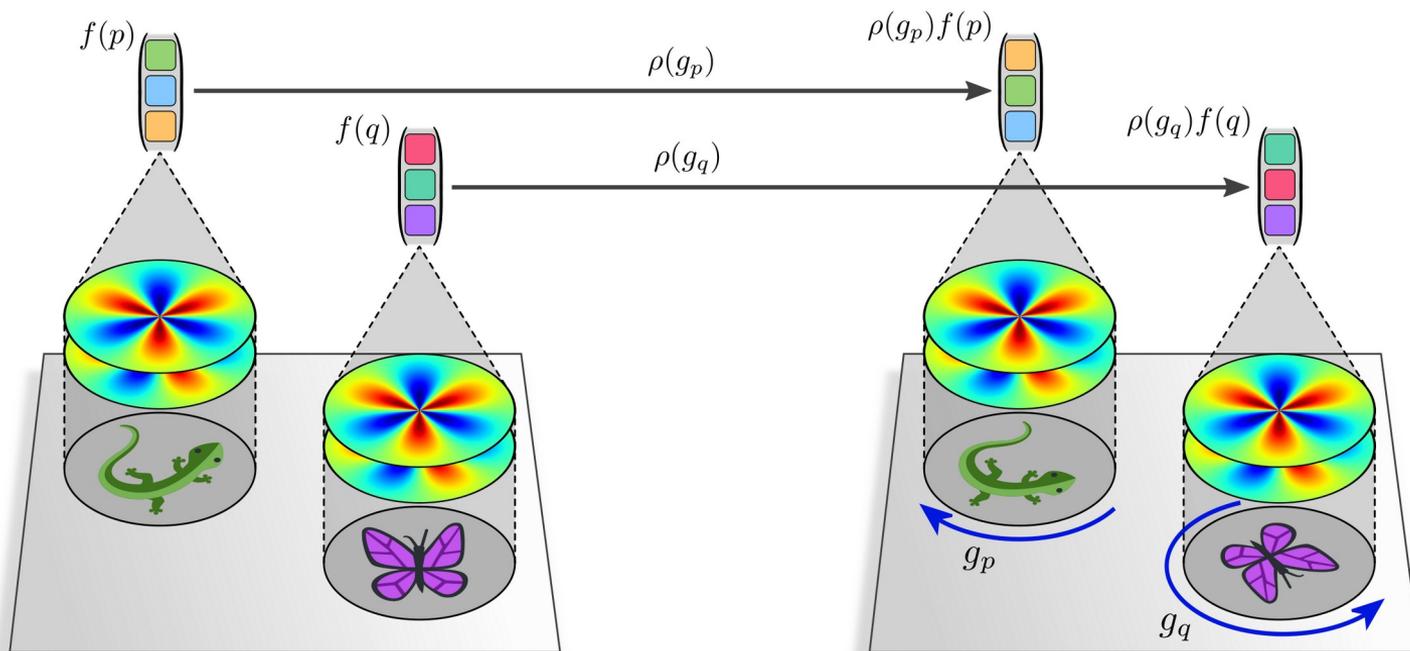
Dian Wang Mingxi Jia Xupeng Zhu Robin Walters Robert Platt
Khoury College of Computer Sciences
Northeastern University
Boston, MA 02115, USA



Local gauge equivariance

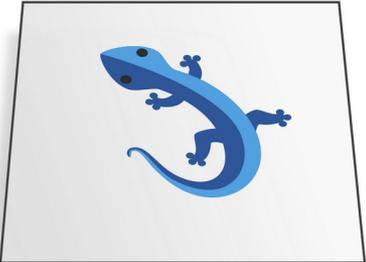
steerable CNNs are not only *globally* $\text{Aff}(G)$ -equivariant, but *locally* G -equivariant (gauge equivariant)

formalized as *coordinate independent CNN*



Active & passive transformations

active transformations - acting on the data itself:

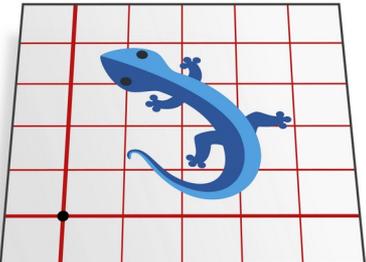


vs.

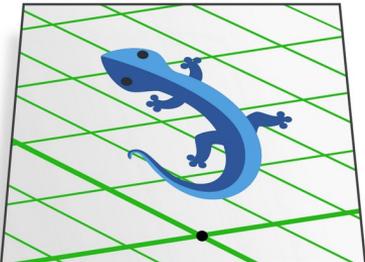


← **global transformations**

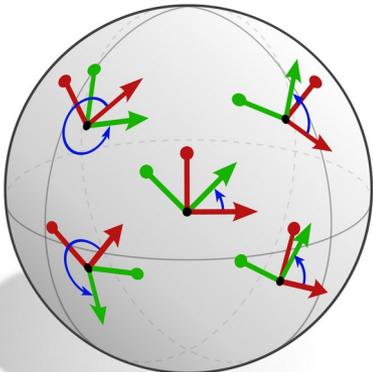
passive transformations - acting on coordinatization of data:



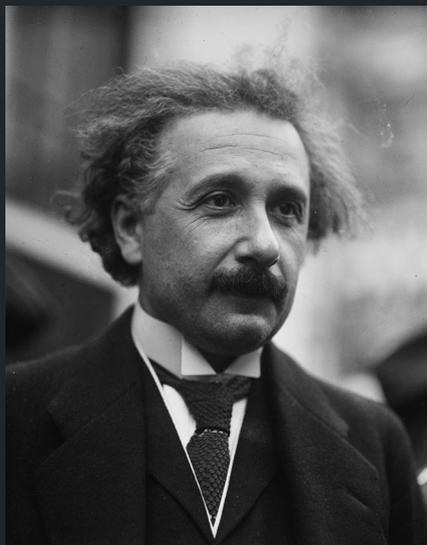
vs.



local gauge trafos

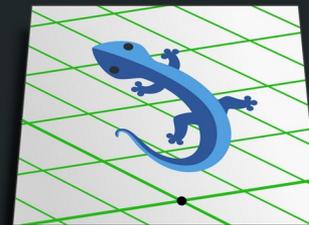
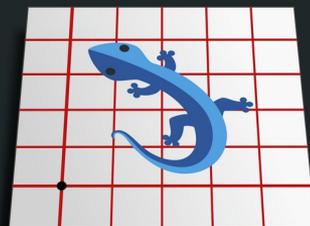


