UNIVERSITY OF AMSTERDAM

AMLAB Amsterdam Machine Learning Lab

Group Equivariant Deep Learning

Lecture 1 - Regular group convolutions

Lecture 1.1 - Introduction

Desirable properties of neural networks, invariance, equivariance, weight-sharing

Erik Bekkers, Amsterdam Machine Learning Lab, University of Amsterdam

This mini-course serves as a module with the UvA Master AI course Deep Learning 2 https://uvadl2c.github.io/

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Lecture 1.1 - Introduction

Desirable properties of neural networks, invariance, equivariance, weight-sharing

Lecture 1.2 - Group Theory | The basics

Groups, group product, inverse, action, representation, affine groups $G = \mathbb{R}^d \rtimes H$

Lecture 1.3 - Regular group convolutions | Template matching viewpoint

General group convolutional NN design with example for roto-translation equivariance (SE(2))

Lecture 1.4 - SE(2) Equivariant NN Example | With histopathology images

Visual example for roto-translation equivariance (SE(2))

Lecture 1.5 - A brief history of G-CNNs

Lecture 1.6 - Group Theory | Homogeneous/quotient spaces

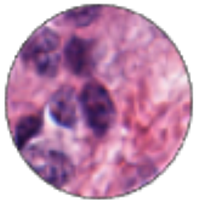
Transitive action, homogeneous space, quotient space, examples

Lecture 1.7 - Group convolutions are all you need!

Equivariant linear layers between feature maps are group convolutions

Geometric guarantees (invariance)

Example: Detection of pathological cells



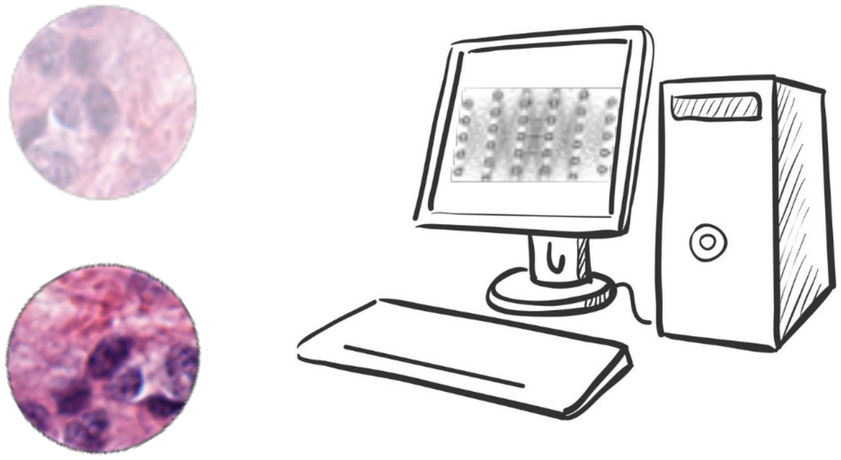
Geometric guarantees (invariance)

Example: Detection of pathological cells

Healthy

Geometric guarantees (invariance)

Example: Detection of pathological cells



Healthy

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Pathological

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Example: Detection of pathological cells

Healthy

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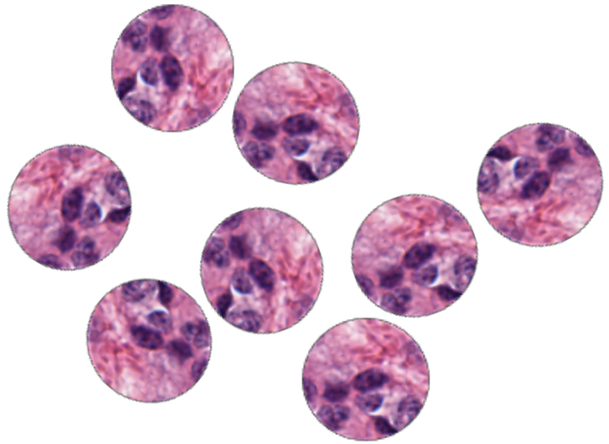
Common approach: data-augmentation



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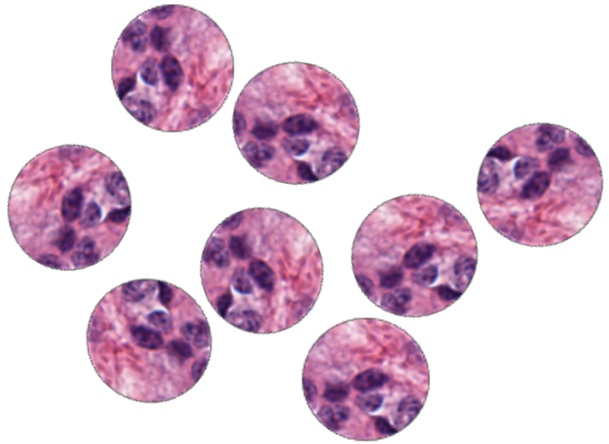
Common approach: data-augmentation



Issues:

- Still no guarantee of invariance
- Valuable net capacity is spend on learning invariance
- Redundancy in feature repr.

https://distill.pub/2020/circuits/equivariance/

Naturally Occurring Equivariance in Neural Networks

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Gabriel Goh	OpenAI

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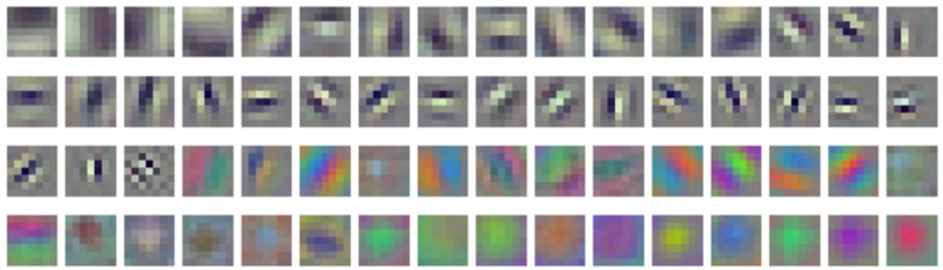
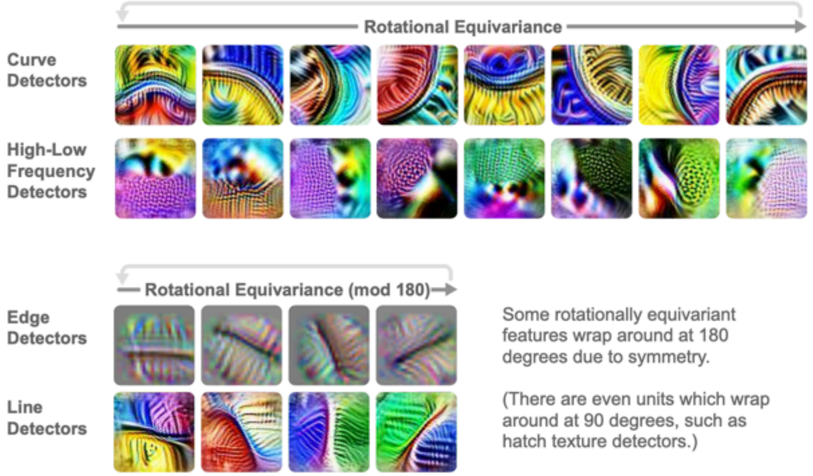
Dec. 8, 2020	10.23915/distill.00024.004



The weights for the units in the first layer of the TF-Slim [11] version of InceptionV1 [8].[5] Units are sorted by the first principal component of the adjacency matrix between the first and second layers. Note how many features are similar except for rotation, scale, and hue.

Equivariant Features

Rotational Equivariance: One example of equivariance is rotated versions of the same feature. These are especially common in early vision, for example curve detectors, high-low frequency detectors, and line detectors.



Some rotationally equivariant features wrap around at 180 degrees due to symmetry.

(There are even units which wrap around at 90 degrees, such as hatch texture detectors.)

Geometric guarantees (equivariance)

CNNs are translation equivariant

Via convolutions

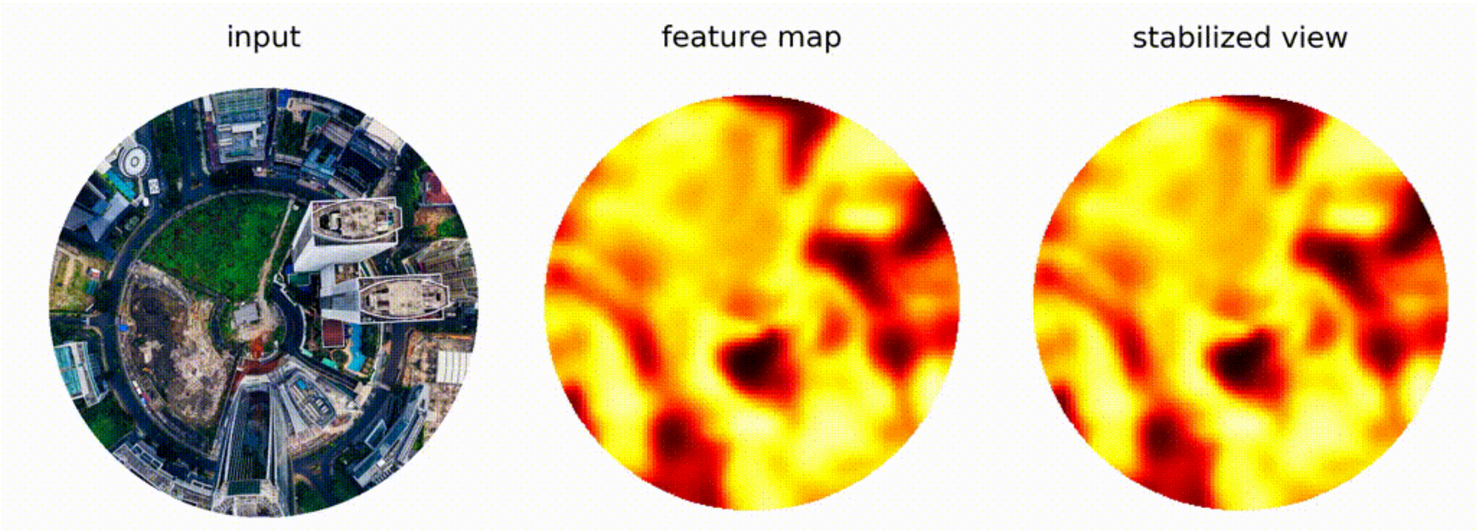
Geometric guarantees (equivariance)

CNNs are translation equivariant

Via convolutions

Geometric guarantees (equivariance)

Normal CNN



Figures source:
https://github.com/QUVA-Lab/e2cnn

Geometric guarantees (equivariance)

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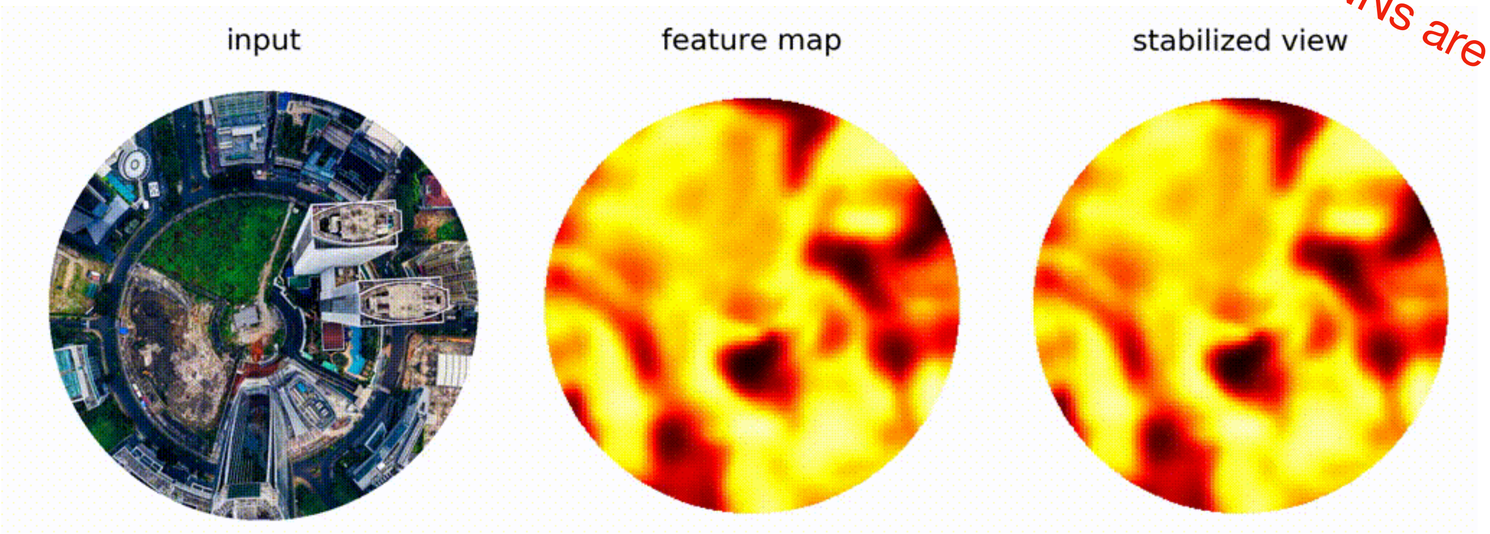

CNNs are not rotation equivariant

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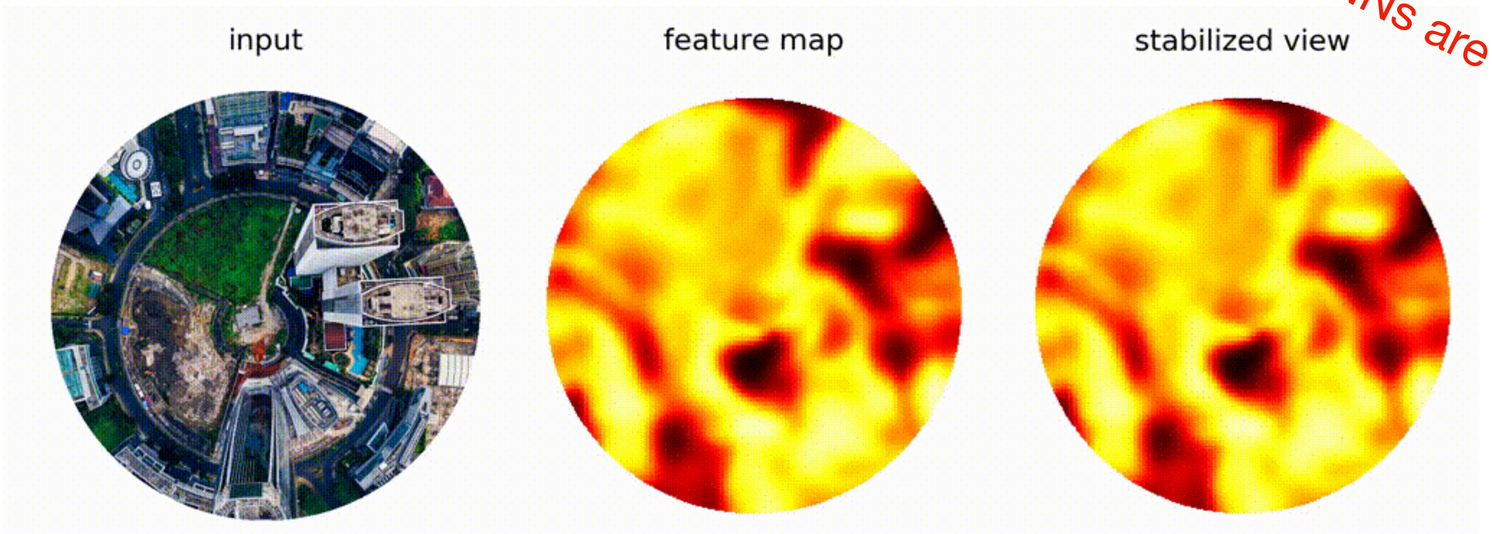
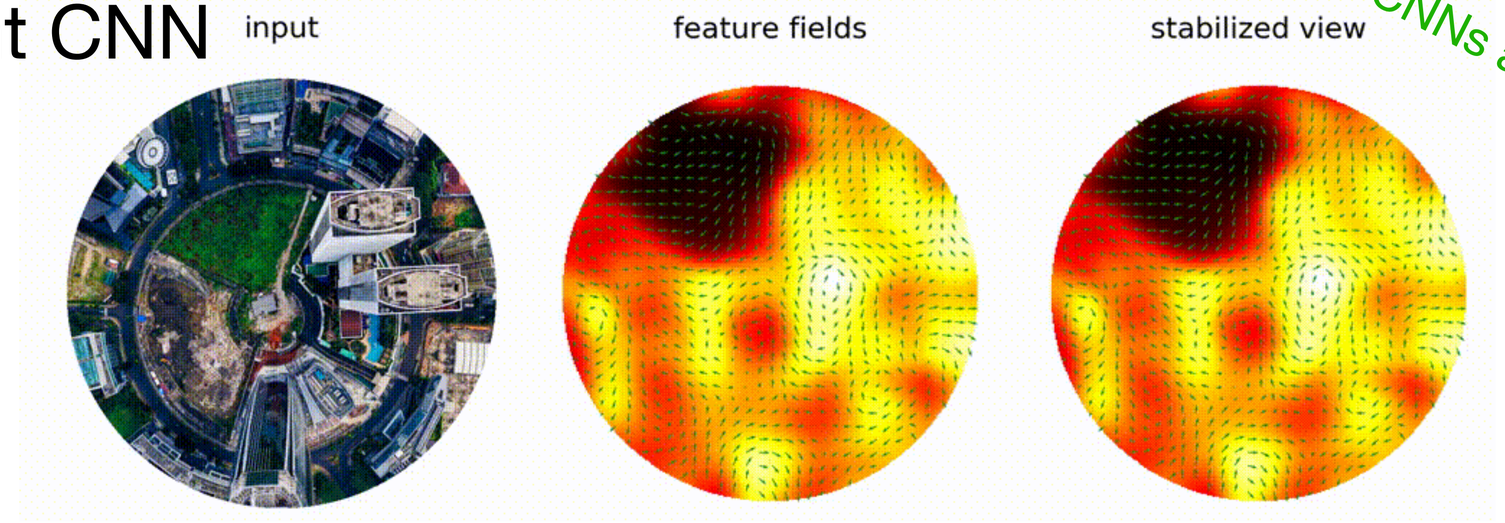


CNNs are not rotation equivariant

Group equivariant CNN



G-CNNs are rotation equivariant!

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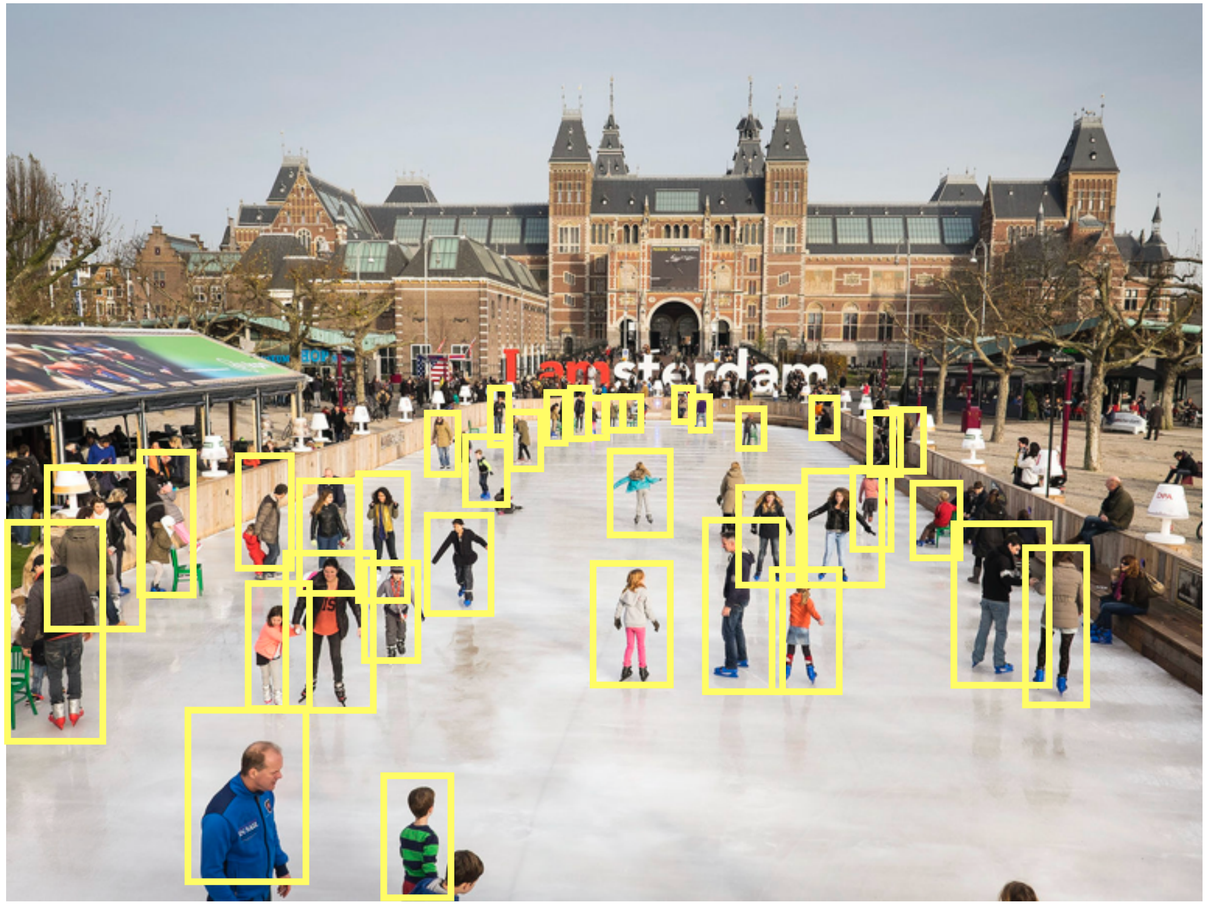
Geometric guarantees (equivariance)



Importance of equivariance:

- No information is lost when the input is transformed

- Guaranteed stability to (local + global) transformations

Group convolutions:

- Equivariance beyond translations

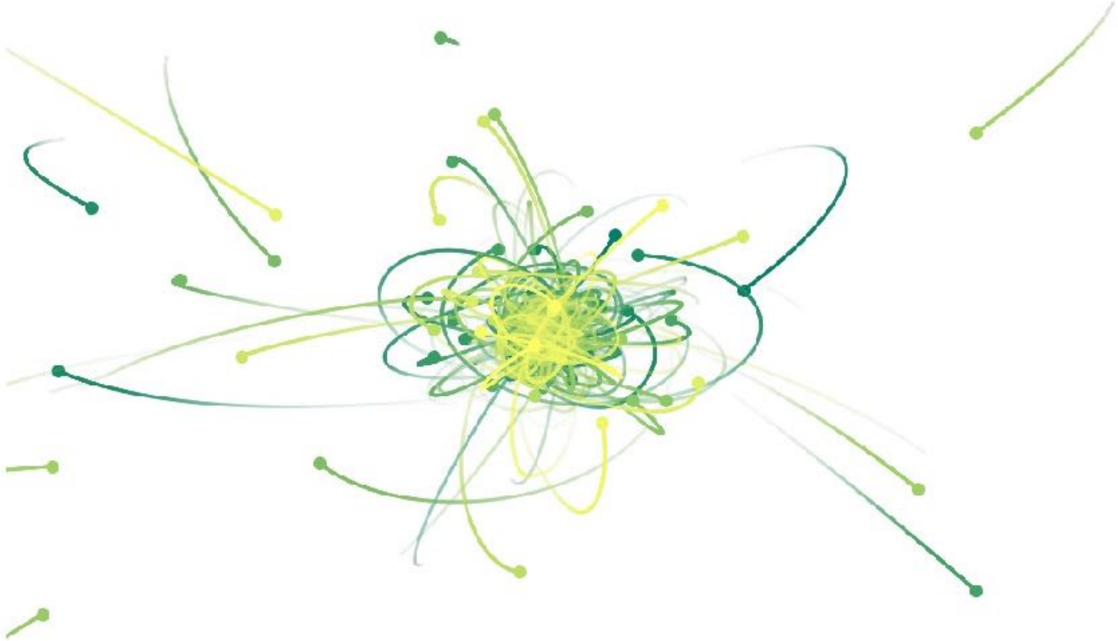
- Geometric guarantees

- Increased weight sharing

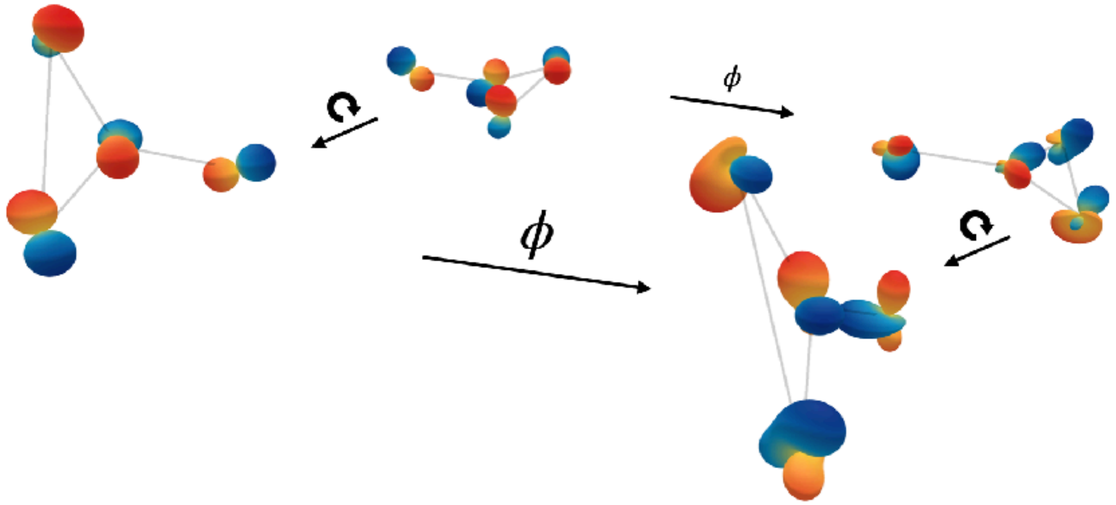
G-CNNs are not only relevant for invariant problems but for any type of structured data!

Geometric guarantees (equivariance)

Equivariant problem:
N-body problem (force/velocity prediction)

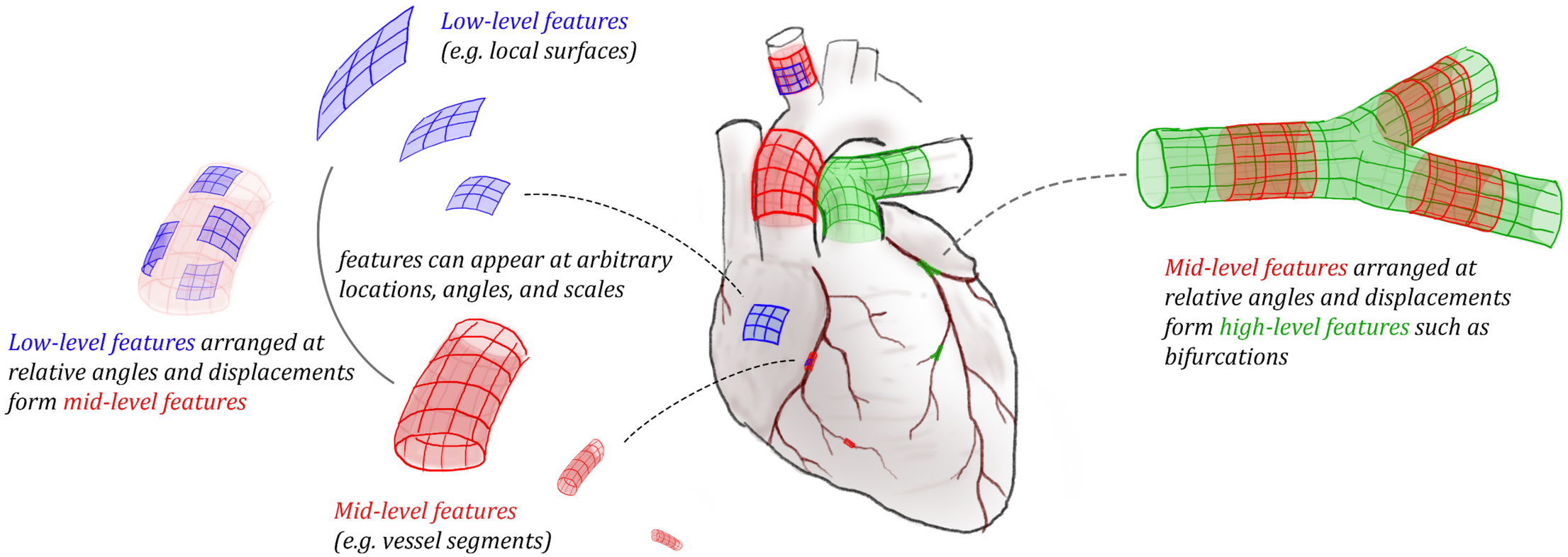


Equivariant problem:
Molecule conformer generation

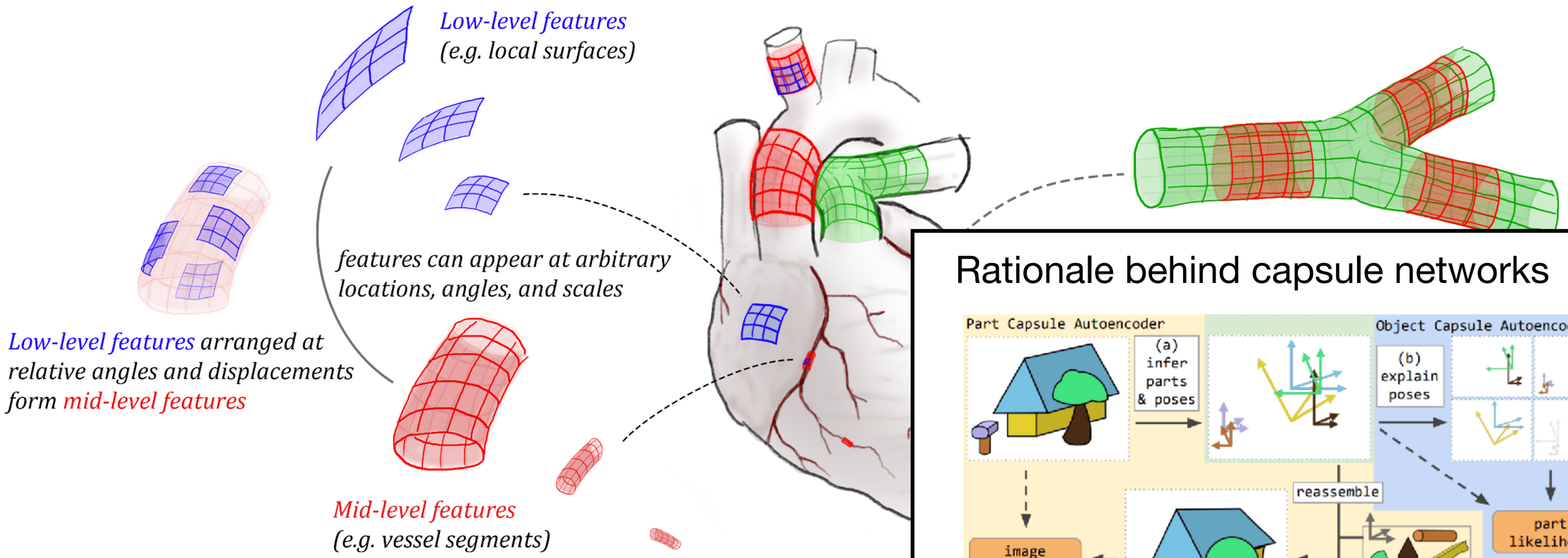


Invariant problem:
Molecule property prediction

Psychology of vision: recognition by components



Psychology of vision: recognition by components



Rationale behind capsule networks

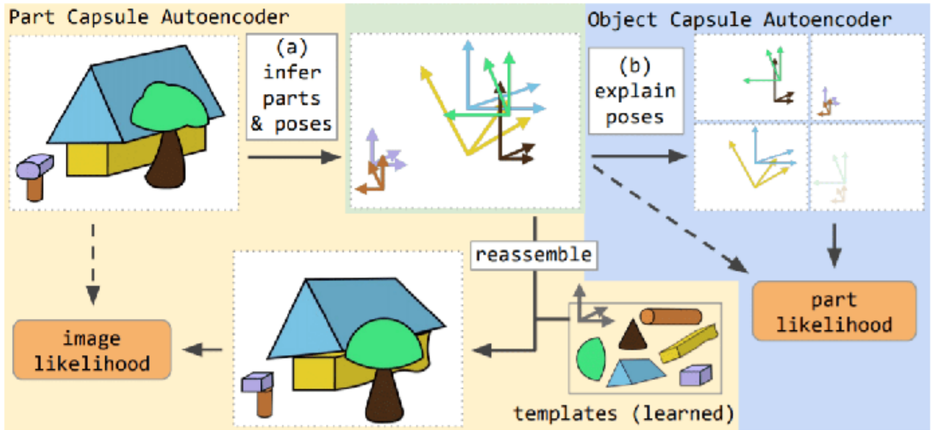
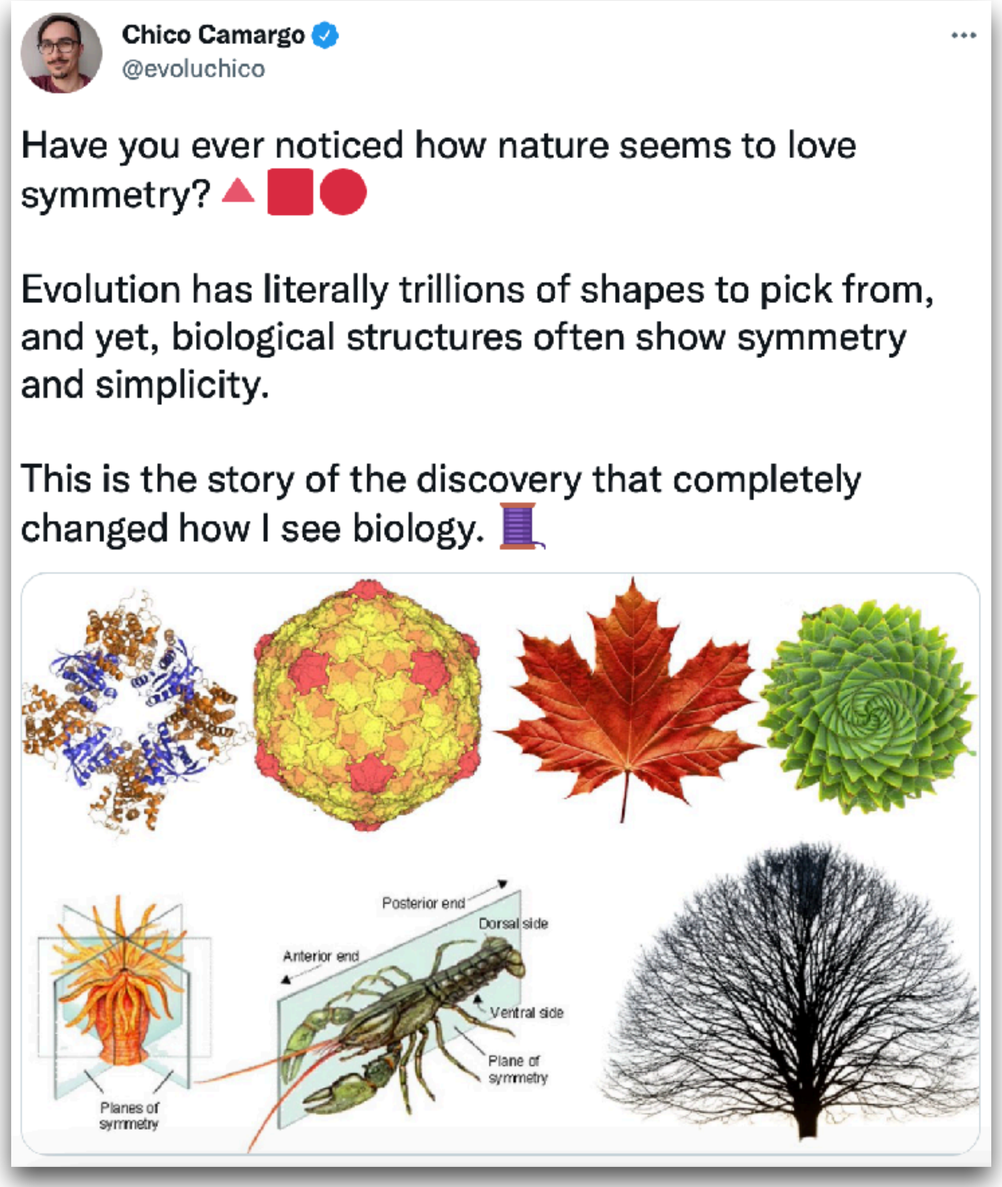


Fig from Kosiorek et al. 2019

Symmetries in nature



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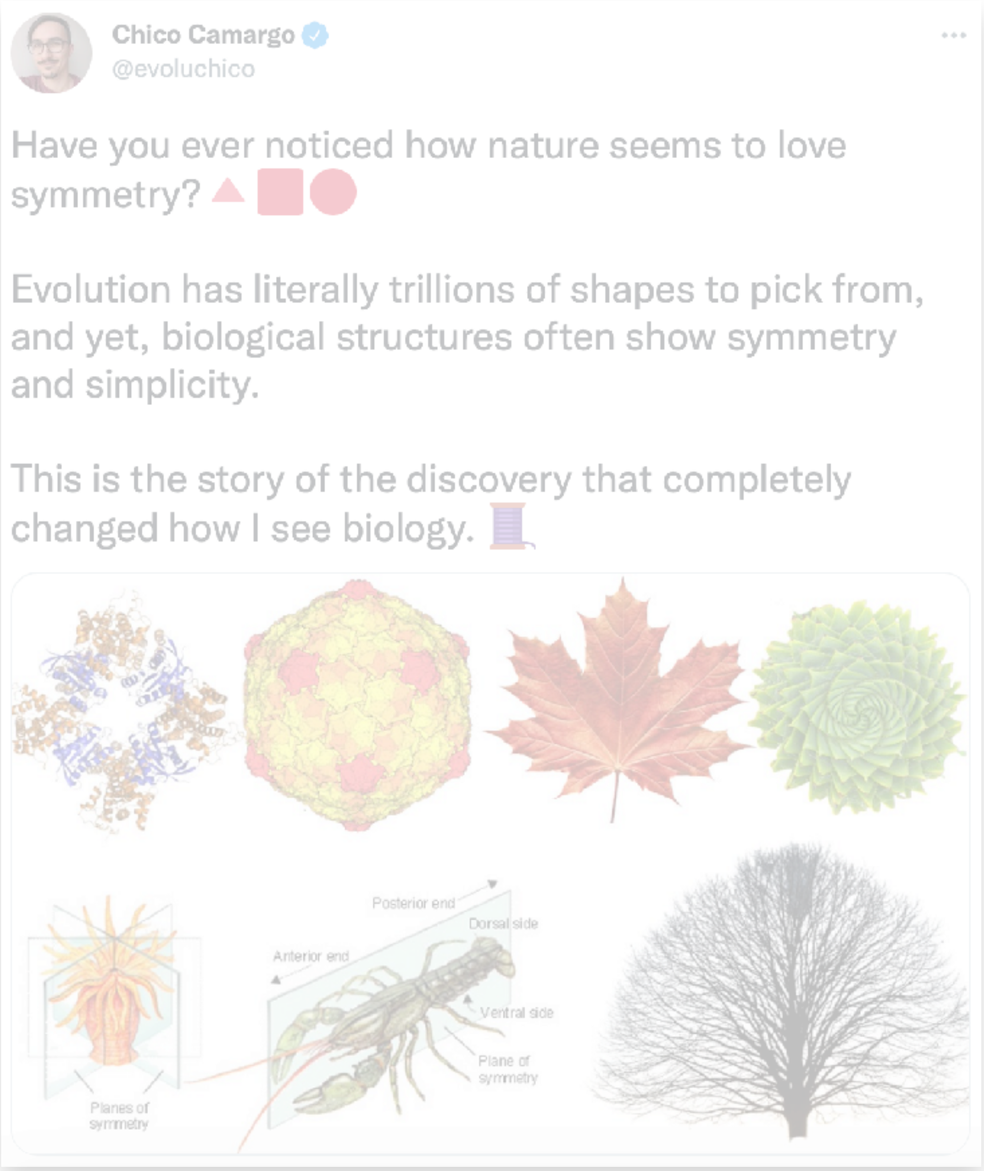