Coordinate independent CNNs on Riemannian manifolds



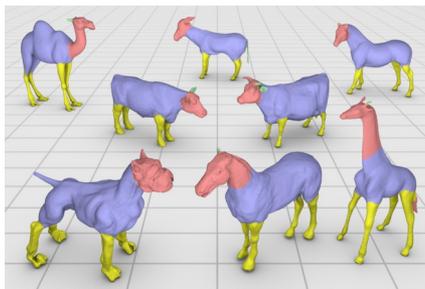
Principle of Covariance (Einstein, 1916)

*“Universal laws of **AI** are to be expressed by equations which hold good for all systems of coordinates.”*

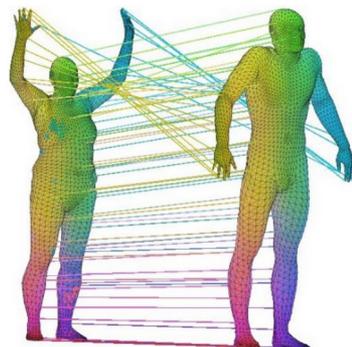


Convolutions on Riemannian manifolds

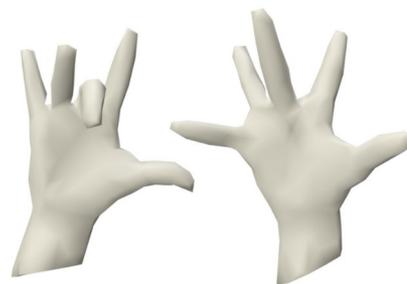
mesh segmentation



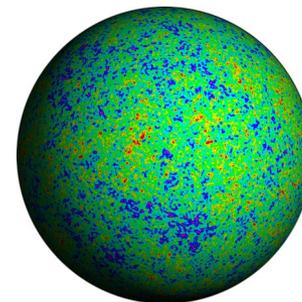
shape correspondence



deformations (metric field)

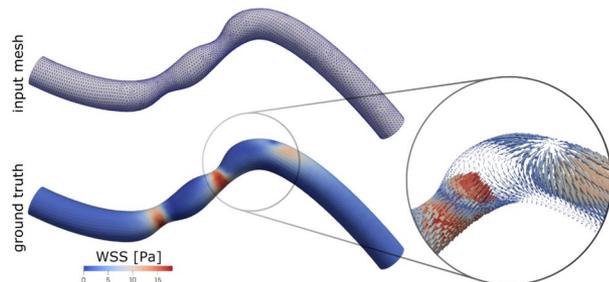


spherical CNNs

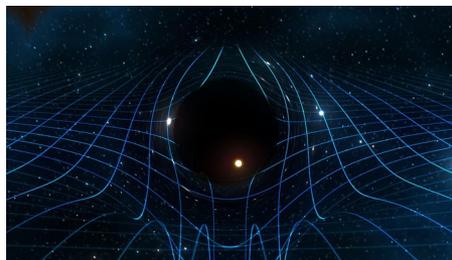


intrinsic convolutions, not in embedding space !

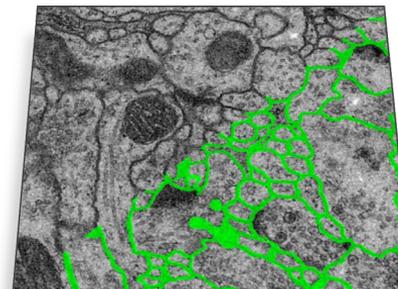
artery wall stress estimation



general relativity



Euclidean CNNs



Design questions

Image adapted from Konakov-Lukovic et al.

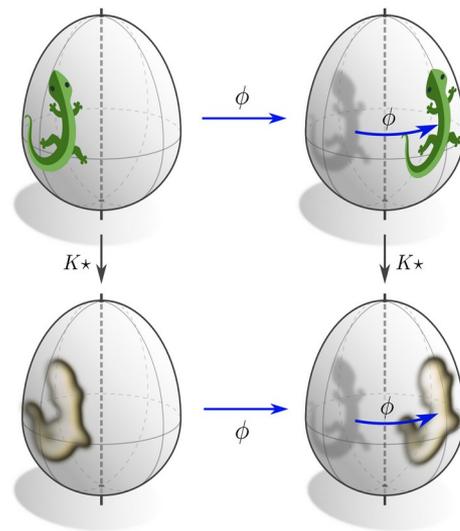
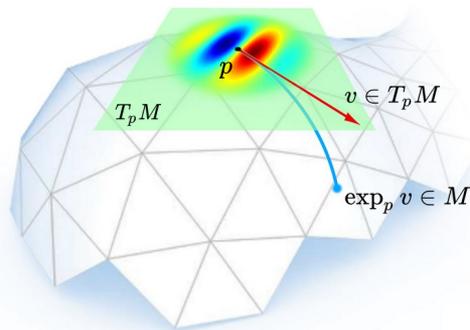
how to ...

... define *feature fields* on M ?

... define *convolution kernels* on M ?

... *share weights* over M ?

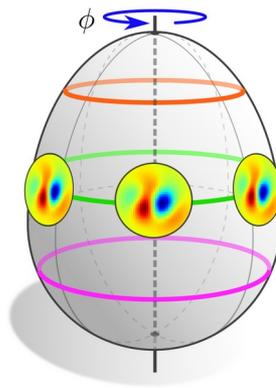
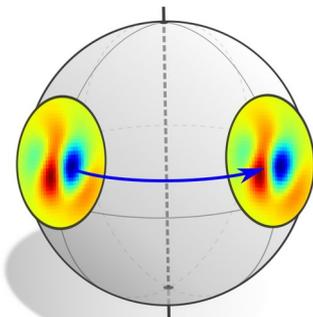
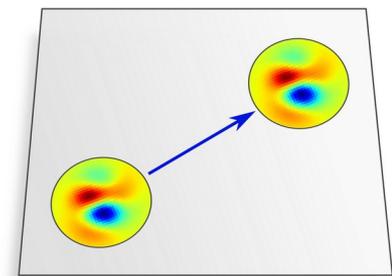
... guarantee *isometry equivariance* ?