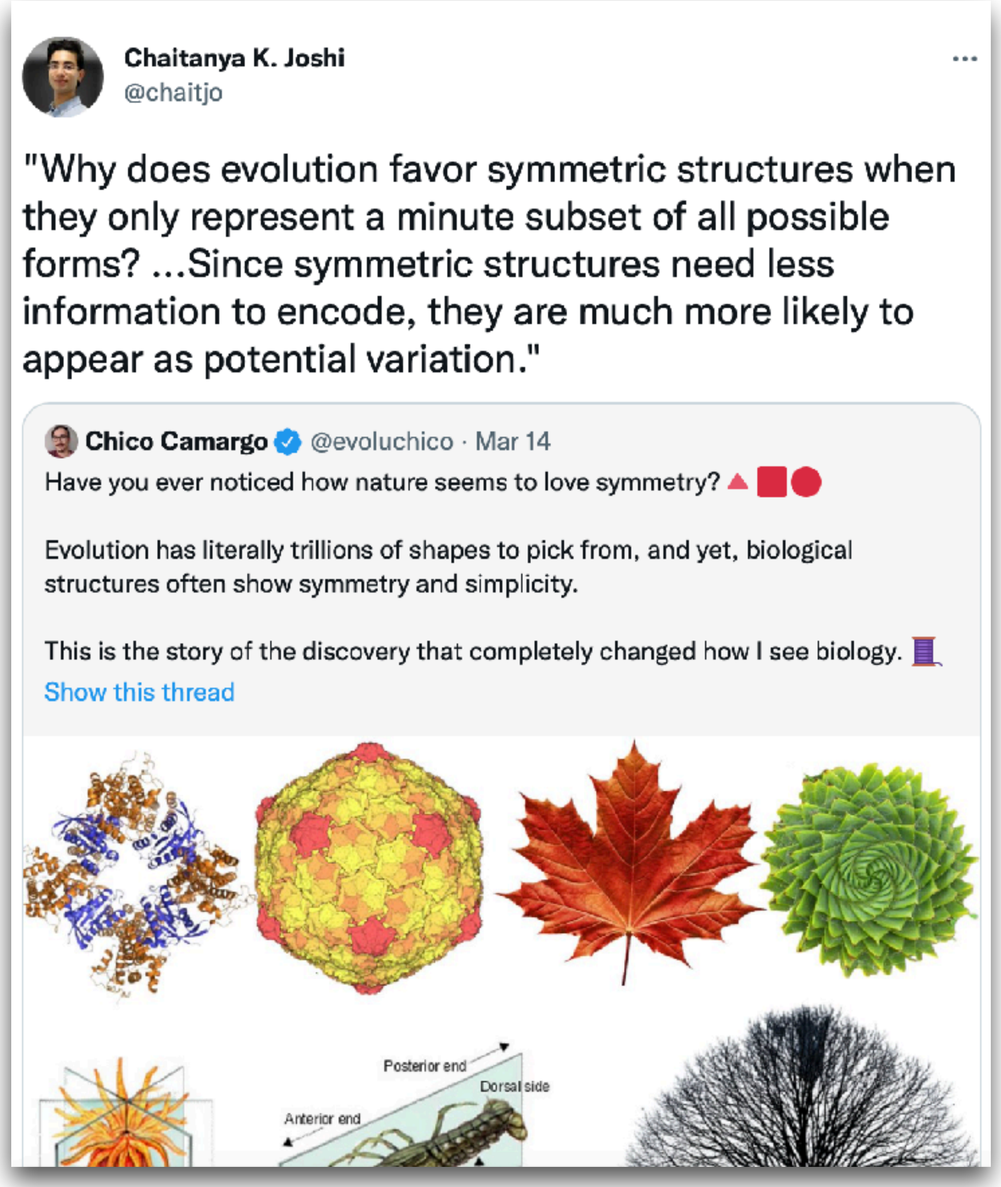

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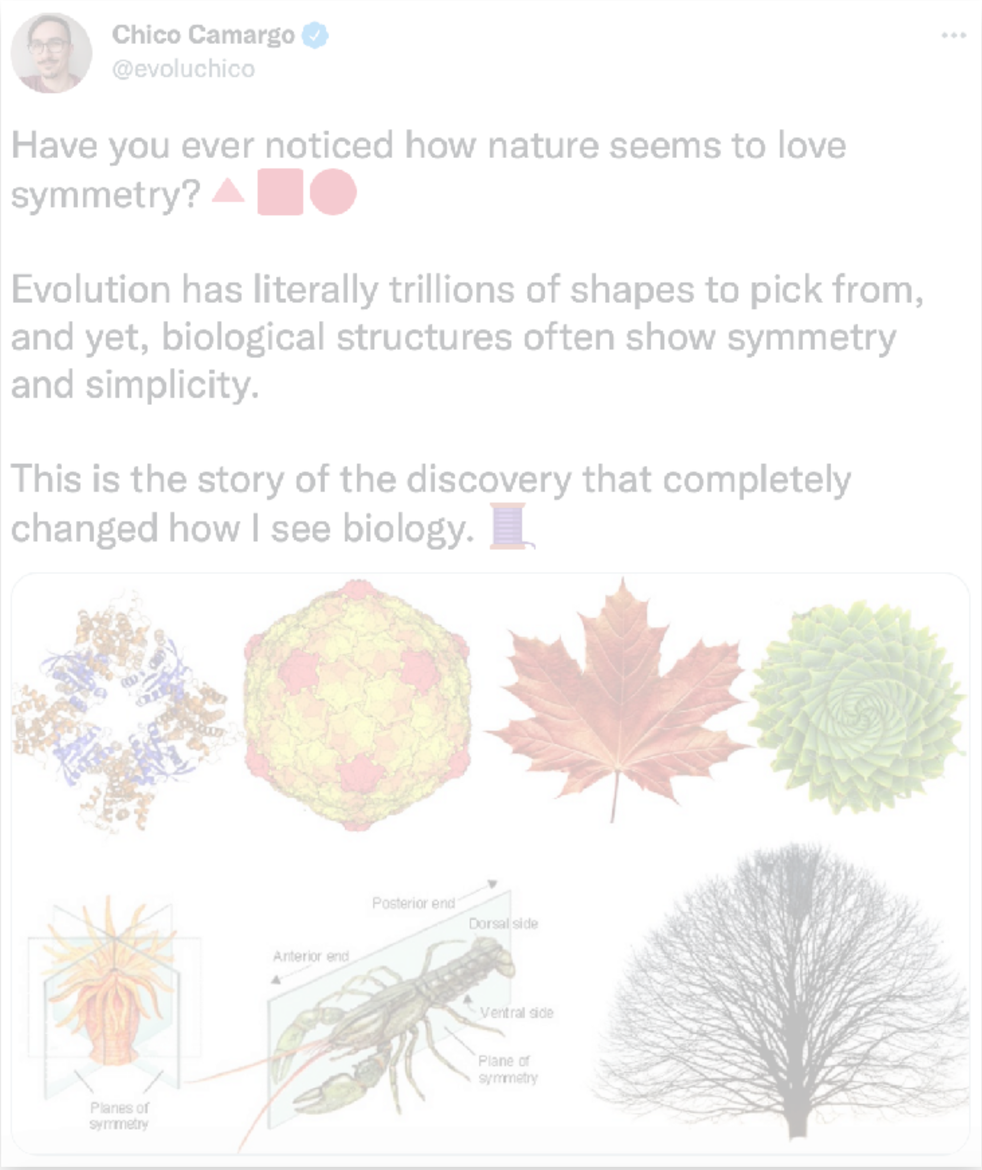
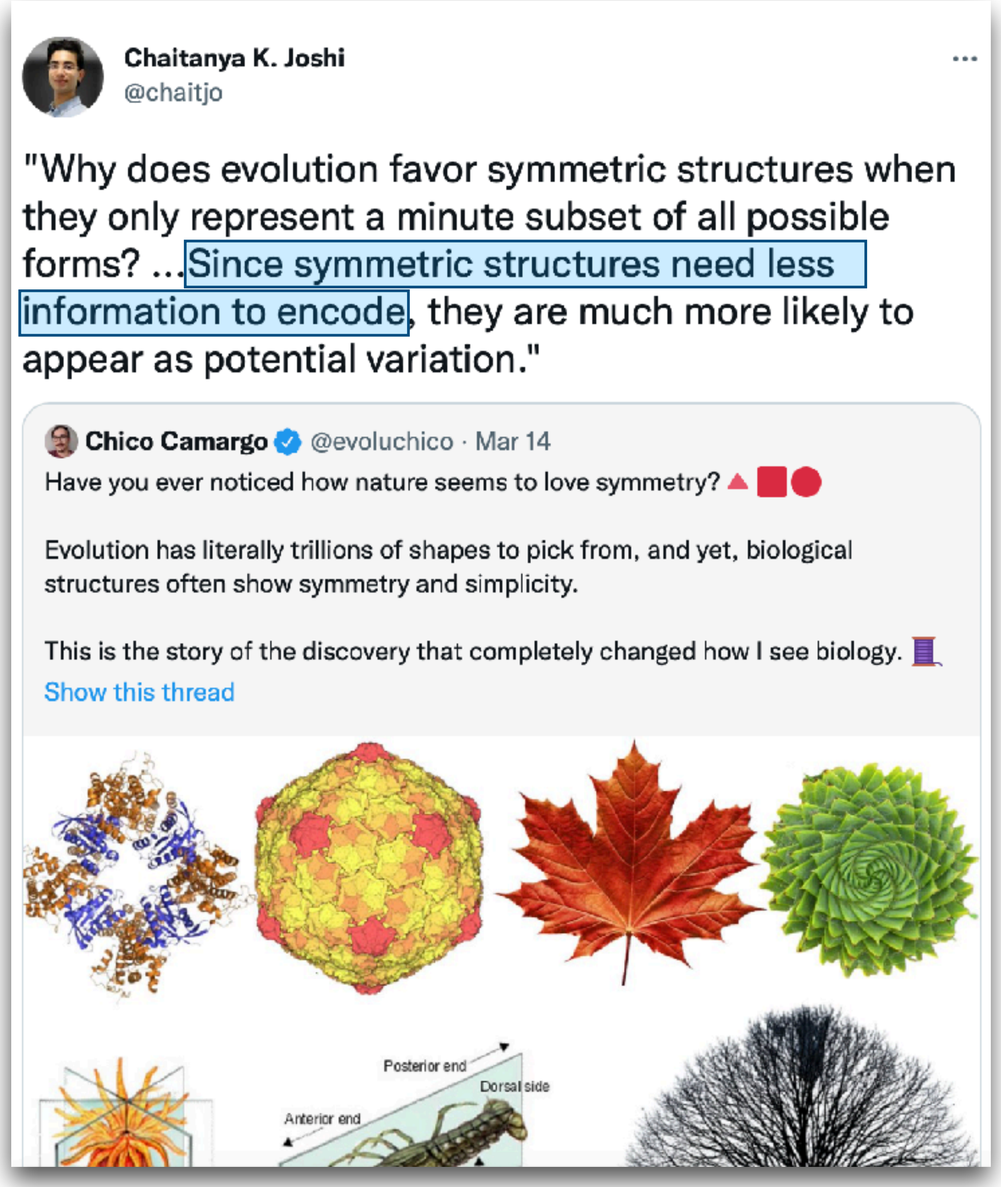
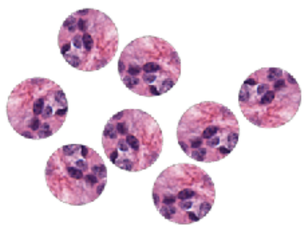
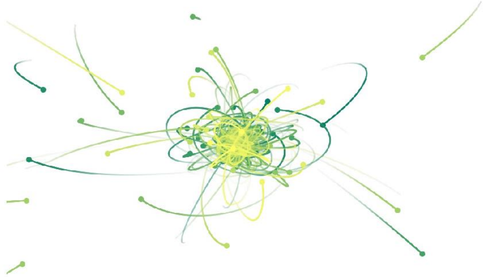


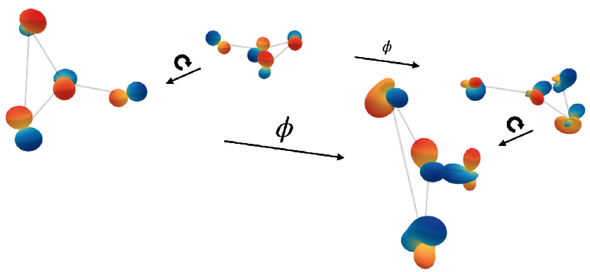


Group equivariant deep learning

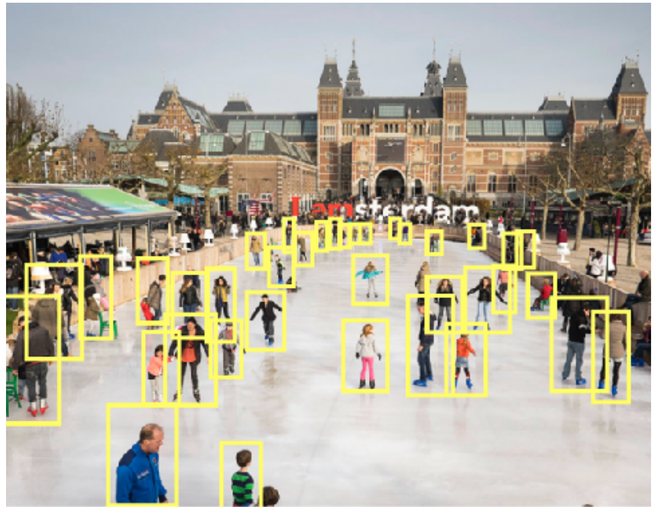
Create architectures with guarantees of invariance or equivariance
(often demanded by problems)



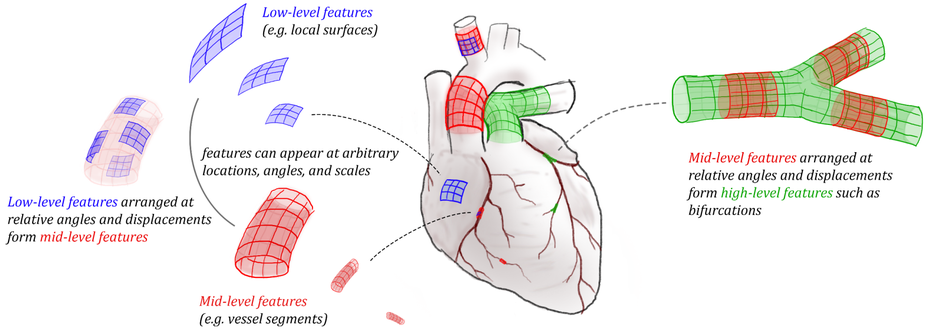




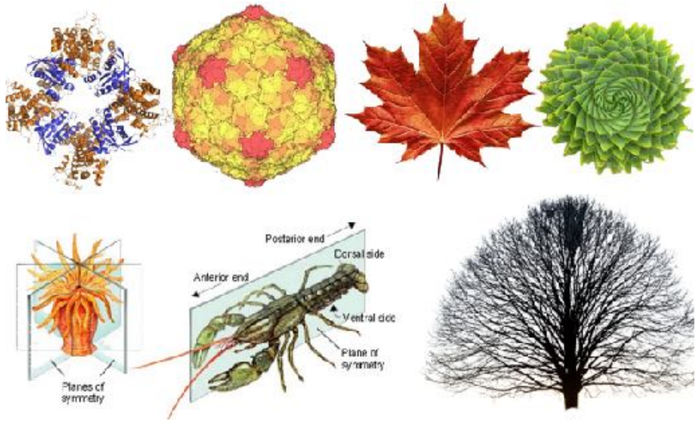
Equivariance allows for
increased weight sharing



Psychology of vision
(recognition by components)



Efficient representation learning
(leverage symmetries)



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Group Equivariant Deep Learning

Lecture 1 - Regular group convolutions

Lecture 1.2 - Group Theory | The basics

Preliminaries for regular group convolutions

Groups, group product, inverse, action, representation, affine groups $G = \mathbb{R}^d \rtimes H$

Erik Bekkers, Amsterdam Machine Learning Lab, University of Amsterdam

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What is a group?

A group $(G, \cdot\,)$ is a set of elements G equipped with a group product $\cdot$, a binary operator, that satisfies the following four axioms:

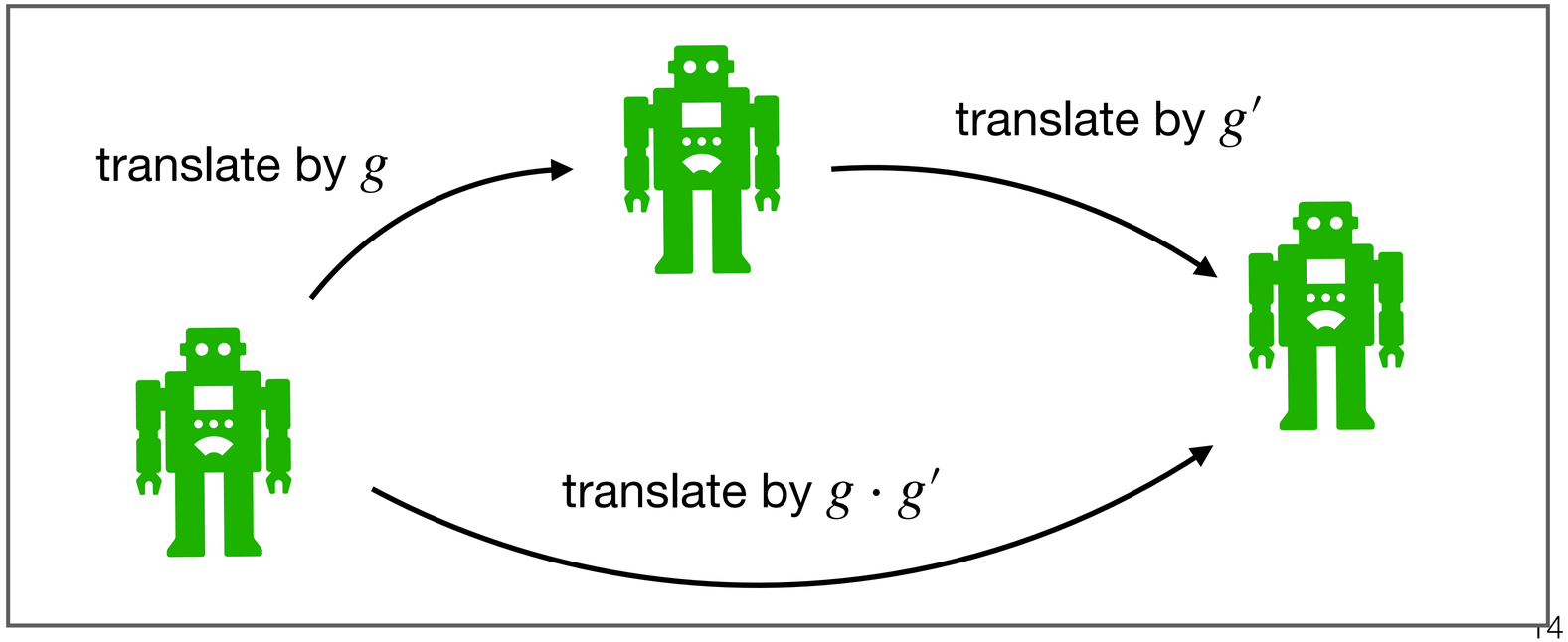
- **Closure**: Given two elements g and h of G, the product $g \cdot h$ is also in G.
- **Associativity**: For $g, h, i \in G$ the product $\cdot$ is associative, i.e., $g \cdot (h \cdot i) = (g \cdot h) \cdot i$.
- **Identity element**: There exists an identity element $e \in G$ such that $e \cdot g = g \cdot e = g$ for any $g \in G$.
- **Inverse element**: For each $g \in G$ there exists an inverse element $g^{-1} \in G$ s.t. $g^{-1} \cdot g = g \cdot g^{-1} = e$.

Translation group $(\mathbb{R}^2, +)$

The translation group consists of all possible translations in $\mathbb{R}^2$ and is equipped with the group product and group inverse:

$$g \cdot g' = (\mathbf{x} + \mathbf{x}')$$
$$g^{-1} = (-\mathbf{x})$$

with $g = (\mathbf{x}), g' = (\mathbf{x}')$ and $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2$.



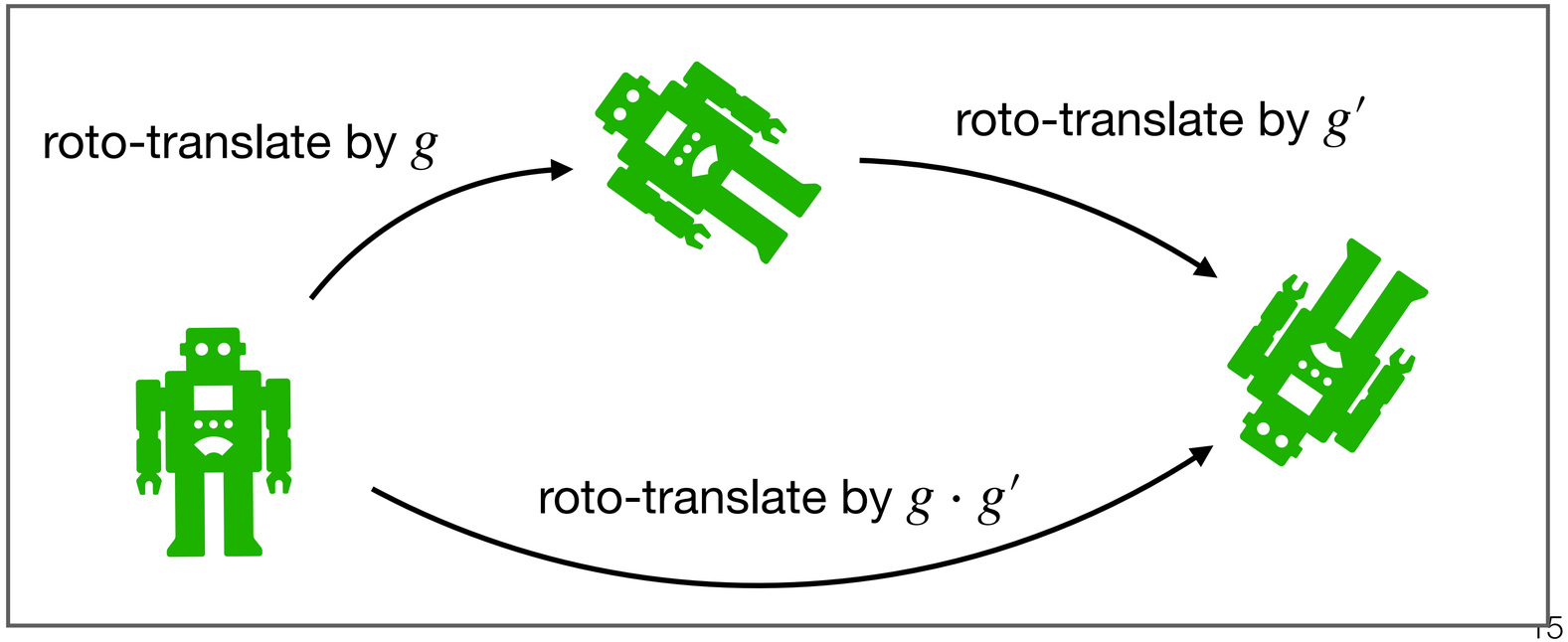
Roto-ranslation group $SE(2)$

***2**D **S**pecial **E**uclidean motion group*

The group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$ consists of the coupled space $\mathbb{R}^2 \times S^1$ of translations vectors in $\mathbb{R}^2$, and rotations in $SO(2)$ (or equivalently orientations in S^1), and is equipped with the group product and group inverse:

$$g \cdot g' = (\mathbf{x}, \mathbf{R}_\theta) \cdot (\mathbf{x}', \mathbf{R}_{\theta'}) = (\mathbf{R}_\theta \mathbf{x}' + \mathbf{x}, \mathbf{R}_{\theta+\theta'})$$
$$g^{-1} = (-\mathbf{R}_\theta^{-1}\mathbf{x}, \mathbf{R}_\theta^{-1})$$

with $g = (\mathbf{x}, \mathbf{R}_\theta)$, $g' = (\mathbf{x}', \mathbf{R}_{\theta'})$.



Roto-ranslation group $SE(2)$

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Matrix representation: The group can also be represented by matrices

$$g = (\mathbf{x}, \mathbf{R}_\theta) \quad \leftrightarrow \quad \mathbf{G} = \begin{pmatrix} \cos\theta & -\sin\theta & x \\ \sin\theta & \cos\theta & y \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \mathbf{R}_\theta & \mathbf{x} \\ \mathbf{0}^T & 1 \end{pmatrix}$$

with the group product and inverse simply given by the matrix product and matrix inverse.

In parametric form:

$$(\mathbf{x}, \theta) \cdot (\mathbf{x}', \theta') = (\mathbf{R}_\theta \mathbf{x}' + \mathbf{x},\ \theta + \theta' \bmod 2\pi)$$

$$\leftrightarrow$$

In matrix form:

$$\begin{pmatrix} \mathbf{R}_\theta & \mathbf{x} \\ \mathbf{0}^T & 1 \end{pmatrix} \begin{pmatrix} \mathbf{R}'_\theta & \mathbf{x}' \\ \mathbf{0}^T & 1 \end{pmatrix} = \begin{pmatrix} \mathbf{R}_{\theta+\theta'} & \mathbf{R}_\theta \mathbf{x}' + \mathbf{x} \\ \mathbf{0}^T & 1 \end{pmatrix}$$

Scale-translation group $R^2 \rtimes \mathbb{R}^+$

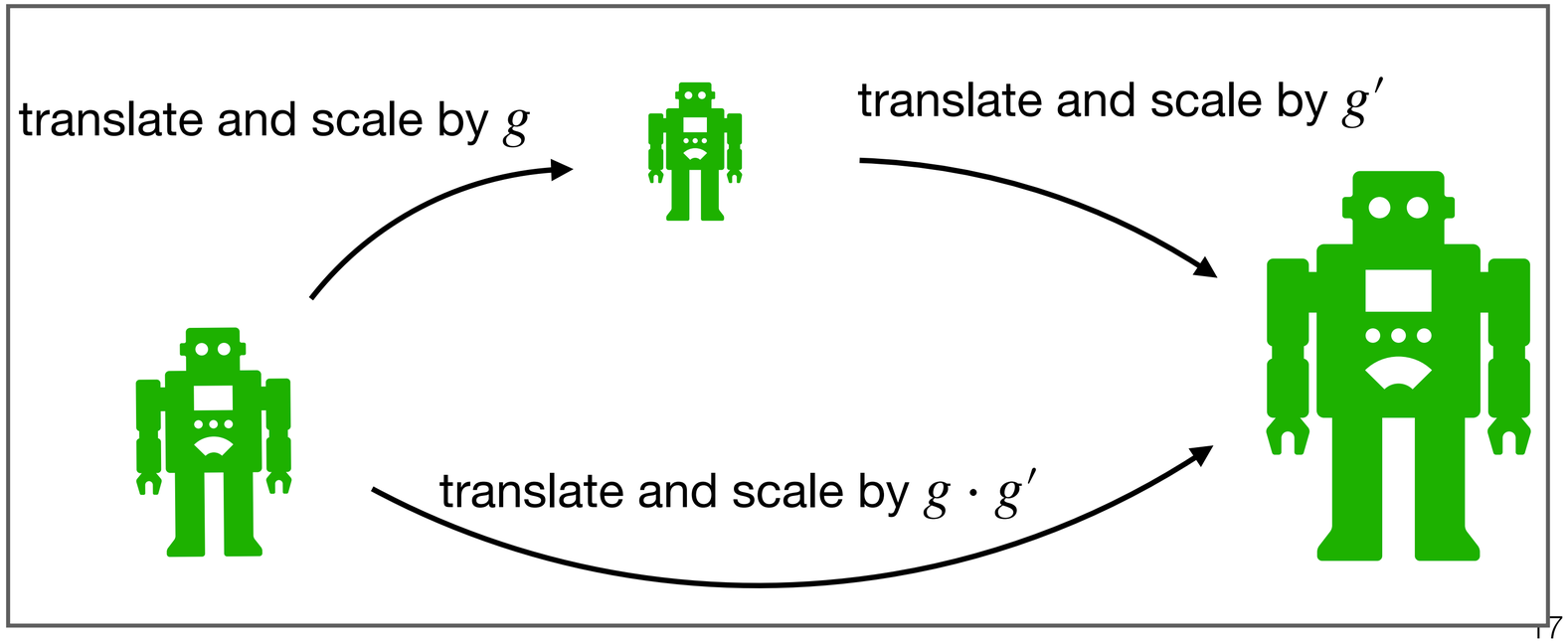
The scale-translation group of space $\mathbb{R}^2 \times \mathbb{R}^+$ of translations vectors in $\mathbb{R}^2$ and scale/dilation factors in $\mathbb{R}^+$, and is equipped with the group product and group inverse:

$$g \cdot g' = (\mathbf{x}, s) \cdot (\mathbf{x}', s') = (s\mathbf{x}' + \mathbf{x}, ss')$$
$$g^{-1} = \left(-\frac{1}{s}\mathbf{x}, \frac{1}{s}\right)$$

with $g = (\mathbf{x}, s), g' = (\mathbf{x}', s')$.

with $g \cdot g^{-1} = e = (\mathbf{0}, 1)$

matrix repr: $\mathbf{G} = \begin{pmatrix} \mathbf{I}_s & \mathbf{x} \\ \mathbf{0}^T & 1 \end{pmatrix}$



Affine groups $G = \mathbb{R}^d \rtimes H$

Affine groups are semi-direct product groups of some group H with an action on $\mathbb{R}^d$ from which we derive the following group product and inverse

transform/shift sub-group

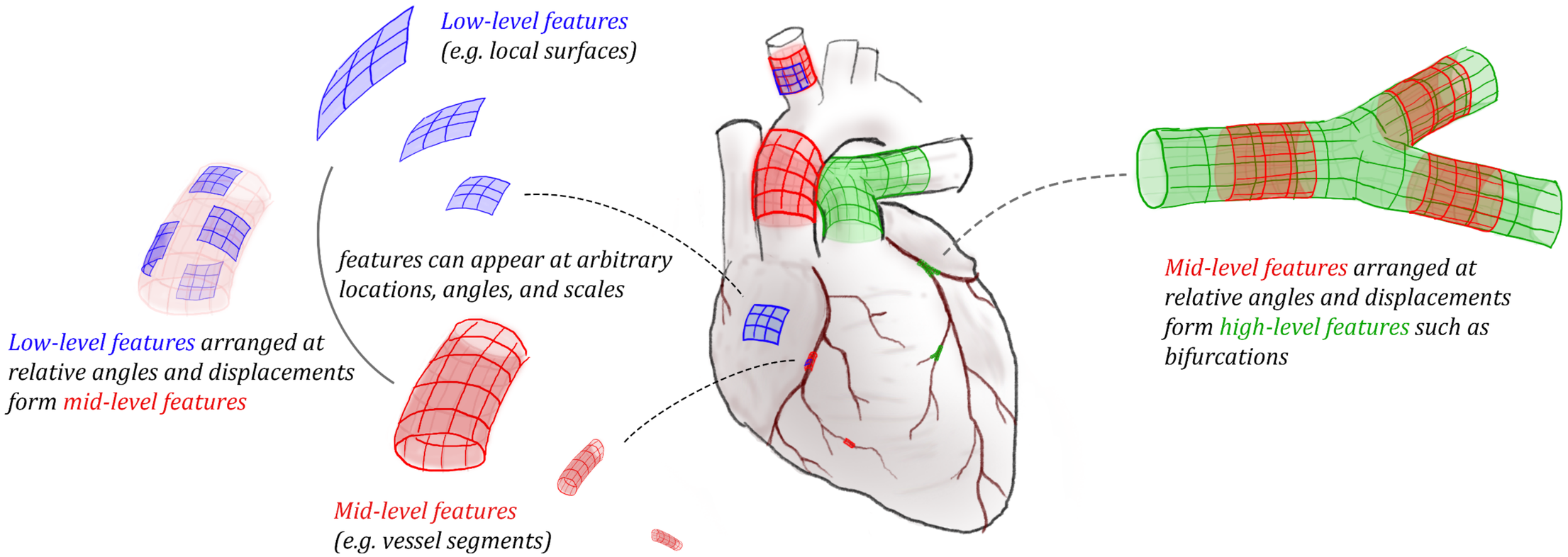
$$g \cdot g' = (\mathbf{x}, h) \cdot (\mathbf{x}', h') = (h \cdot \mathbf{x}' + \mathbf{x}, h \cdot h')$$

Transform point + shift point

$$g^{-1} = \left(-h^{-1} \cdot \mathbf{x}, h^{-1}\right)$$

with group elements $g = (\mathbf{x}, h), g' = (\mathbf{x}', h')$.

Psychology of vision: recognition by components



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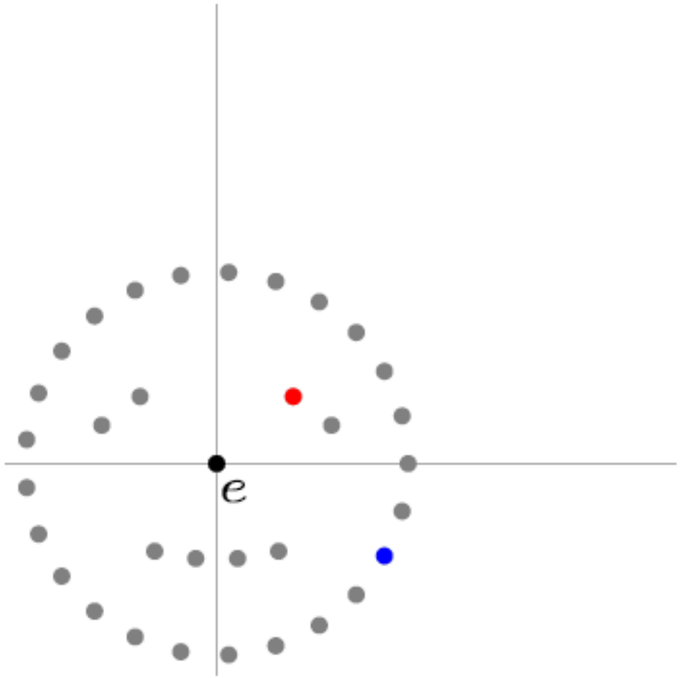

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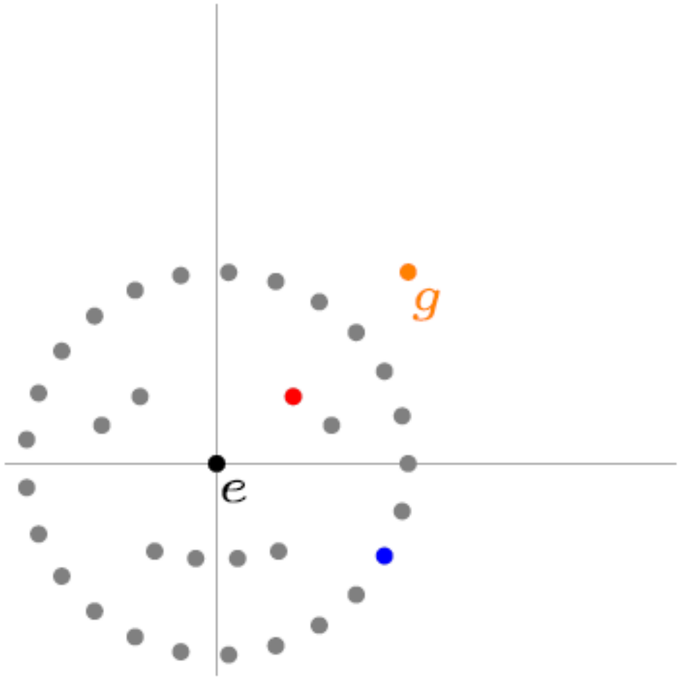

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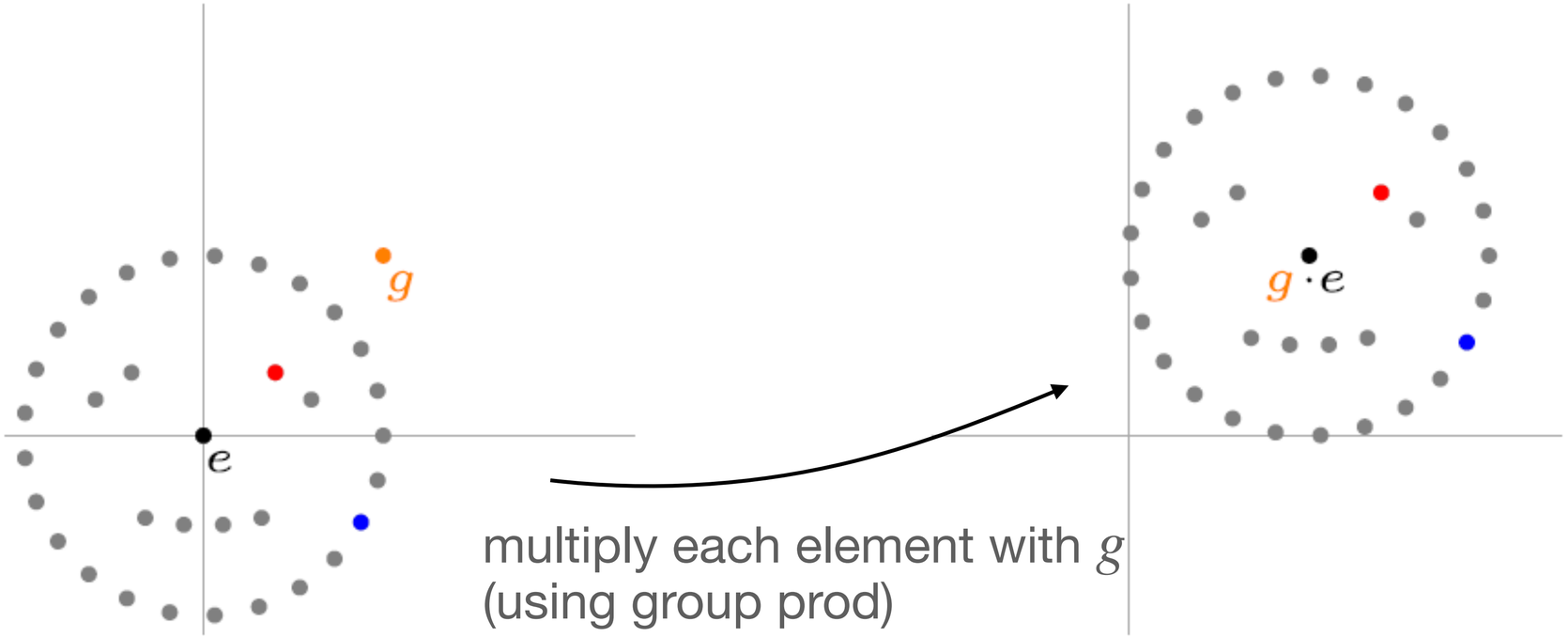

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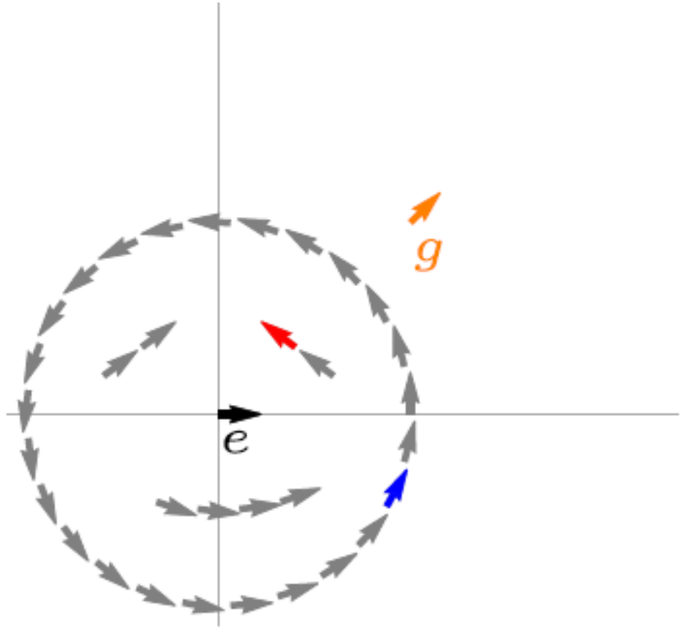

Roto-ranslation group $SE(2)$

***2**D **S**pecial **E**uclidean motion group*

The group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$ consists of the coupled space $\mathbb{R}^2 \times S^1$ of translations vectors in $\mathbb{R}^2$, and rotations in $SO(2)$ (or equivalently orientations in S^1), and is equipped with the group product and group inverse:

$$g \cdot g' = (\mathbf{x}, \mathbf{R}_\theta) \cdot (\mathbf{x}', \mathbf{R}_{\theta'}) = (\mathbf{R}_\theta \mathbf{x}' + \mathbf{x}, \mathbf{R}_{\theta+\theta'})$$
$$g^{-1} = (-\mathbf{R}_\theta^{-1}\mathbf{x}, \mathbf{R}_\theta^{-1})$$

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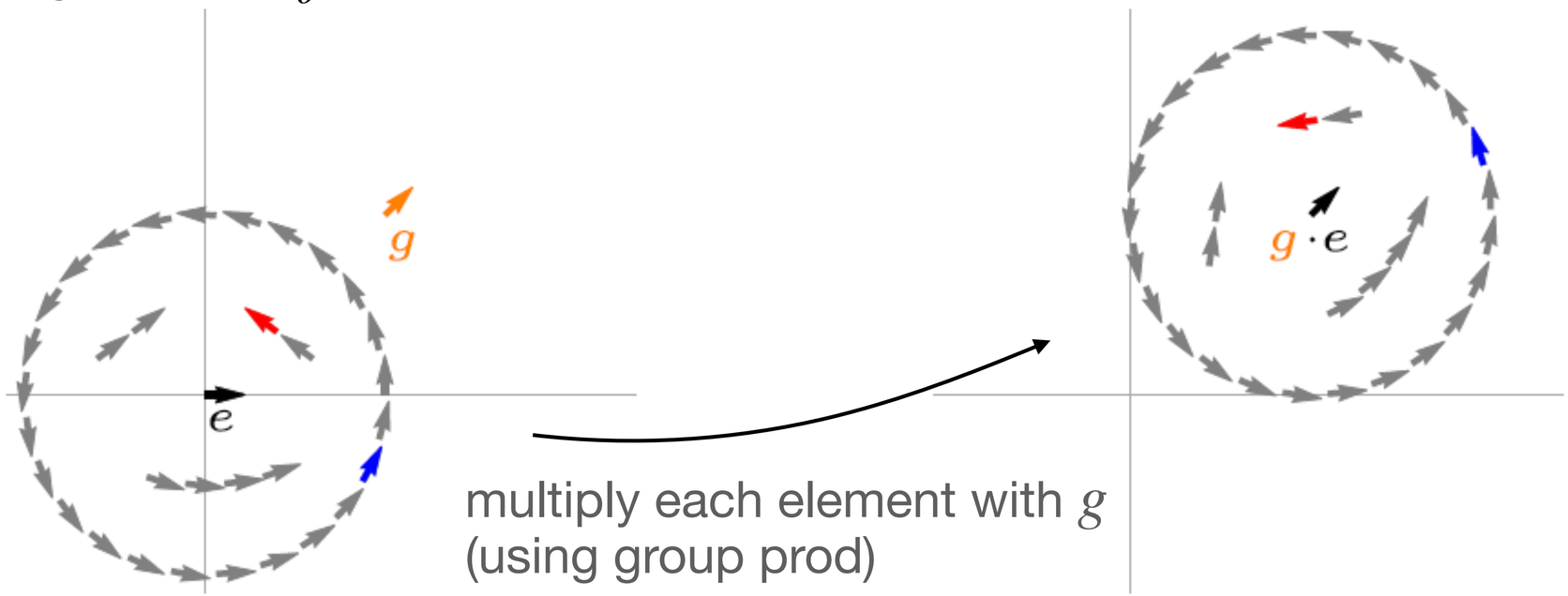
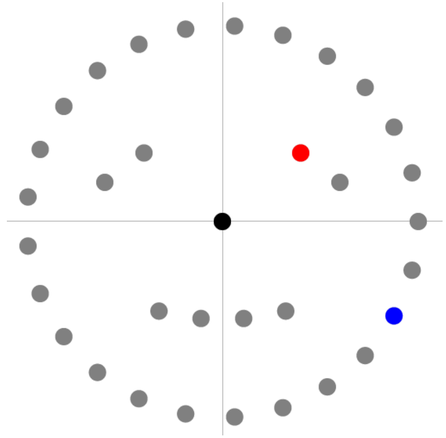


So… How to translate this to (G-)CNNs?