Weight sharing - via global symmetries

weight sharing by *demanding equivariance* w.r.t. global symmetries (isometries)

⚡ can only share over *symmetry orbits* (in general non-transitive)



homogeneous spaces,
transitive orbits

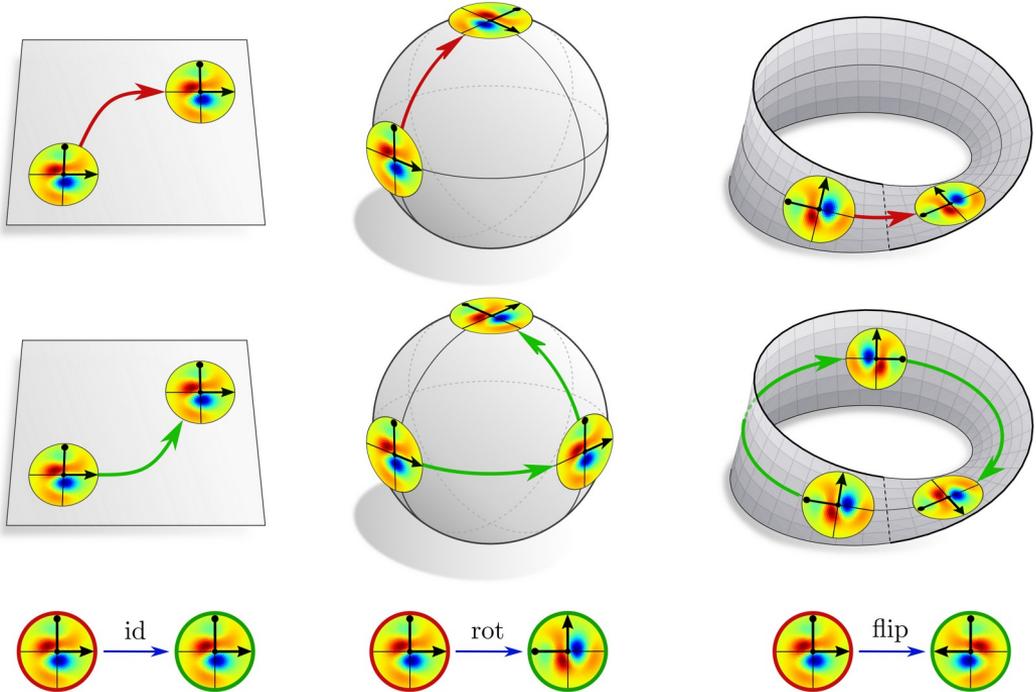
SO(2) orbits

trivial orbits

Weight sharing - via parallel transport

sharing weights by “shifting” kernel over manifold ?

⚡ parallel transport in general path dependent



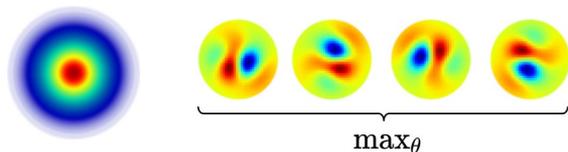
Weight sharing - approaches in the literature

the kernel alignment (“*gauge*”) on manifolds is *inherently ambiguous!*

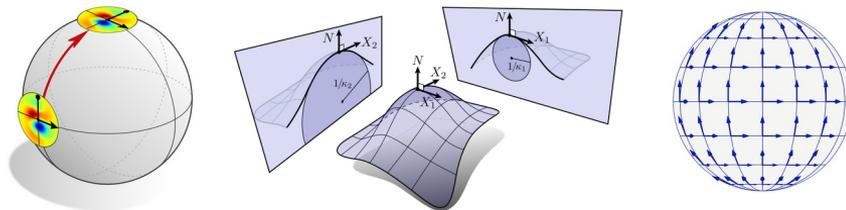
\Leftrightarrow topological obstructions to the existence of G -structures

solution approaches in the literature:

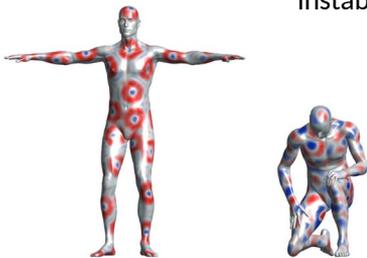
1) **gauge invariant** features \searrow low expressiveness



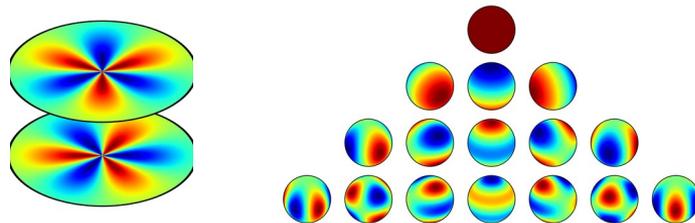
2) **heuristic gauges** \searrow instable under deformations



3) **spectral** approaches \searrow gauge independent but instable under deformations

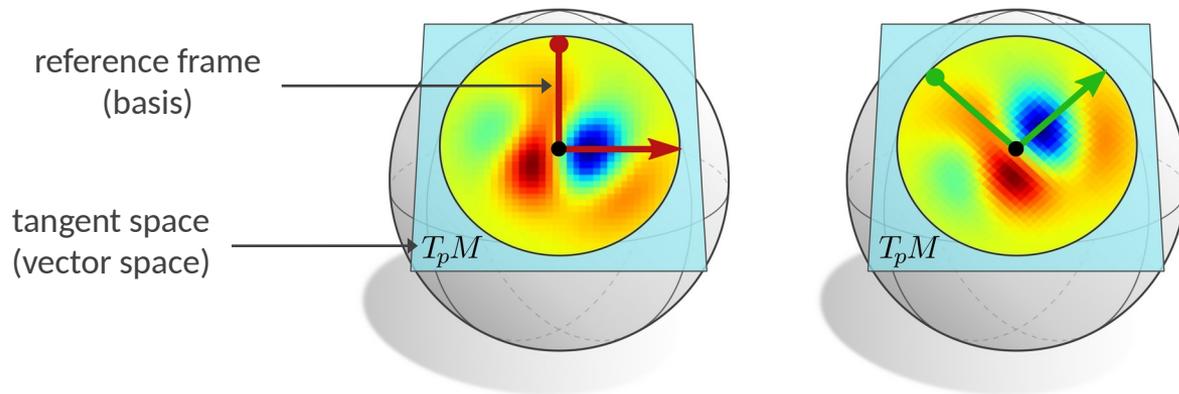


4) **gauge equivariant** features (ours, covers 1,2 as special cases)



Reference frames and kernel alignments

identify kernel alignment with a choice of reference frame

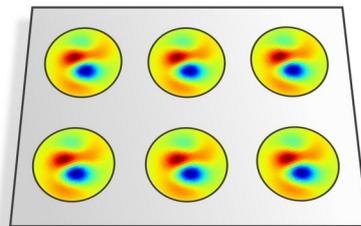
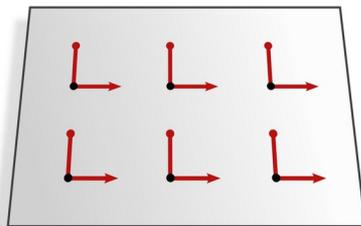