Set of points (group elements)



Convolution kernel

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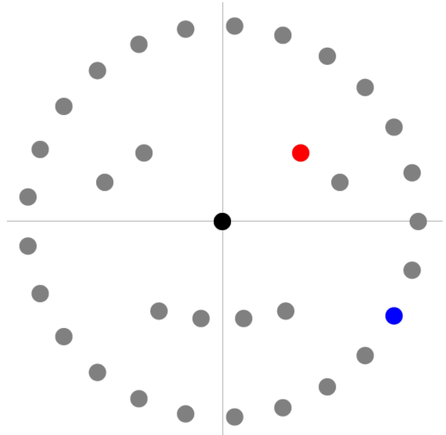

Convolution kernel

$$\{g_1, g_2, \ldots\} \subset G = (\mathbb{R}^2, +)$$

“A collection of parts in certain poses”

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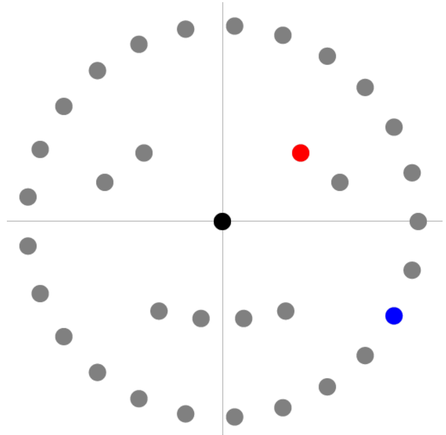

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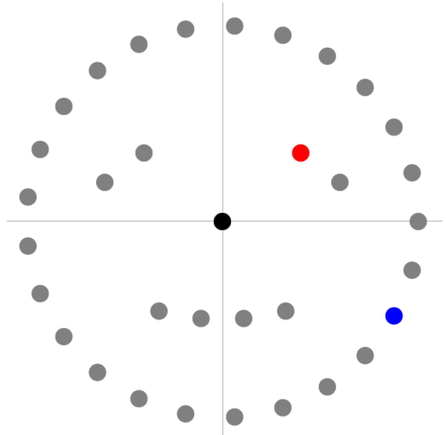

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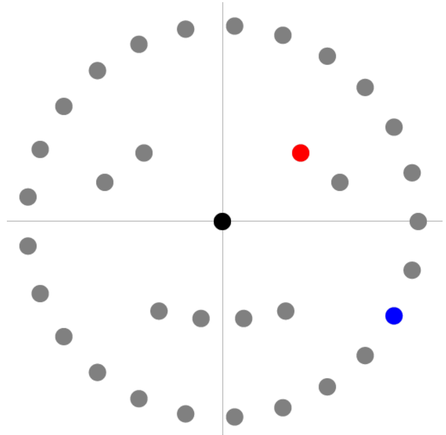

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Transforms via group representations

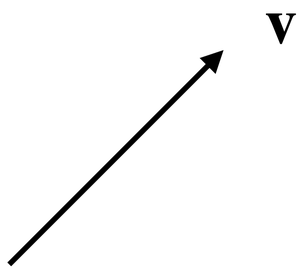
Representations

A representation $\rho : G \rightarrow GL(V)$ is a group homomorphism from G to the general linear group $GL(V)$.

That is $\rho(g)$ is a linear transformation that is parameterized by group elements $g \in G$ that transforms some vector $\mathbf{v} \in V$ (e.g. an image) such that

$$\rho(g') \circ \rho(g)[\mathbf{v}] = \rho(g' \cdot g)\,[\mathbf{v}]$$

Representations



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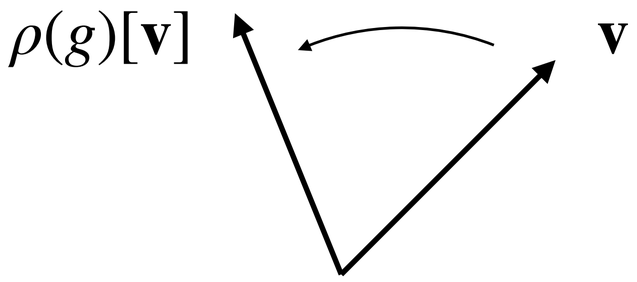

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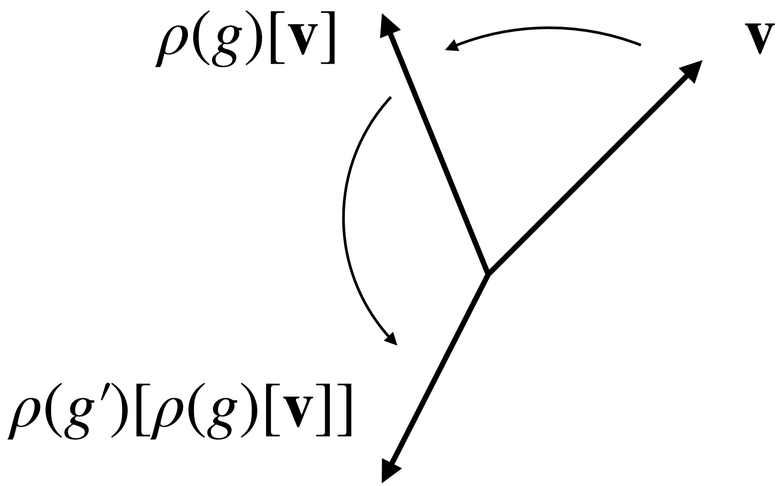

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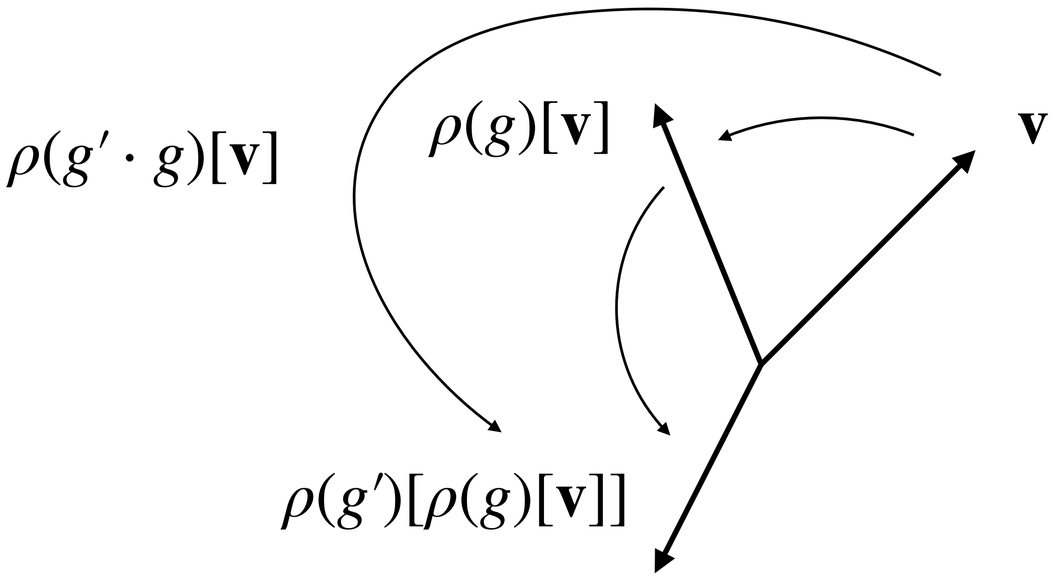

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Left-regular Representations

A left-regular representation $\mathscr{L}_g$ is a representation that transforms functions f by transforming their domains via the inverse group action

$$\mathscr{L}_g[f](x) := f(g^{-1} \cdot x)$$

"group action" equals group product when domain is G

Left-regular Representations

Example:

$f \in \mathbb{L}_2(\mathbb{R}^2)$

- a 2D image

$G = SE(2)$

- the roto-translation group

$\mathscr{L}_g(f)(\mathbf{y}) = f(\mathbf{R}_\theta^{-1}(\mathbf{y} - \mathbf{x}))$

- a roto-translation of the image

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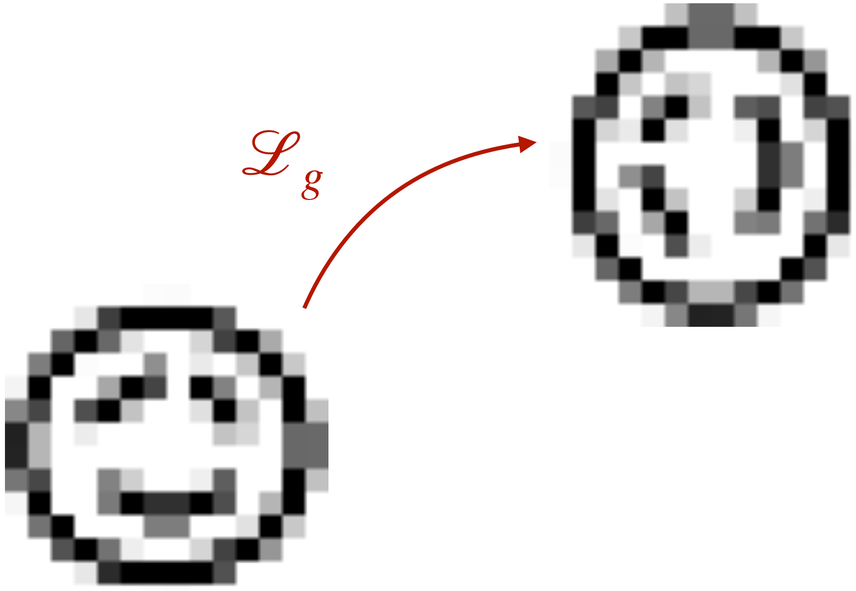

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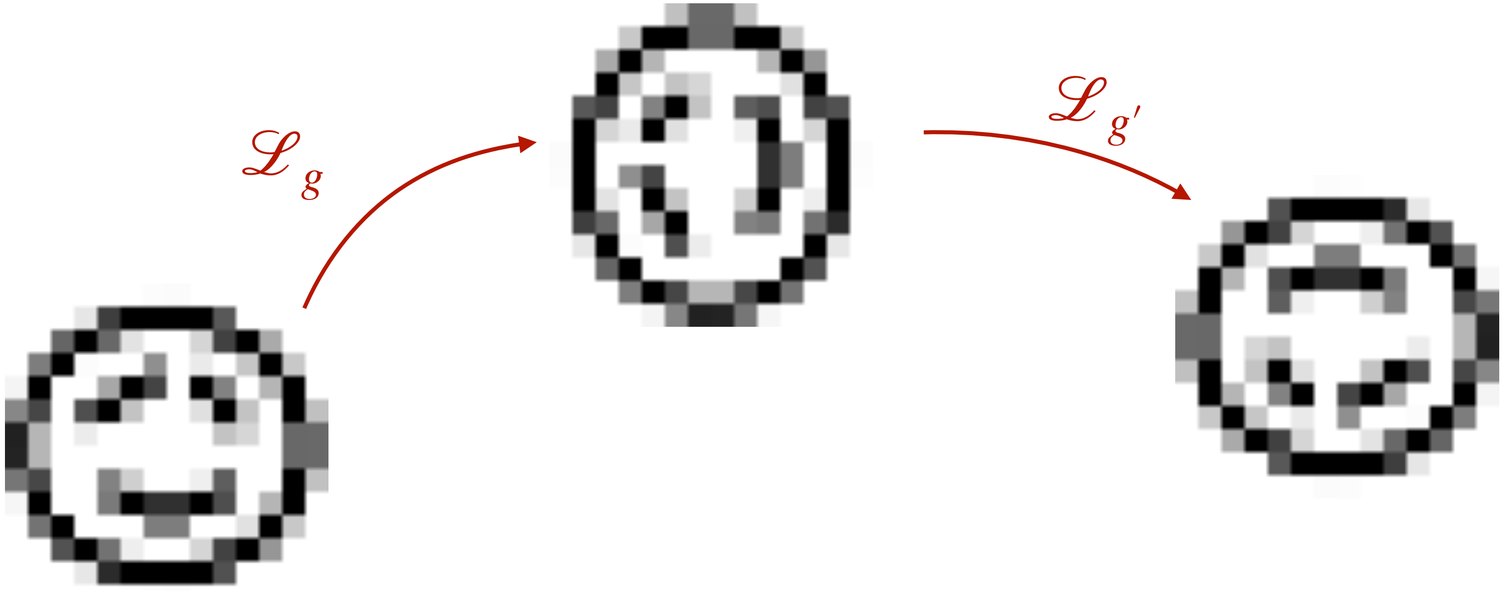

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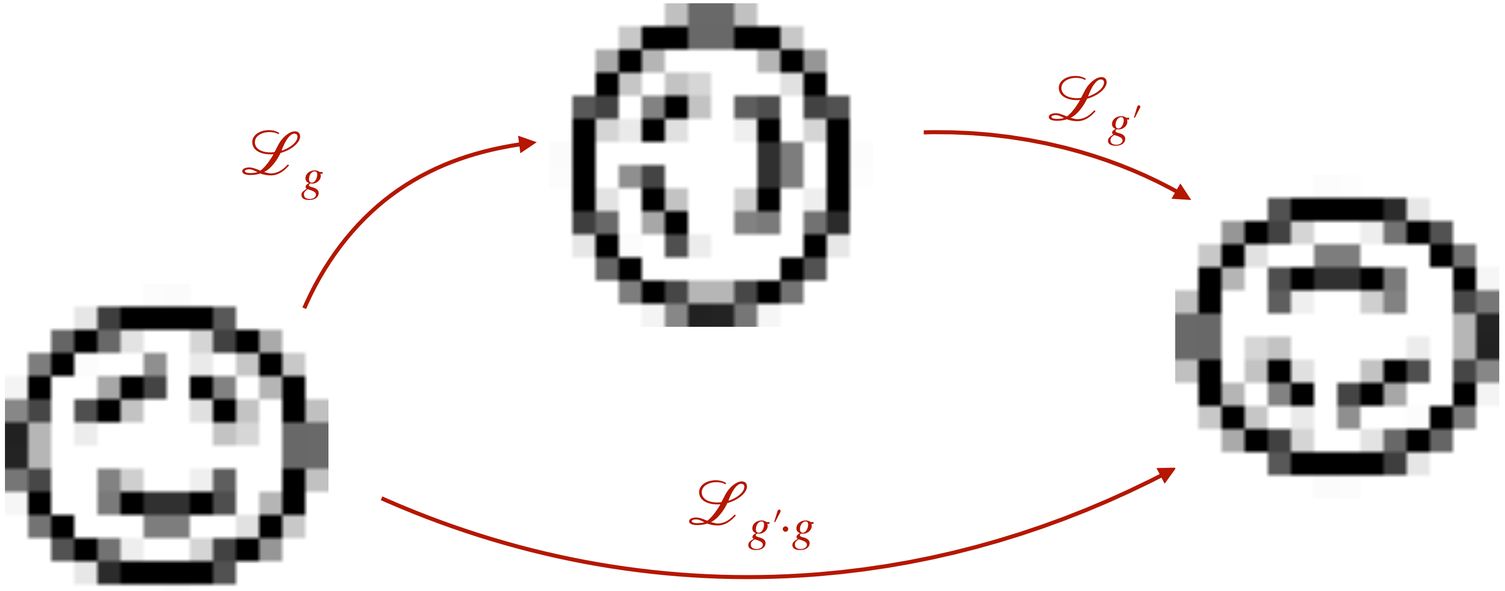

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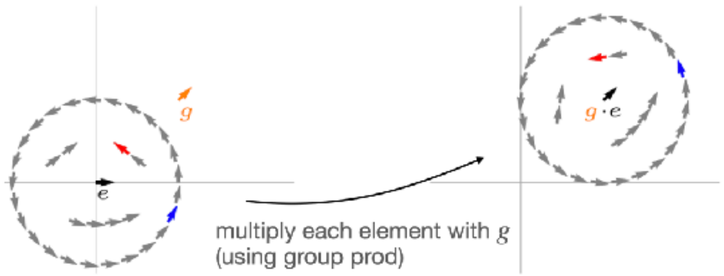
Group actions

Group product (the action on G)

$$g \cdot g'$$



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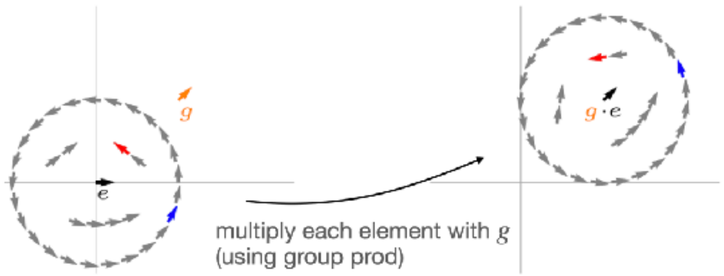
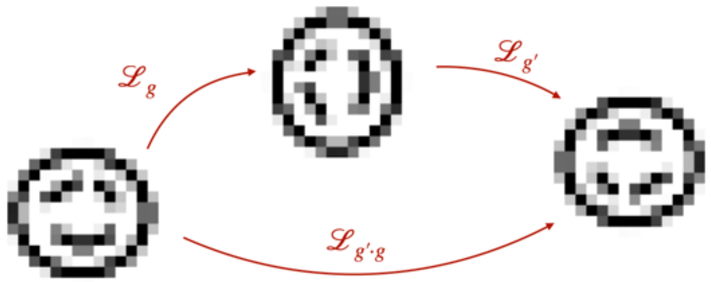


Left regular representation (the action on $\mathbb{L}_2(X)$)

$$\mathscr{L}_g f$$



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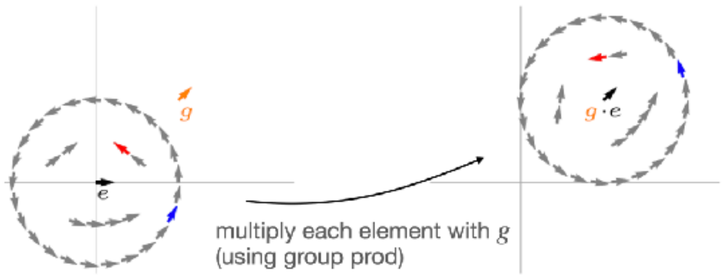

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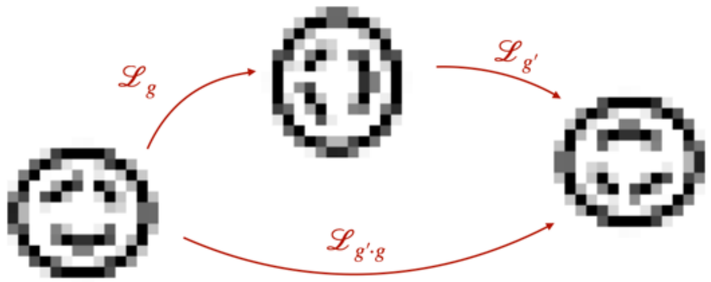
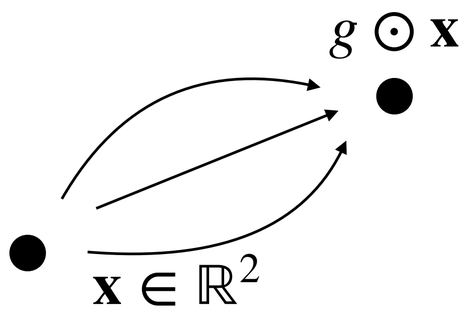


Group action (the action on $\mathbb{R}^d$)

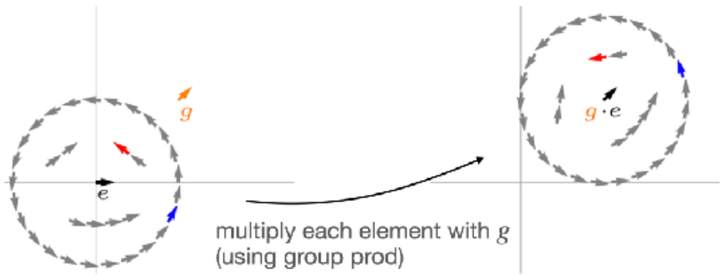
$$g \odot \mathbf{x}$$



Group actions

Group product (the action on G)

$$g \cdot g' \qquad\qquad gg'$$



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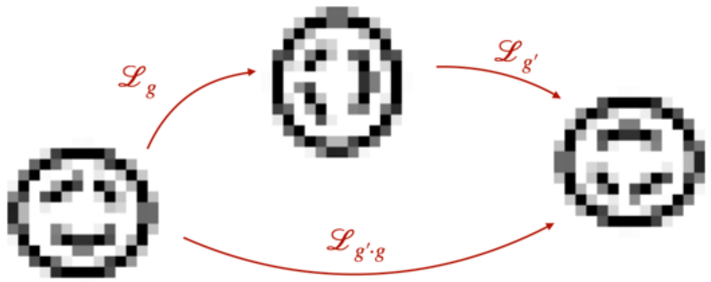