Reference frames and kernel alignments

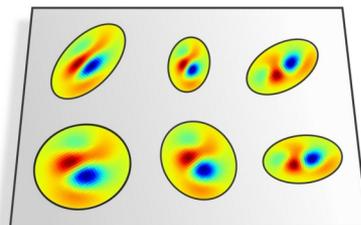
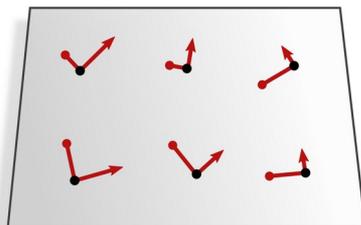
identify kernel alignment with a choice of reference frame

frame field \longleftrightarrow kernel field

standard (canonical)
frame / kernel field / CNN
on \mathbb{R}^2



alternative
frame / kernel field / CNN
on \mathbb{R}^2



Reference frames and kernel alignments

identify kernel alignment with a choice of reference frame

frame field \longleftrightarrow kernel field

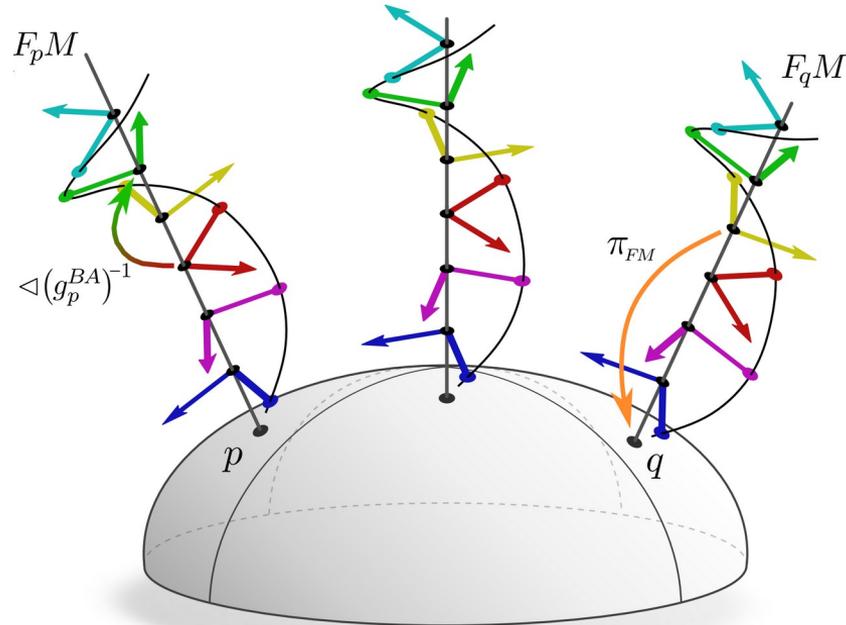
ambiguity of kernel alignments == ambiguity of reference frames

↑
“G-structure”

G-structures

frame bundle FM = “set” (bundle) of all frames (GL(d)-valued transition functions)

G-structures GM = sub-bundles of frames with $G \leq GL(d)$ valued transition functions



G-structures

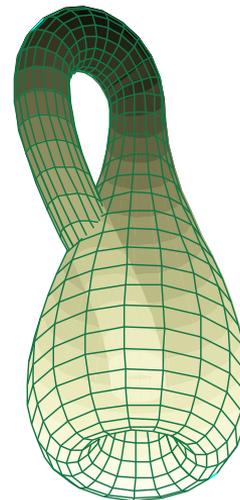
frame bundle FM = “set” (bundle) of all frames (GL(d)-valued transition functions)

G-structures GM = sub-bundles of frames with $G \leq GL(d)$ valued transition functions

G-structures encode **additional geometric structure on M** in a unified way:

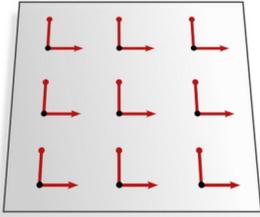
structure on M	distinguished frames	structure group $G \leq GL(d)$
smooth structure only	all reference frames	$GL(d)$
orientation of M	positively oriented frames	$GL^+(d)$
volume form	unit volume frames	$SL(d)$
Riemannian metric	orthonormal frames	$O(d)$
pseudo-Riemannian metric	pseudo-orthonormal frames	$O(d - n, n)$
global trivialization	global frame field	$\{e\}$

Klein bottle
non-orientable

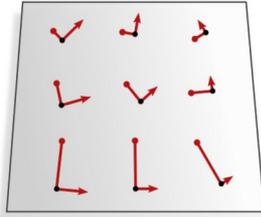


topological obstructions may prevent the existence of (continuous) G-structures

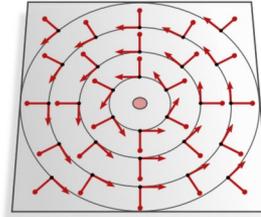
G-structures



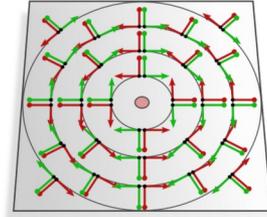
$$M = \mathbb{R}^2, G = \{e\}$$



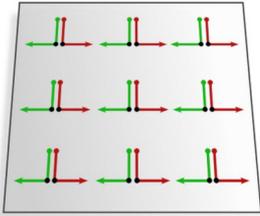
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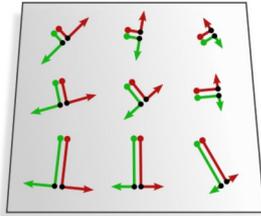
$$M = \mathbb{R}^2 \setminus \{0\}, G = \{e\}$$