Group action (the action on $\mathbb{R}^d$)

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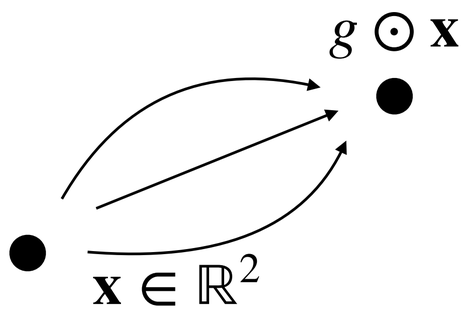
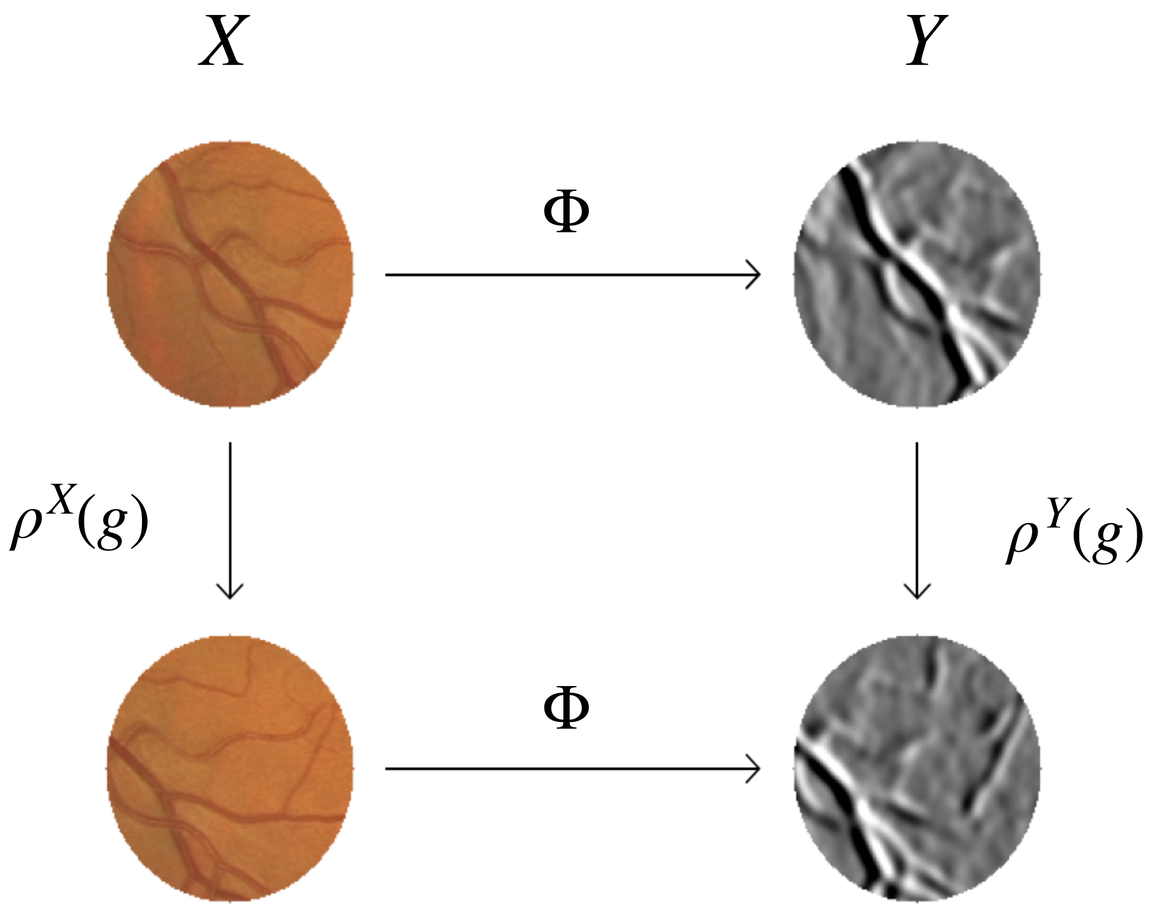


Equivariance

Equivariance is a property of an operator $\Phi : X \to Y$ (such as a neural network layer) by which it commutes with the group action:

$$\Phi \circ \rho^X(g) = \rho^Y(g) \circ \Phi$$

group representation action on X



UNIVERSITY OF AMSTERDAM

AMLAB Amsterdam Machine Learning Lab

Group Equivariant Deep Learning

Lecture 1 - Regular group convolutions

Lecture 1.3 - Regular group convolutions | Template matching viewpoint

General group convolutional NN design with example for roto-translation equivariance (SE(2))

Erik Bekkers, Amsterdam Machine Learning Lab, University of Amsterdam

This mini-course serves as a module with the UvA Master AI course Deep Learning 2 https://uvadl2c.github.io/

Cross-correlations

$$(k \star_{\mathbb{R}^2} f)(\mathbf{x}) = \int_{\mathbb{R}^2} k(\mathbf{x}' - \mathbf{x}) f(\mathbf{x}') \mathrm{d}\mathbf{x}'$$

Cross-correlations

Representation of the translation group!

$$(k \star_{\mathbb{R}^2} f)(\mathbf{x}) = \int_{\mathbb{R}^2} k(\mathbf{x}' - \mathbf{x}) f(\mathbf{x}') \mathrm{d}\mathbf{x}' = (\mathscr{L}_g \, k \, , f)_{\mathbb{L}_2(\mathbb{R}^2)}$$

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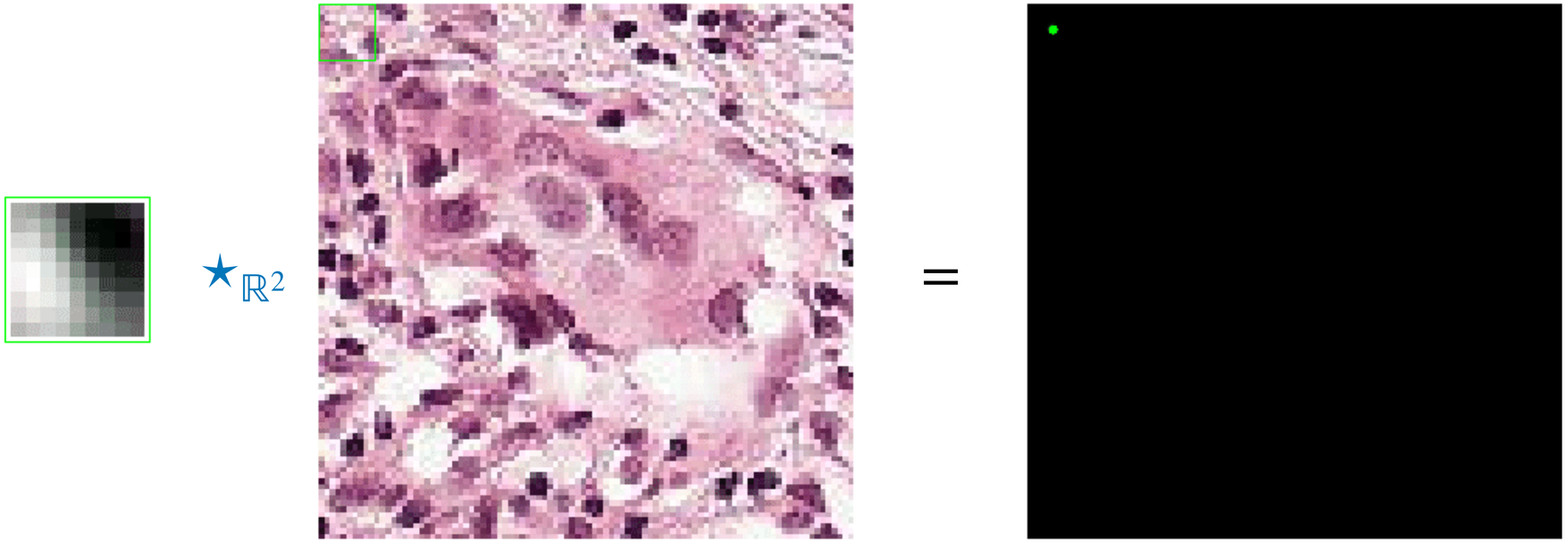


k
2D convolution kernel

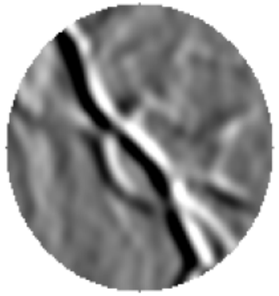
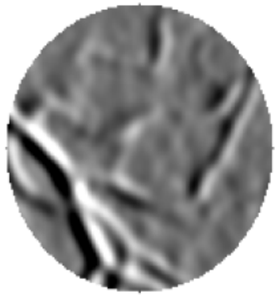
f^{in}
2D feature map

f^{out}
2D feature map (after ReLU)

Equivariance

Convolutions/cross-correlations are translation equivariant

$$(k \star_{\mathbb{R}^2} f)(\mathbf{x}) = (\mathscr{L}^{\mathbb{R}^2 \to \mathbb{L}_2(\mathbb{R}^2)}_{(\mathbf{x})} k \, , f)_{\mathbb{L}_2(\mathbb{R}^2)}$$

$$\begin{tikzcd}
\text{ } \arrow[r, "\Phi"] \arrow[d, "\mathscr{L}^{\mathbb{R}^2 \to \mathbb{L}_2(\mathbb{R}^2)}_{(\mathbf{x})}"'] & \text{  } \arrow[d, "\mathscr{L}^{\mathbb{R}^2 \to \mathbb{L}_2(\mathbb{R}^2)}_{(\mathbf{x})}"] \\
\text{ } \arrow[r, "\Phi"'] & \text{  }
\end{tikzcd}$$

Representation of the translation group

Equivariance

Convolutions are generally **not equivariant to roto-translations**

$$(k \star_{\mathbb{R}^2} f)(\mathbf{x}) = (\mathscr{L}^{\mathbb{R}^2 \to \mathbb{L}_2(\mathbb{R}^2)}_{(\mathbf{x})} k \, , f)_{\mathbb{L}_2(\mathbb{R}^2)}$$

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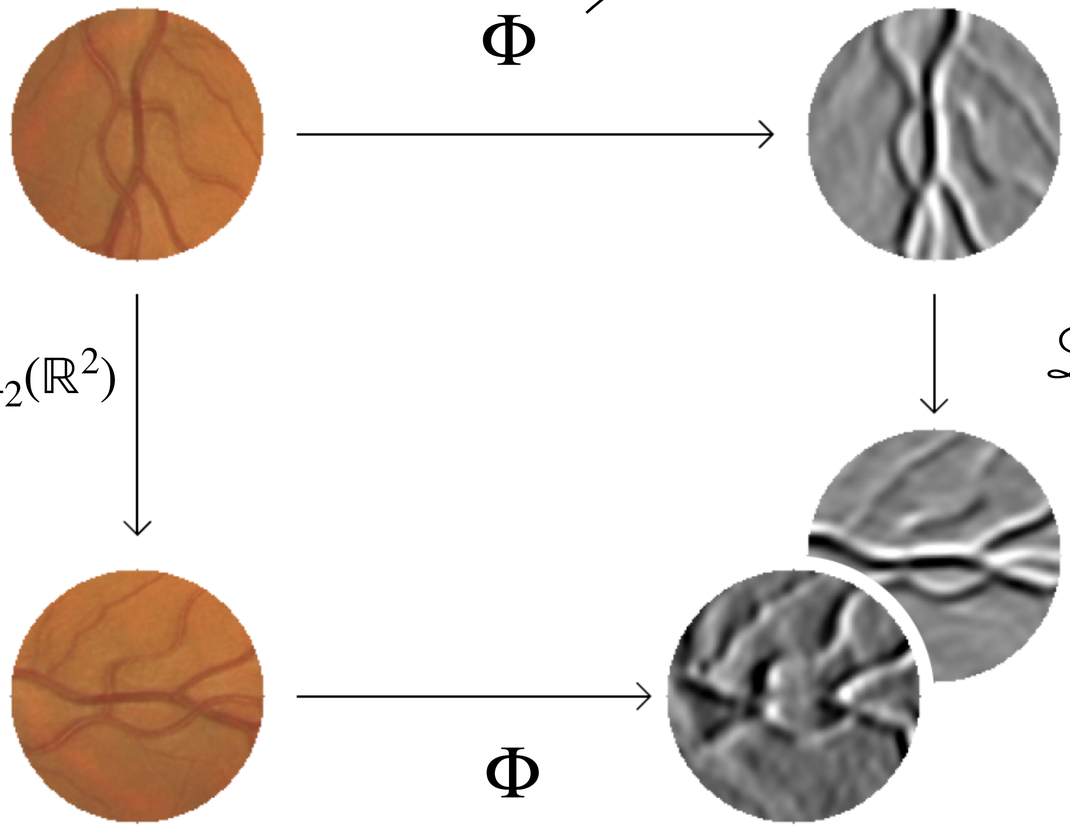

Representation of the rotation group

SE(2) equivariant cross-correlations

Representation of the roto-translation group!

Lifting correlations: $(k \tilde{\star} f)(\mathbf{x}, \theta) = (\mathscr{L}_g^{SE(2) \to \mathbb{L}_2(\mathbb{R}^2)} k \, , f)_{\mathbb{L}_2(\mathbb{R}^2)}$

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translation *rotation*

SE(2) equivariant cross-correlations

Representation of the roto-translation group!

$k(\mathbf{R}_\theta^{-1}(\mathbf{x}'-\mathbf{x}))$

Lifting correlations: $(k \tilde{\star} f)(\mathbf{x}, \theta) = (\mathscr{L}_g^{SE(2)\to\mathbb{L}_2(\mathbb{R}^2)}\, k\,, f)_{\mathbb{L}_2(\mathbb{R}^2)} = (\overbrace{\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2\to\mathbb{L}_2(\mathbb{R}^2)}\, \mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(\mathbb{R}^2)}\, k}\,, f)_{\mathbb{L}_2(\mathbb{R}^2)}$

translation *rotation*

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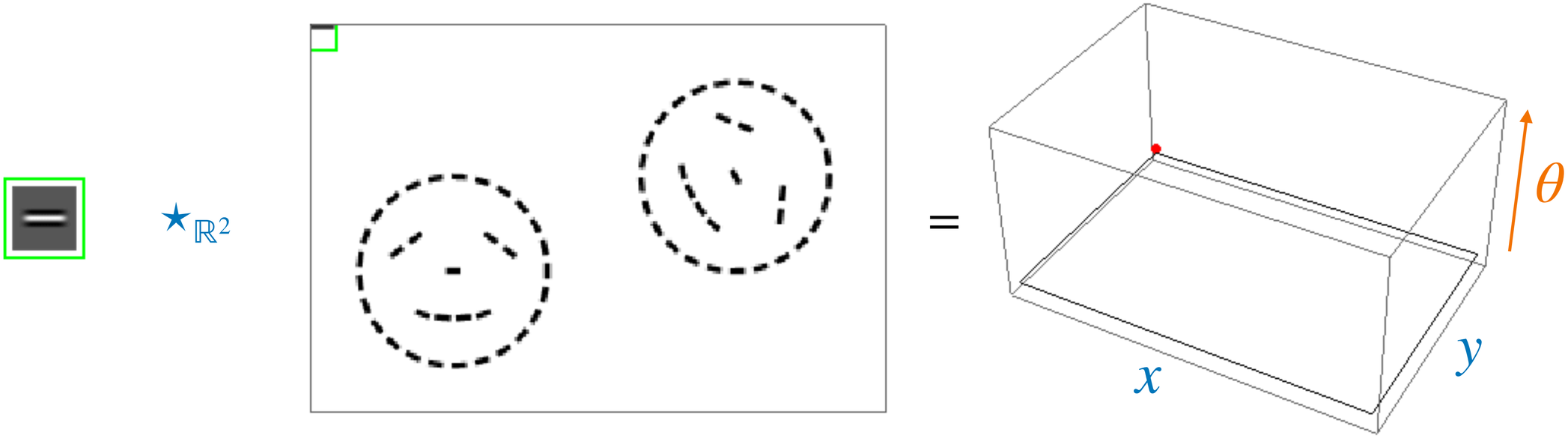
translation *rotation*



$\mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(\mathbb{R}^2)} k$
Rotated 2D convolution kernel

f^{in}
2D feature map

f^{out}
3D (*SE(2)*) feature map (after ReLU)

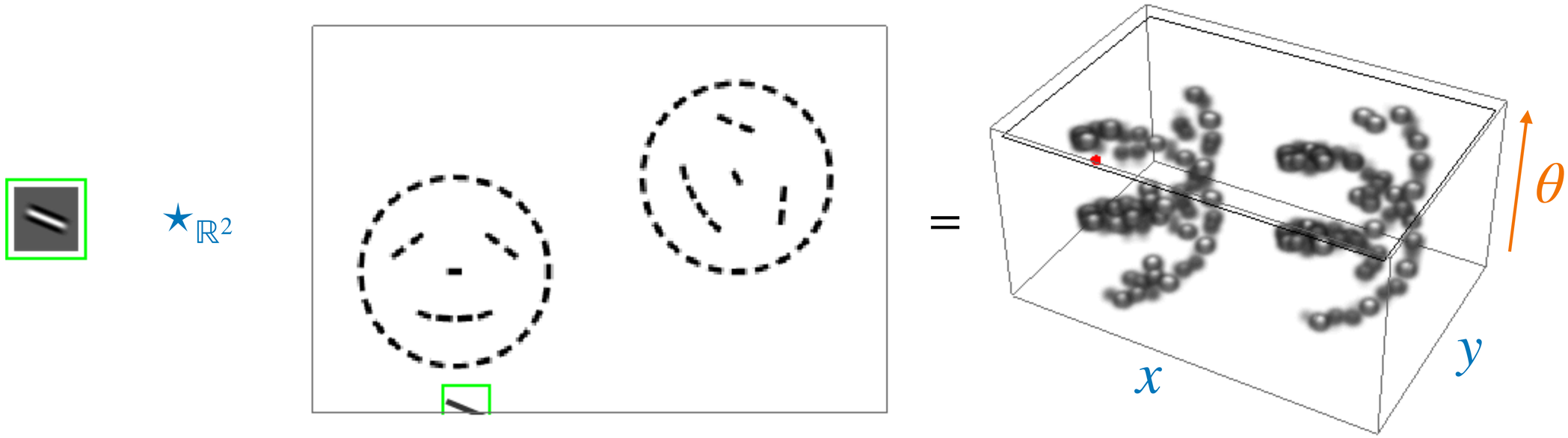
SE(2) equivariant cross-correlations

Representation of the roto-translation group!