$$M = \mathbb{R}^2 \setminus \{0\}, G = \mathcal{R}$$



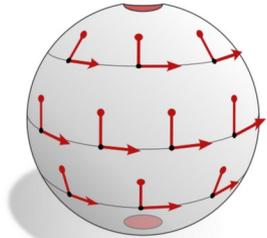
$$M = \mathbb{R}^2, G = \mathcal{R}$$



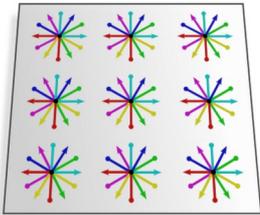
$$M = \mathbb{R}^2, G = \mathcal{R}$$



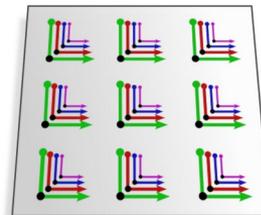
$$M = S^2, G = \text{SO}(2)$$



$$M = S^2 \setminus \text{poles}, G = \{e\}$$



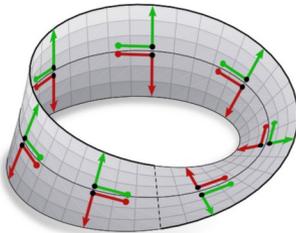
$$M = \mathbb{R}^2, G = \text{SO}(2)$$



$$M = \mathbb{R}^2, G = \mathcal{S}$$



$$M = \text{"Suzanne"}, G = \text{SO}(2)$$

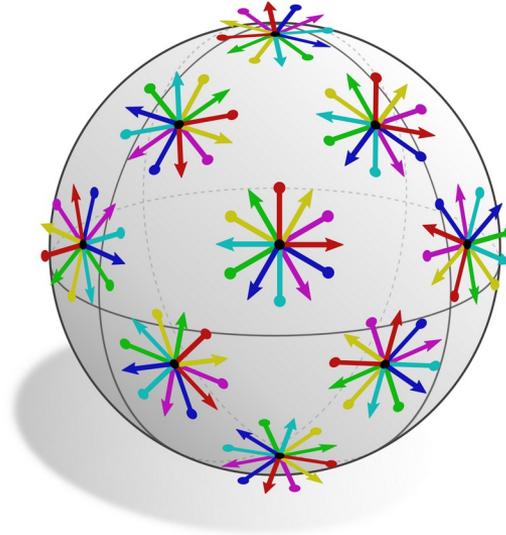


$$M = \text{Möbius}, G = \mathcal{R}$$

GM-coordinate independence - tangent vectors

all frames of the G-structure are equally valid

⇒ any *object* or *morphism* should be expressible relative to any frame in GM



GM-coordinate independence - tangent vectors

all frames of the G -structure are equally valid

\Rightarrow any *object* or *morphism* should be expressible relative to any frame in GM

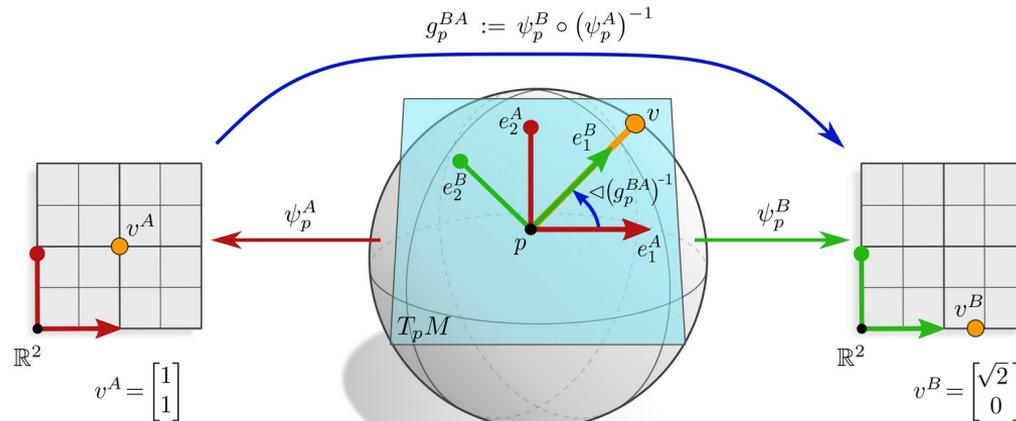
example: - tangent vectors $v \in T_p M$ are *coordinate free*

- in gauge A, v is expressed by coefficients $v^A \in \mathbb{R}^d$

- in gauge B, v is expressed by coefficients $v^B \in \mathbb{R}^d$

- gauge trafos $g^{BA} \in G$ relate coefficients: $v^B = g^{BA} v^A$

different coefficients,
same information content!



GM-coordinate independence - feature vector fields

all frames of the G -structure are equally valid

\Rightarrow any *object* or *morphism* should be expressible relative to any frame in GM

coordinate independent *feature vectors* transform according to G -representation ρ :

$$f^A, f^B \in \mathbb{R}^c \quad f^B = \rho(g^{BA})f^A$$

scalar field	trivial representation	$\rho(g) = id$
tangent vector field	standard representation	$\rho(g) = g$
tensor field	tensor representation	$\rho(g) = (g^{-T})^{\otimes s} \otimes g^{\otimes r}$
irrep field	irreducible representation	
regular feature field	regular representation	

formally, feature vectors are elements of a G -associated feature vector bundle $(GM \times \mathbb{R}^c) / \sim_\rho$

GM-coordinate independence - linear maps on $T_p M$

all frames of the G-structure are equally valid

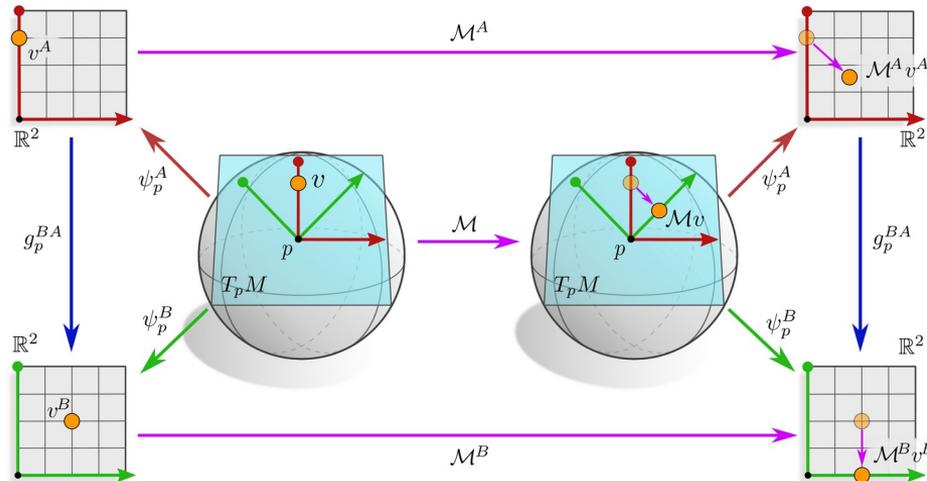
\Rightarrow any *object* or *morphism* should be expressible relative to any frame in GM

example: - linear maps $\mathcal{M} : T_p M \rightarrow T_p M$ are *coordinate free*

- in gauge A, \mathcal{M} is expressed by coefficients $\mathcal{M}^A \in \mathbb{R}^{d \times d}$

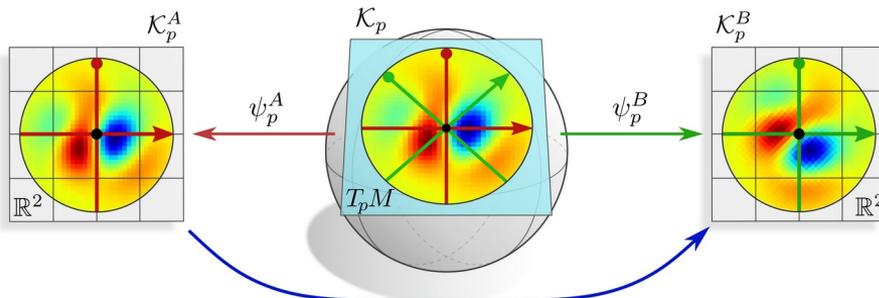
- in gauge B, \mathcal{M} is expressed by coefficients $\mathcal{M}^B \in \mathbb{R}^{d \times d}$

- gauge trafos $g^{BA} \in G$ relate coefficients: $\mathcal{M}^B = g^{BA} \mathcal{M}^A (g^{BA})^{-1}$



GM-coordinate independence - kernels

coordinate independence of kernels:



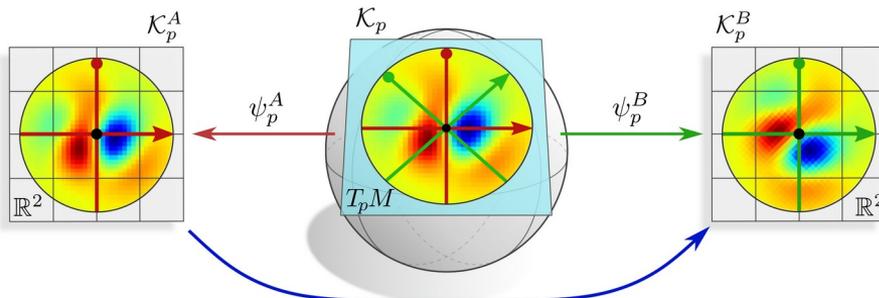
G-steerability constraint \neq gauge trafo: $\mathcal{K}_p^B = \frac{1}{|\det g_p^{BA}|} (\rho_{\text{in}}^{-\top} \otimes \rho_{\text{out}}) (g_p^{BA}) \circ \mathcal{K}_p^A \circ (g_p^{BA})^{-1}$

$$\begin{array}{ccc}
 \mathbb{R}^d & \xrightarrow{K} & \mathbb{R}^{C_{\text{out}} \times C_{\text{in}}} \\
 \downarrow g \cdot & & \downarrow \frac{\rho_{\text{in}}^* \otimes \rho_{\text{out}}}{|\det|}(g) \\
 \mathbb{R}^d & \xrightarrow{K} & \mathbb{R}^{C_{\text{out}} \times C_{\text{in}}}
 \end{array}$$

$$\begin{array}{ccc}
 \mathbb{R}^d & \xrightarrow{\mathcal{K}_p^A} & \mathbb{R}^{C_{\text{out}} \times C_{\text{in}}} \\
 \downarrow g_p^{BA} \cdot & & \downarrow \frac{\rho_{\text{in}}^* \otimes \rho_{\text{out}}}{|\det|}(g_p^{BA}) \\
 \mathbb{R}^d & \xrightarrow{\mathcal{K}_p^B} & \mathbb{R}^{C_{\text{out}} \times C_{\text{in}}}
 \end{array}$$

GM-coordinate independence - kernels

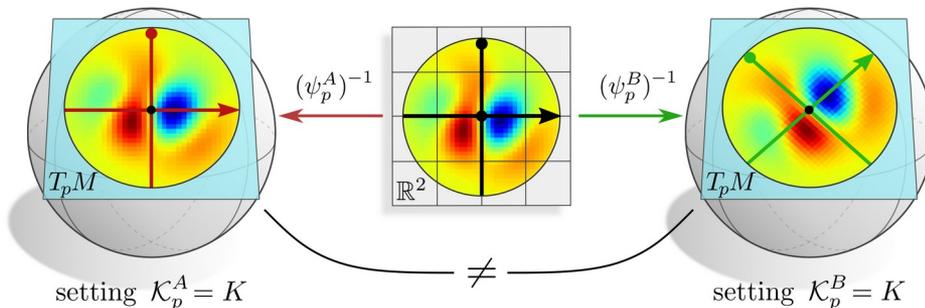
coordinate independence of kernels:



equivariance constraint \neq gauge trafo: $\mathcal{K}_p^B = \frac{1}{|\det g_p^{BA}|} (\rho_{\text{in}}^{-\top} \otimes \rho_{\text{out}}) (g_p^{BA}) \circ \mathcal{K}_p^A \circ (g_p^{BA})^{-1}$

weight sharing of kernels:

depends in general on chosen gauge!



coordinate independent iff:

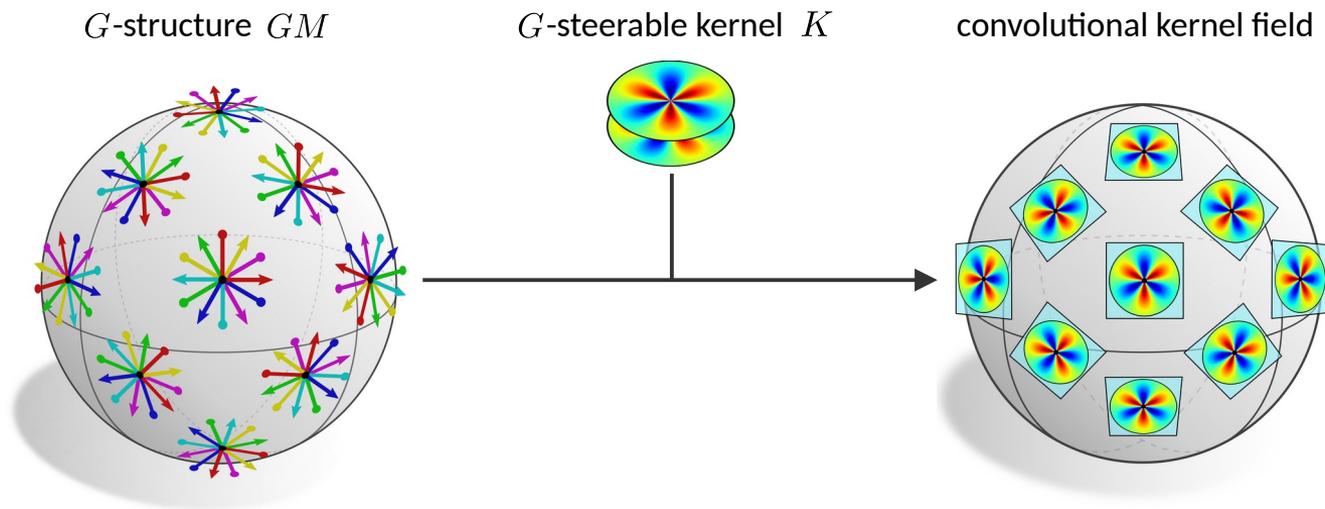
$$\mathcal{K}_p^X = K \quad \text{for any gauge } X$$

coordinate independence } \rightarrow G -steerability
weight sharing }

$$K = \frac{1}{|\det g|} (\rho_{\text{in}}^{-\top} \otimes \rho_{\text{out}}) (g) \circ K \circ g^{-1} \quad \forall g \in G$$