$k(\mathbf{R}_\theta^{-1}(\mathbf{x}'-\mathbf{x}))$

Lifting correlations: $(k \tilde{\star} f)(\mathbf{x}, \theta) = (\mathscr{L}_g^{SE(2)\to\mathbb{L}_2(\mathbb{R}^2)} k\,, f)_{\mathbb{L}_2(\mathbb{R}^2)} = (\overbrace{\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2\to\mathbb{L}_2(\mathbb{R}^2)} \mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(\mathbb{R}^2)} k}\,, f)_{\mathbb{L}_2(\mathbb{R}^2)}$

translation *rotation*



$\mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(\mathbb{R}^2)} k$
Rotated 2D convolution kernel

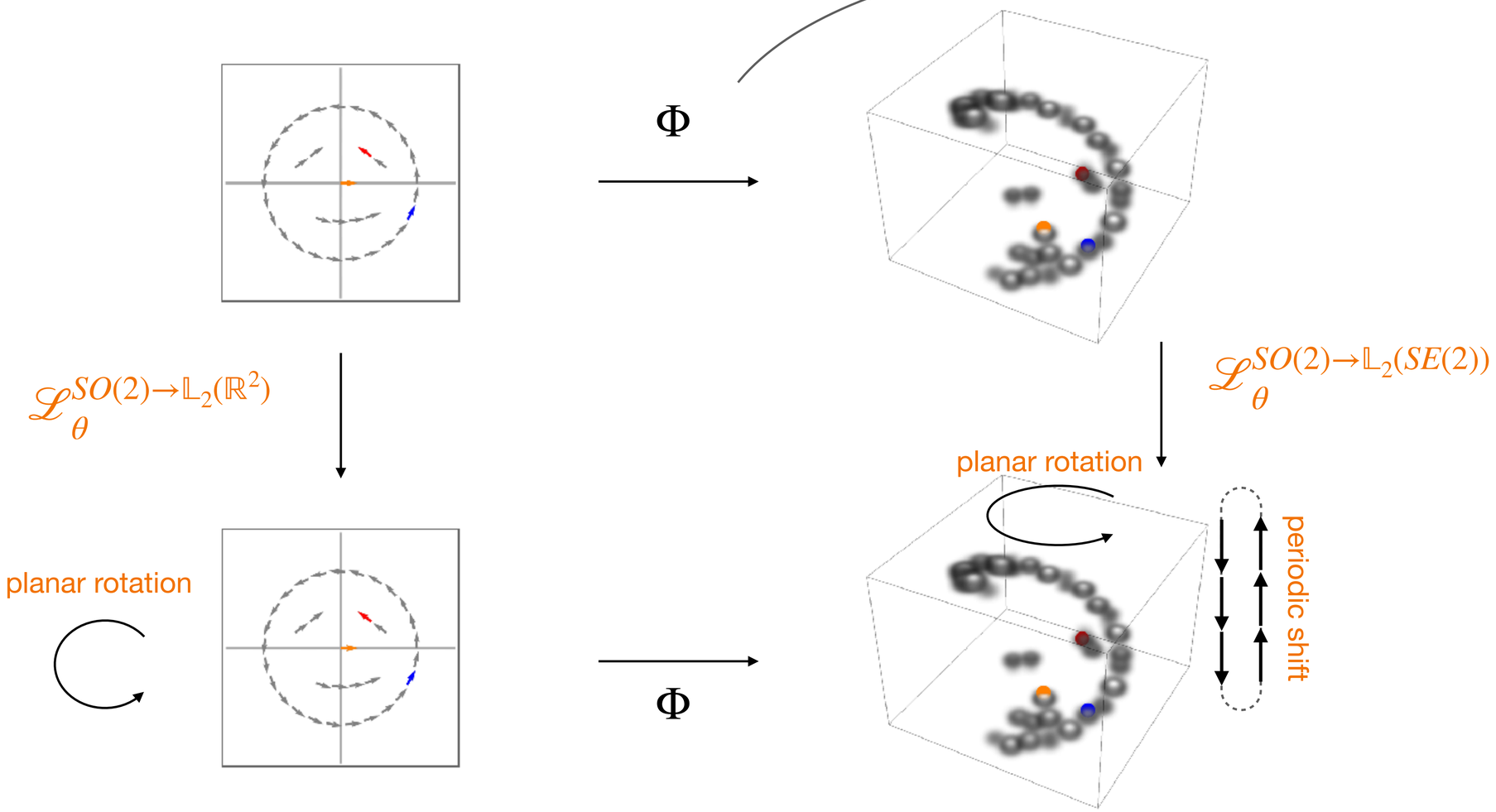
f^{in}
2D feature map

f^{out}
3D (*SE(2)*) feature map (after ReLU)

Equivariance

SE(2) group **lifting convolutions** are roto-translation equivariant

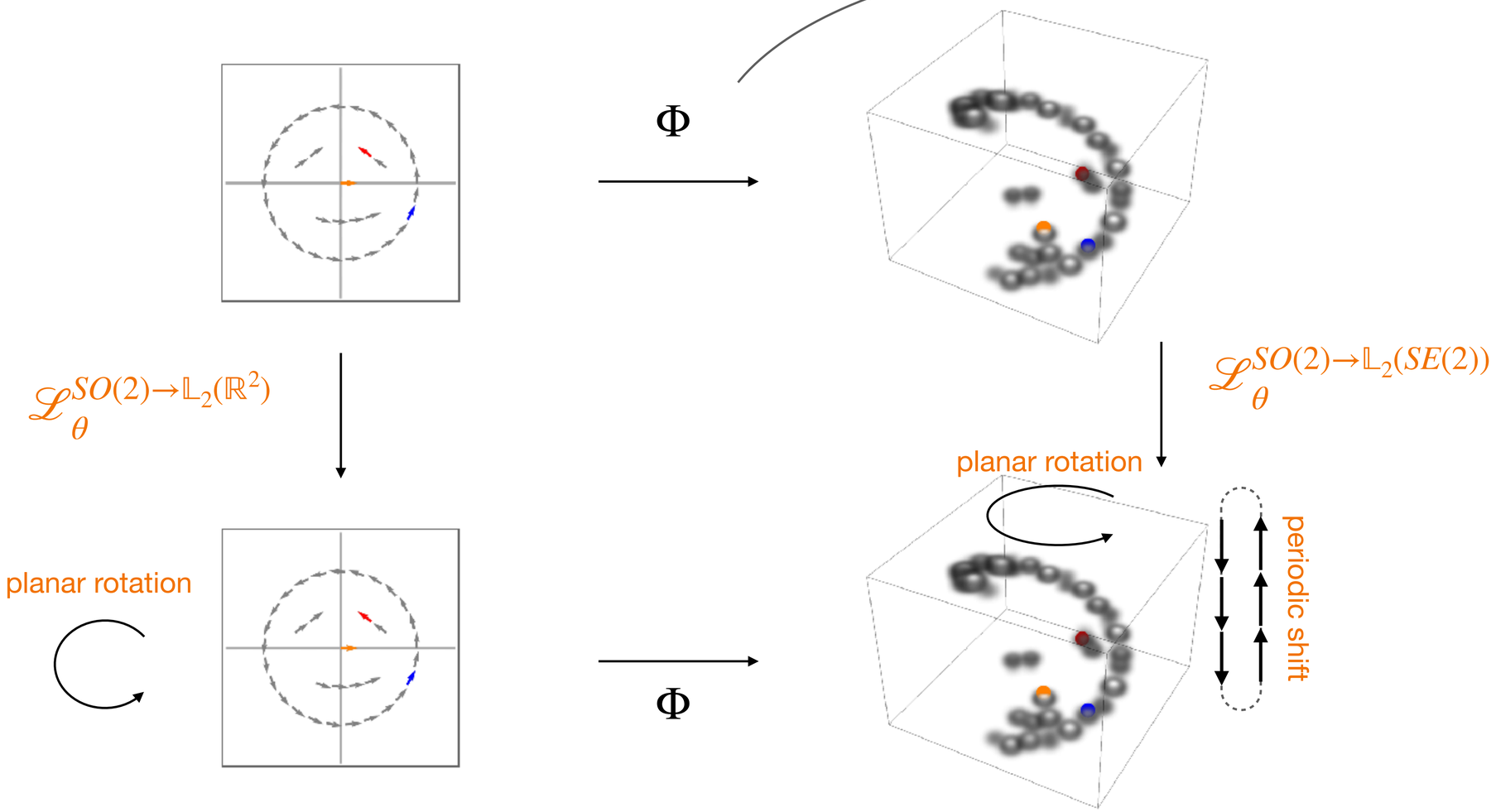
$$(k \tilde{\star} f)(\mathbf{x}, \theta) = (\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2 \to \mathbb{L}_2(\mathbb{R}^2)} \mathscr{L}_{\theta}^{SO(2) \to \mathbb{L}_2(\mathbb{R}^2)} k \, , f)_{\mathbb{L}_2(\mathbb{R}^2)}$$



Equivariance

SE(2) group **lifting convolutions** are roto-translation equivariant

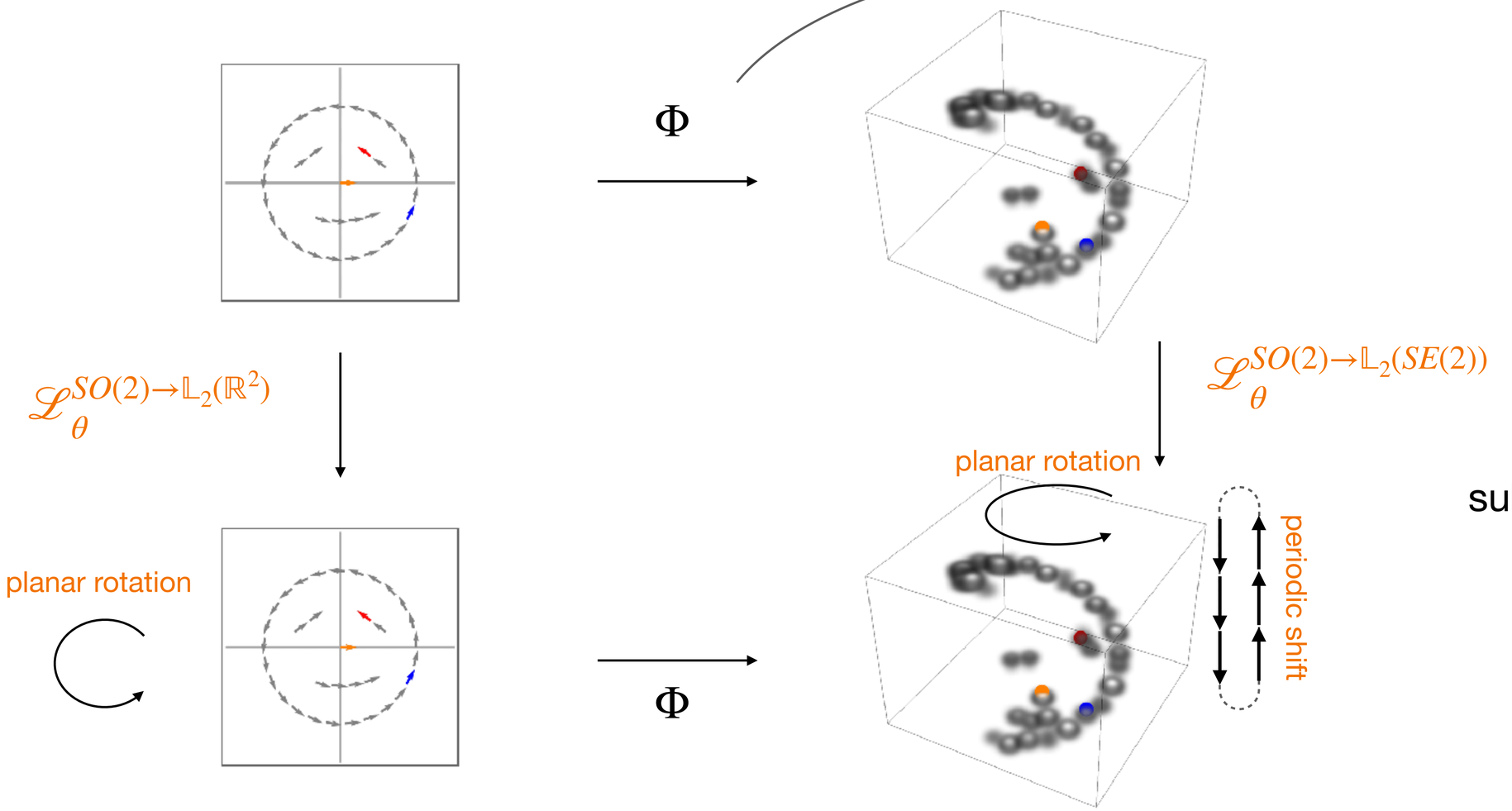
$$(k \tilde{\star} f)(\mathbf{x}, \theta) = (\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2 \to \mathbb{L}_2(\mathbb{R}^2)} \mathscr{L}_{\theta}^{SO(2) \to \mathbb{L}_2(\mathbb{R}^2)} k \, , f)_{\mathbb{L}_2(\mathbb{R}^2)}$$



Equivariance

SE(2) group **lifting convolutions** are roto-translation equivariant

$$(k \tilde{\star} f)(\mathbf{x}, \theta) = (\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2 \to \mathbb{L}_2(\mathbb{R}^2)} \mathscr{L}_{\theta}^{SO(2) \to \mathbb{L}_2(\mathbb{R}^2)} k \, , f)_{\mathbb{L}_2(\mathbb{R}^2)}$$



What about subsequent layers?

SE(2) equivariant cross-correlations

Group correlations:

$$(k \star f)(\mathbf{x}, \theta) = (\mathscr{L}_g^{SE(2)\to\mathbb{L}_2(SE(2))}\, k\,,\, f)_{\mathbb{L}_2(SE(2))} = (\overbrace{\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2\to\mathbb{L}_2(SE(2))}\, \mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(SE(2))}\, k}^{k(\mathbf{R}_\theta^{-1}(\mathbf{x}'-\mathbf{x}),\mathbf{R}_{\theta'-\theta})}\,,\, f)_{\mathbb{L}_2(SE(2)}$$

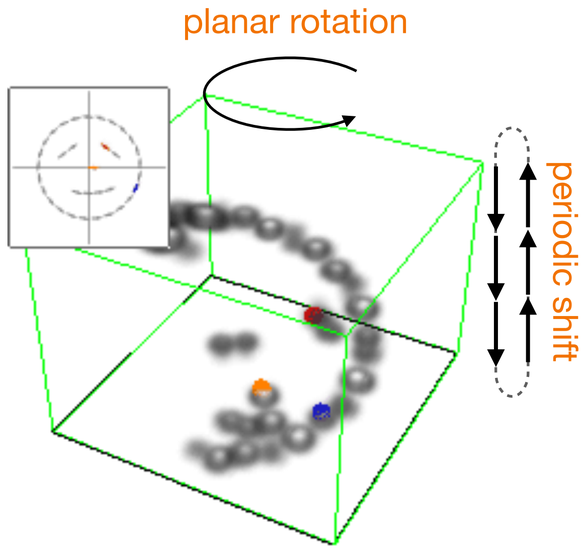
translation *rotation*

SE(2) equivariant cross-correlations

Group correlations:

$$(k \star f)(\mathbf{x}, \theta) = (\mathscr{L}_g^{SE(2)\to\mathbb{L}_2(SE(2))}\, k\,,\, f)_{\mathbb{L}_2(SE(2))} = (\overbrace{\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2\to\mathbb{L}_2(SE(2))}\, \mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(SE(2))}\, k}^{k(\mathbf{R}_\theta^{-1}(\mathbf{x}'-\mathbf{x}),\mathbf{R}_{\theta'-\theta})}\,,\, f)_{\mathbb{L}_2(SE(2)}$$

translation *rotation*



$\mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(SE(2)}k$

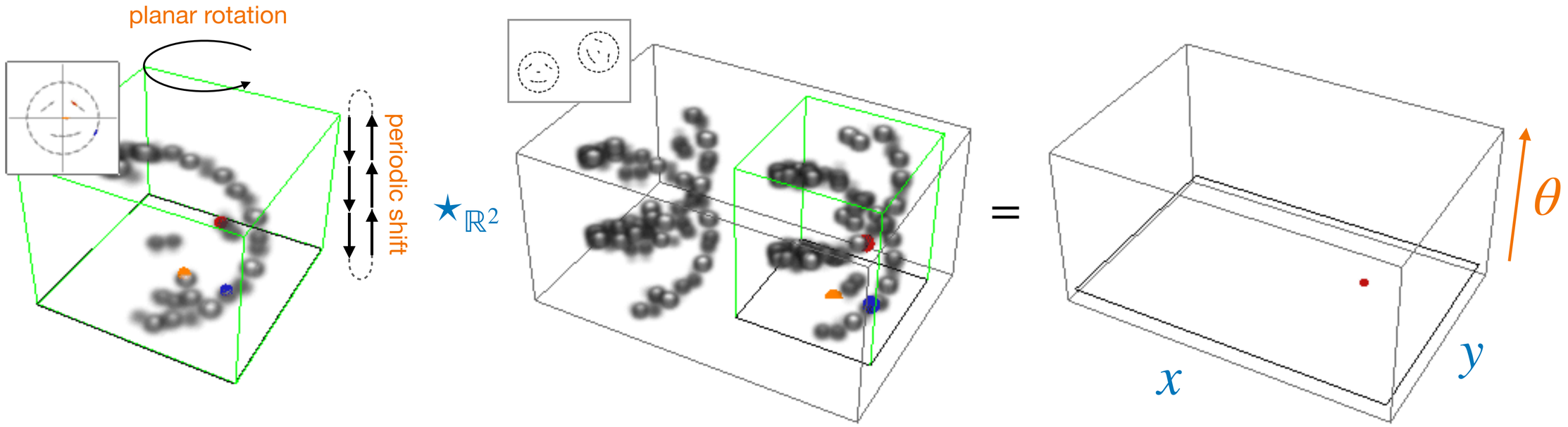
Rotated SE(2) convolution kernel

SE(2) equivariant cross-correlations

Group correlations:

$$(k \star f)(\mathbf{x}, \theta) = (\mathscr{L}_g^{SE(2)\to\mathbb{L}_2(SE(2))}\, k\,,\, f)_{\mathbb{L}_2(SE(2))} = (\overbrace{\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2\to\mathbb{L}_2(SE(2))}\, \mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(SE(2))}\, k}^{k(\mathbf{R}_\theta^{-1}(\mathbf{x}'-\mathbf{x}),\mathbf{R}_{\theta'-\theta})}\,,\, f)_{\mathbb{L}_2(SE(2)}$$

translation *rotation*



$\mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(SE(2)}k$
Rotated SE(2) convolution kernel

f^{in}
SE(2) feature map

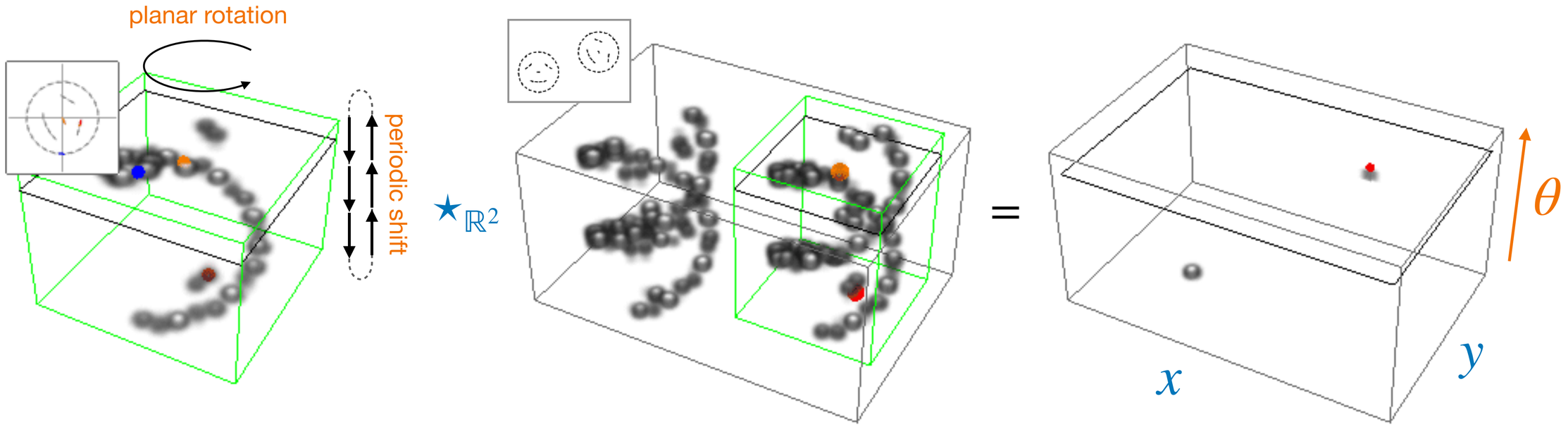
f^{out}
SE(2) feature map (after ReLU)

SE(2) equivariant cross-correlations

Group correlations:

$$(k \star f)(\mathbf{x}, \theta) = (\mathscr{L}_g^{SE(2)\to\mathbb{L}_2(SE(2))}\, k\,,\, f)_{\mathbb{L}_2(SE(2))} = (\overbrace{\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2\to\mathbb{L}_2(SE(2))}\, \mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(SE(2))}\, k}^{k(\mathbf{R}_\theta^{-1}(\mathbf{x}'-\mathbf{x}),\mathbf{R}_{\theta'-\theta})}\,,\, f)_{\mathbb{L}_2(SE(2)}$$

translation *rotation*



$\mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(SE(2)}k$
Rotated SE(2) convolution kernel

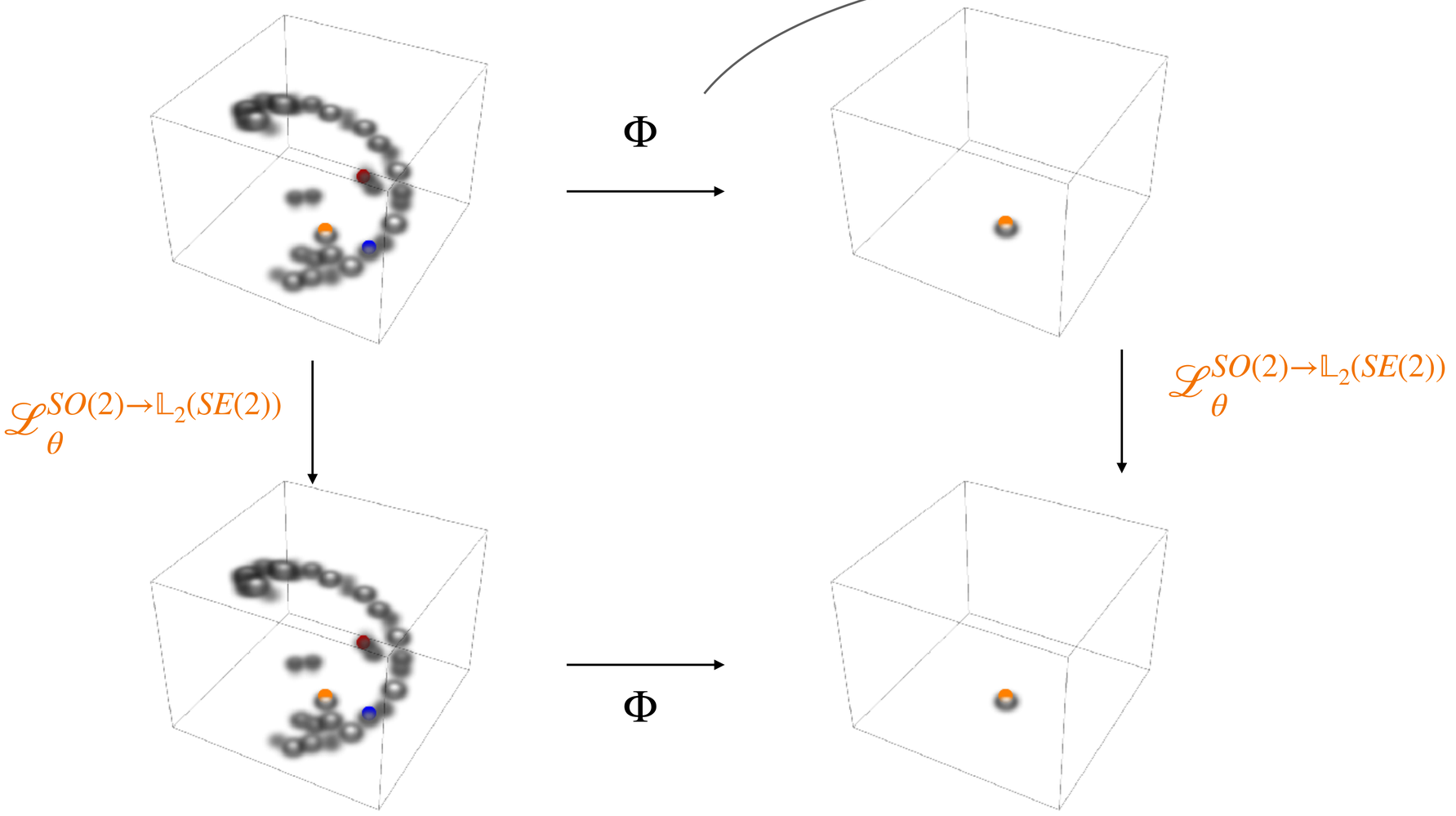
f^{in}
SE(2) feature map

f^{out}
SE(2) feature map (after ReLU)