GM-convolutions

GM-coordinate independent convolutions operate by applying a *convolutional kernel field* to a feature field

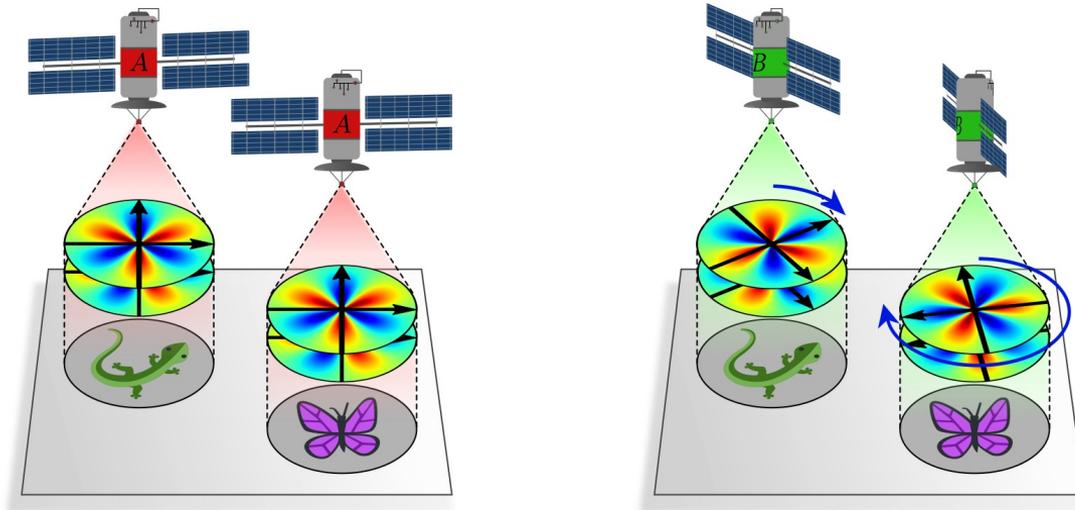


symmetry properties:

- 1) GM -coordinate independence (passive)
- 2) local gauge equivariance (active)
- 3) global isometry equivariance (active)

GM-convolutions

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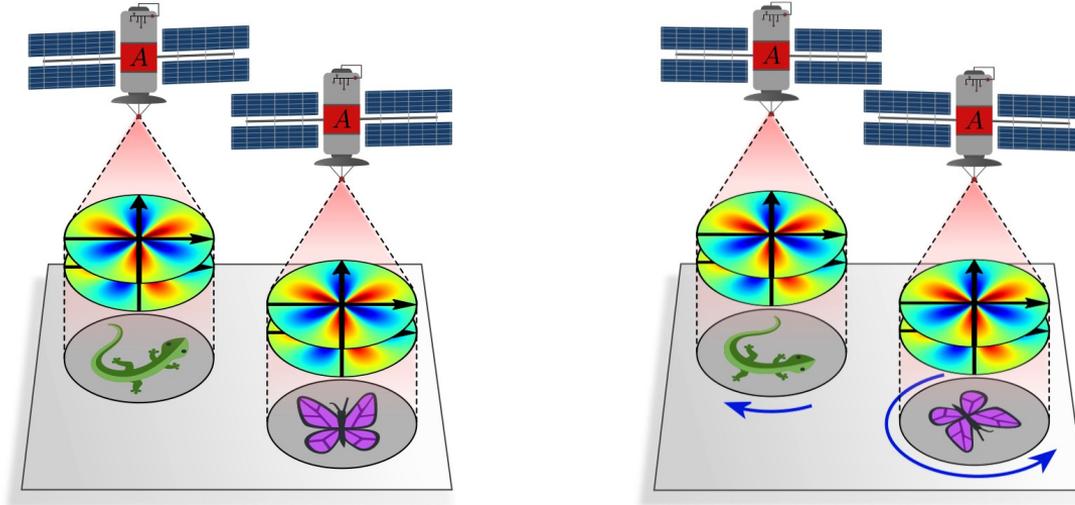


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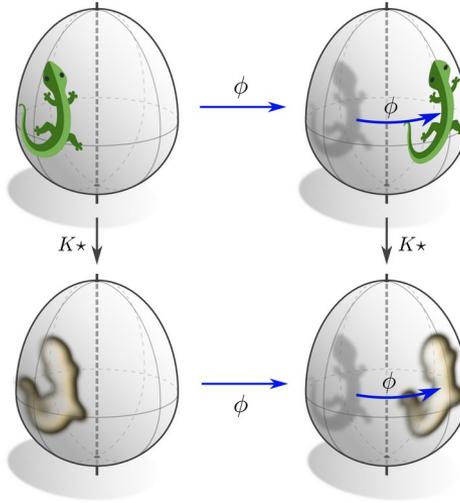


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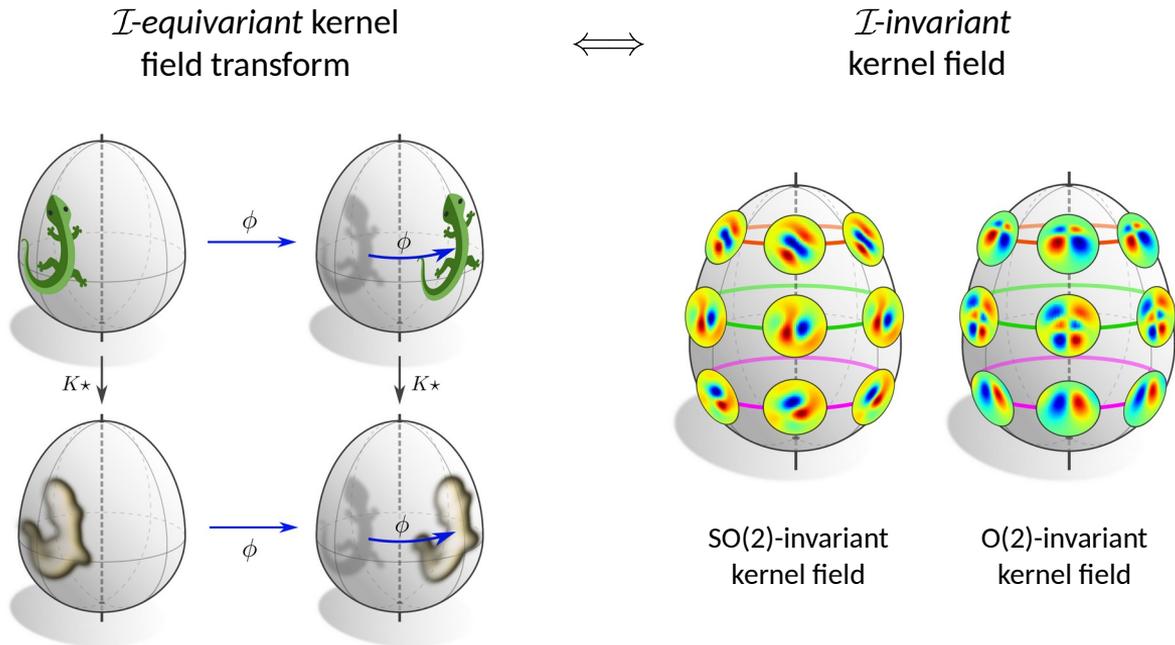
symmetry properties:

- 1) GM-coordinate independence (passive)
- 2) local gauge equivariance (active)
- 3) global isometry equivariance (active)

Isometry equivariance

“kernel field transform”: similar to convolution, but not assuming weight sharing
parameterized by a *kernel field*

Theorem: let $\mathcal{I} \leq \text{Isom}(M)$, then:



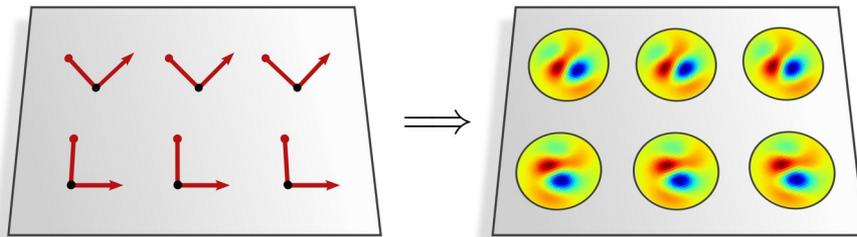
Isometry equivariance - GM-convolutions

Let $\text{Isom}_{GM} \leq \text{Isom}(M)$ be the subgroup of isometries that are symmetries of GM

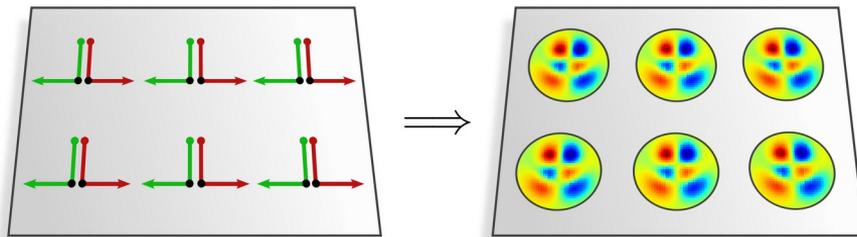
G-steerable (convolutional) kernel fields inherit this Isom_{GM} -invariance

\implies GM-convolutions are Isom_{GM} -equivariant

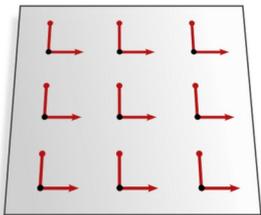
- horizontal translations



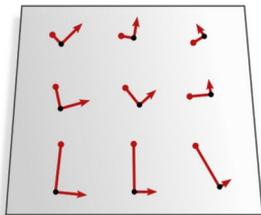
- horizontal translations
- vertical translations
- horizontal reflections



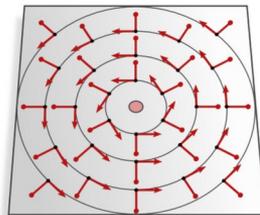
Isometry equivariance - GM-convolutions



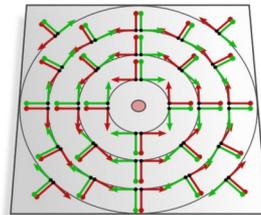
$M = \mathbb{R}^2, G = \{e\}$



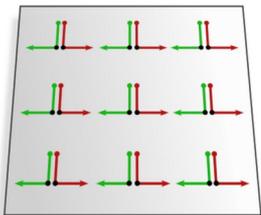
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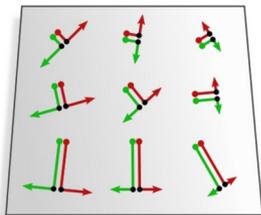
$M = \mathbb{R}^2 \setminus \{0\}, G = \{e\}$



$M = \mathbb{R}^2 \setminus \{0\}, G = \mathcal{R}$



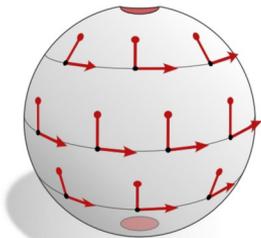
$M = \mathbb{R}^2, G = \mathcal{R}$



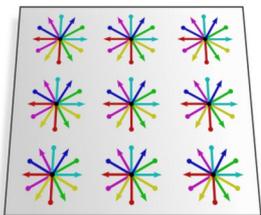
$M = \mathbb{R}^2, G = \mathcal{R}$



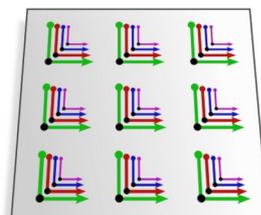
$M = S^2, G = \text{SO}(2)$



$M = S^2 \setminus \text{poles}, G = \{e\}$



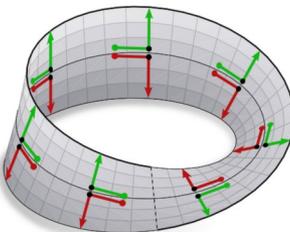
$M = \mathbb{R}^2, G = \text{SO}(2)$



$M = \mathbb{R}^2, G = \mathcal{S}$



$M = \text{"Suzanne"}, G = \text{SO}(2)$



$M = \text{Möbius}, G = \mathcal{R}$

COORDINATE INDEPENDENT CONVOLUTIONAL NETWORKS

ISOMETRY AND GAUGE EQUIVARIANT CONVOLUTIONS ON RIEMANNIAN MANIFOLDS

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mathematical structure
(group/representation theory & differential geometry)



tensor fields

feature fields

Minkowski space + global Poincaré symmetry
curved spacetime + local Lorentz transformations

Euclidean space + global $\text{Aff}(G)$ symmetry
Riemannian manifold + local gauge transformations

invariant laws of nature (relativity)
equivariant system dynamics

invariant neural connectivity
equivariant inference

scalar / vector / tensor operators in QM
quantum state transition rules

G -steerable kernels
feature transition rules