Equivariance

SE(2) group convolutions are roto-translation equivariant

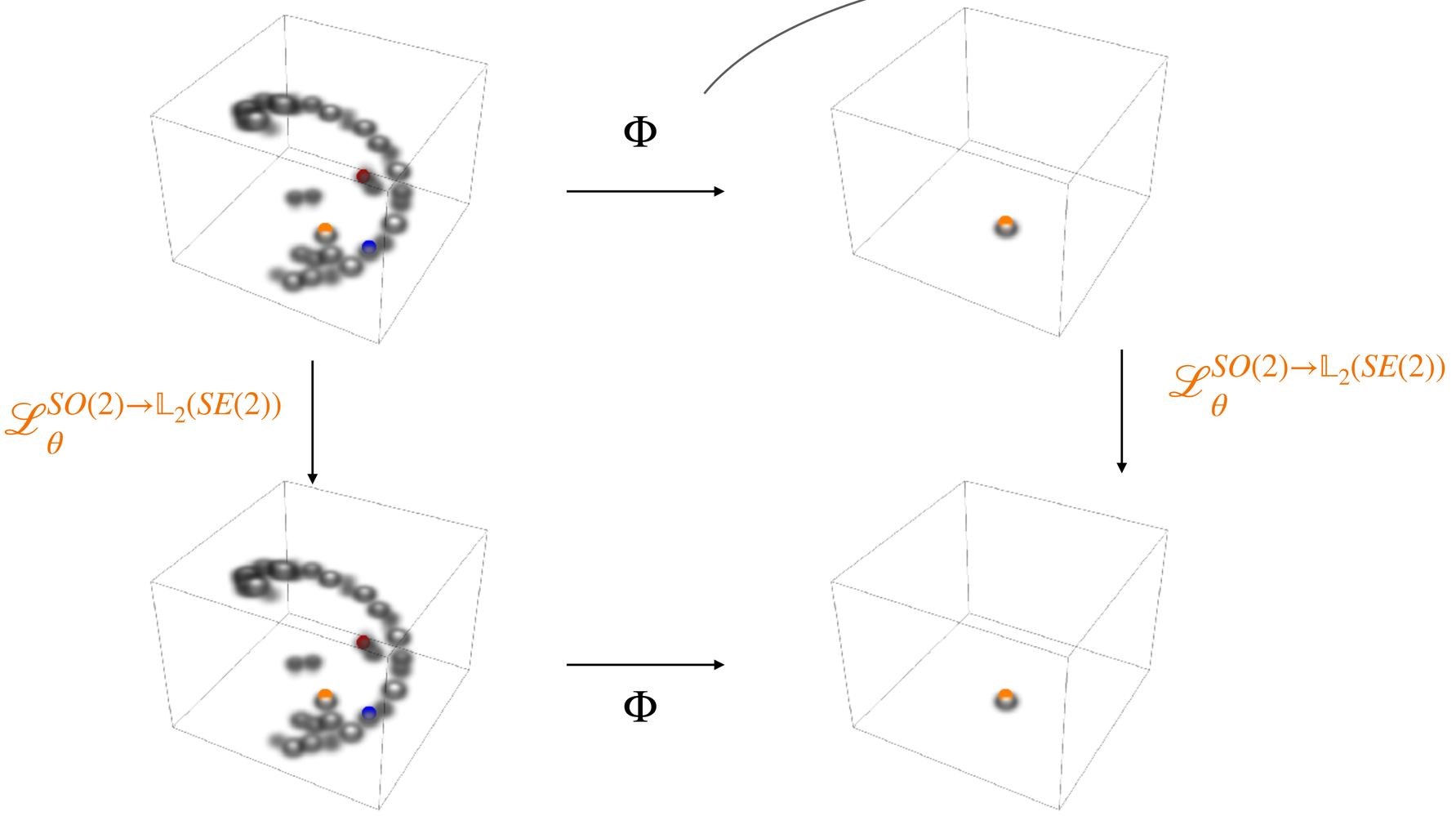
$$(k \star f)(\mathbf{x}, \theta) = (\mathscr{L}_{\mathbf{x}}^{\mathbb{R}^2 \to \mathbb{L}_2(SE(2))} \mathscr{L}_{\theta}^{SO(2) \to \mathbb{L}_2(SE(2))} k \, , f)_{\mathbb{L}_2(SE(2))}$$



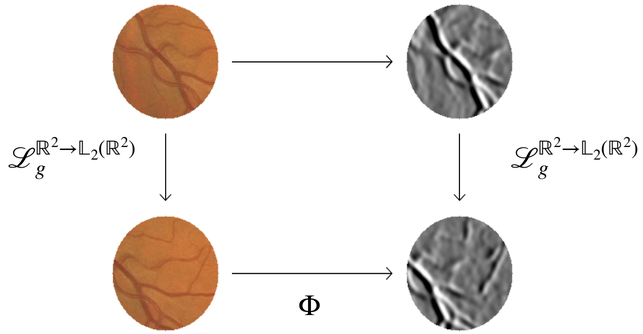
Equivariance

SE(2) group convolutions are roto-translation equivariant

$$(k \star f)(\mathbf{x}, \theta) = (\mathscr{L}_{\mathbf{x}}^{\mathbb{R}^2 \to \mathbb{L}_2(SE(2))} \mathscr{L}_{\theta}^{SO(2) \to \mathbb{L}_2(SE(2))} k \, , f)_{\mathbb{L}_2(SE(2))}$$



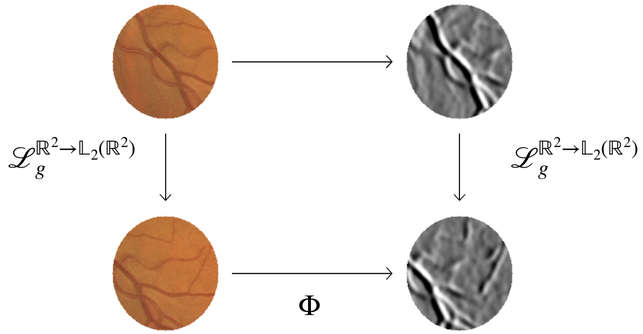
2D cross-correlation (translation equivariant)



$$(k \star_{\mathbb{R}^2} f)(\mathbf{x}) = (\mathscr{L}_{\mathbf{x}}^{\mathbb{R}^2 \to \mathbb{L}_2(\mathbb{R}^2)} k, f)_{\mathbb{L}_2(\mathbb{R}^2)}$$

$$= \int_{\mathbb{R}^2} k(\mathbf{x}' - \mathbf{x}) f(\mathbf{x}') \mathrm{d}\mathbf{x}'$$

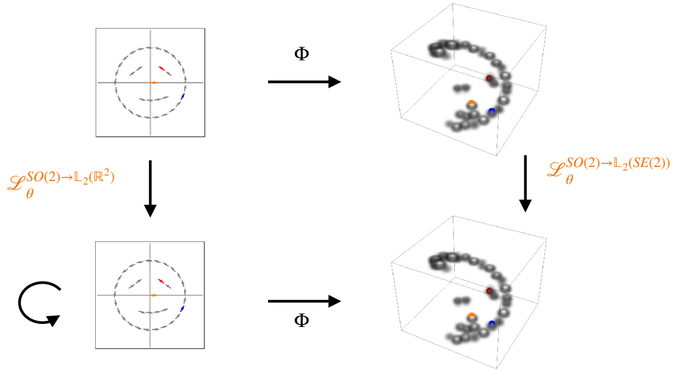
2D cross-correlation (translation equivariant)



$$(k \star_{\mathbb{R}^2} f)(\mathbf{x}) = (\mathscr{L}_{\mathbf{x}}^{\mathbb{R}^2 \to \mathbb{L}_2(\mathbb{R}^2)} k, f)_{\mathbb{L}_2(\mathbb{R}^2)}$$

$$= \int_{\mathbb{R}^2} k(\mathbf{x}' - \mathbf{x}) f(\mathbf{x}') \mathrm{d}\mathbf{x}'$$

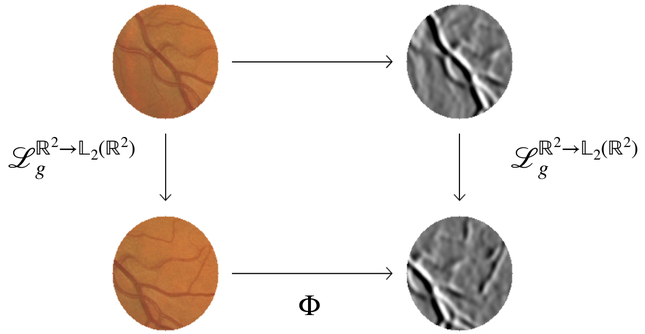
SE(2) lifting correlations (roto-translation equivariant)



$$(k \tilde{\star} f)(\mathbf{x}, \theta) = (\mathscr{L}_g^{SE(2) \to \mathbb{L}_2(\mathbb{R}^2)} k \, , f)_{\mathbb{L}_2(\mathbb{R}^2)}$$

$$= \int_{\mathbb{R}^2} k(\mathbf{R}_\theta^{-1}(\mathbf{x}' - \mathbf{x})) f(\mathbf{x}') \mathrm{d}\mathbf{x}'$$

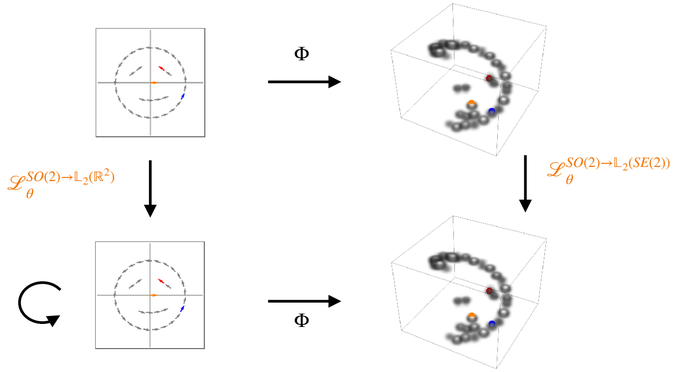
2D cross-correlation (translation equivariant)



$$(k \star_{\mathbb{R}^2} f)(\mathbf{x}) = (\mathscr{L}_{\mathbf{x}}^{\mathbb{R}^2 \to \mathbb{L}_2(\mathbb{R}^2)} k, f)_{\mathbb{L}_2(\mathbb{R}^2)}$$

$$= \int_{\mathbb{R}^2} k(\mathbf{x}' - \mathbf{x}) f(\mathbf{x}') \mathrm{d}\mathbf{x}'$$

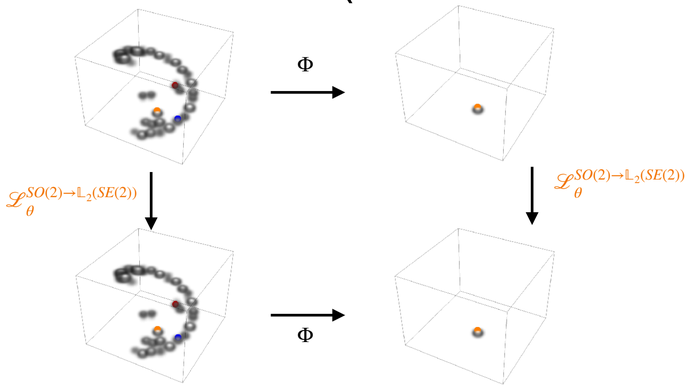
SE(2) lifting correlations (roto-translation equivariant)



$$(k \tilde{\star} f)(\mathbf{x}, \theta) = (\mathscr{L}_g^{SE(2) \to \mathbb{L}_2(\mathbb{R}^2)} k \, , f)_{\mathbb{L}_2(\mathbb{R}^2)}$$

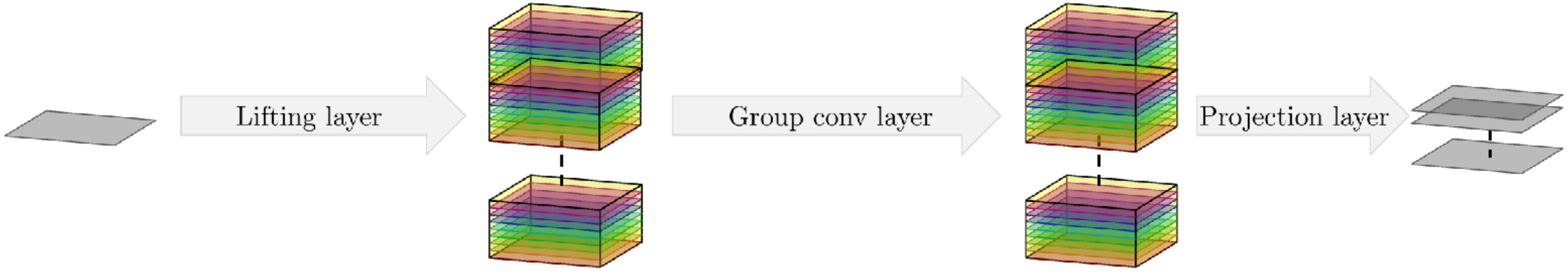
$$= \int_{\mathbb{R}^2} k(\mathbf{R}_\theta^{-1}(\mathbf{x}' - \mathbf{x})) f(\mathbf{x}') \mathrm{d}\mathbf{x}'$$

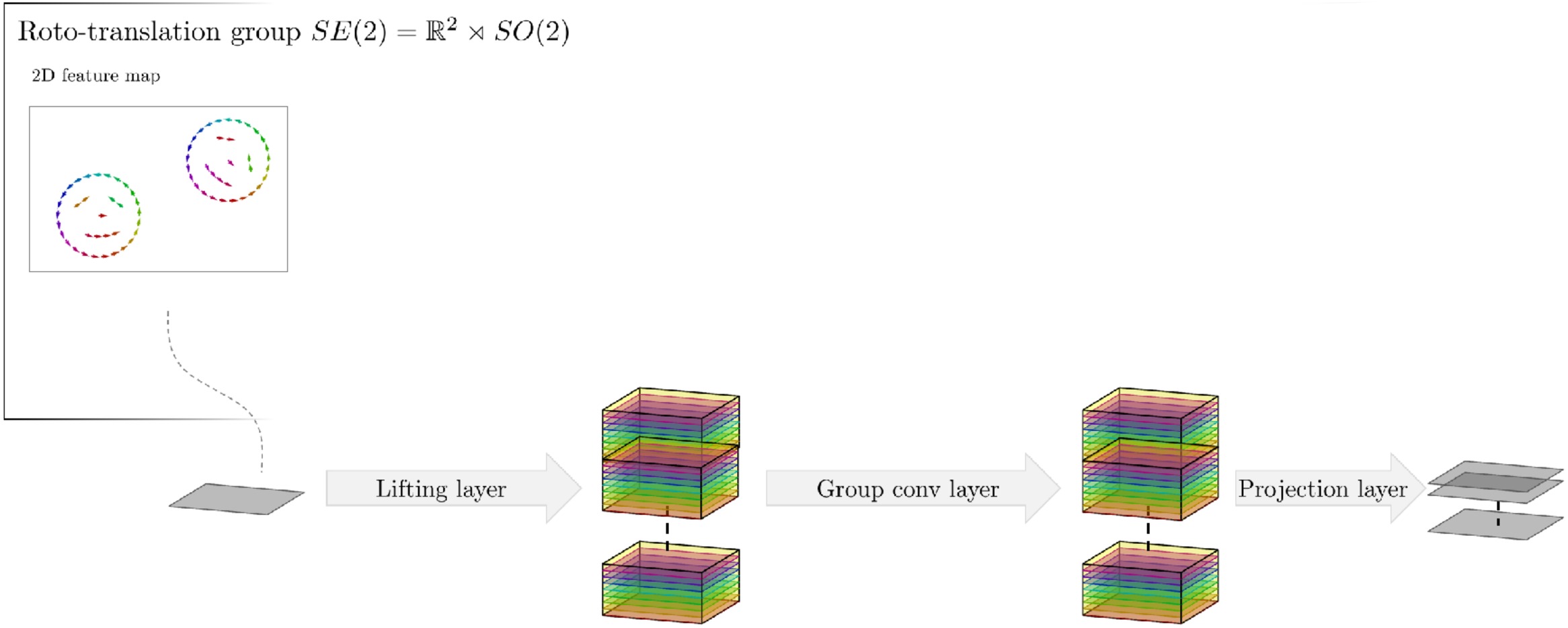
SE(2) G-correlations (roto-translation equivariant)

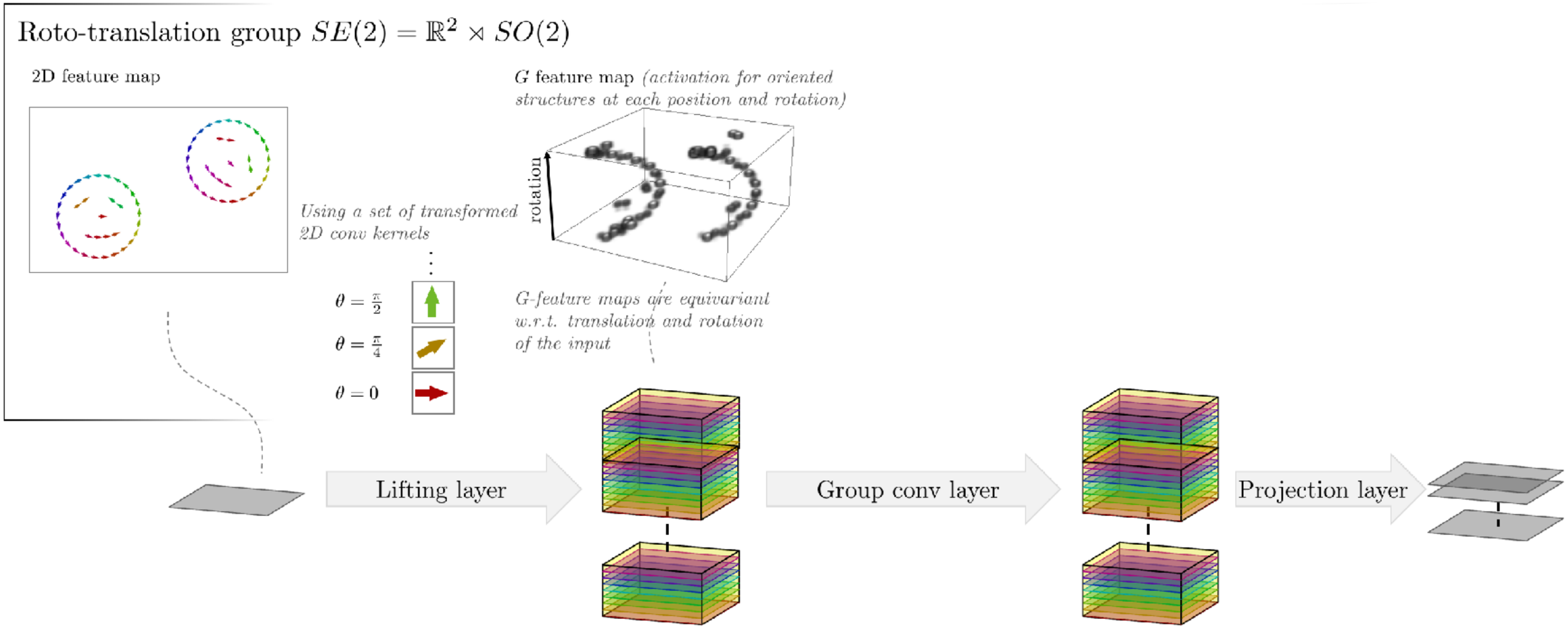


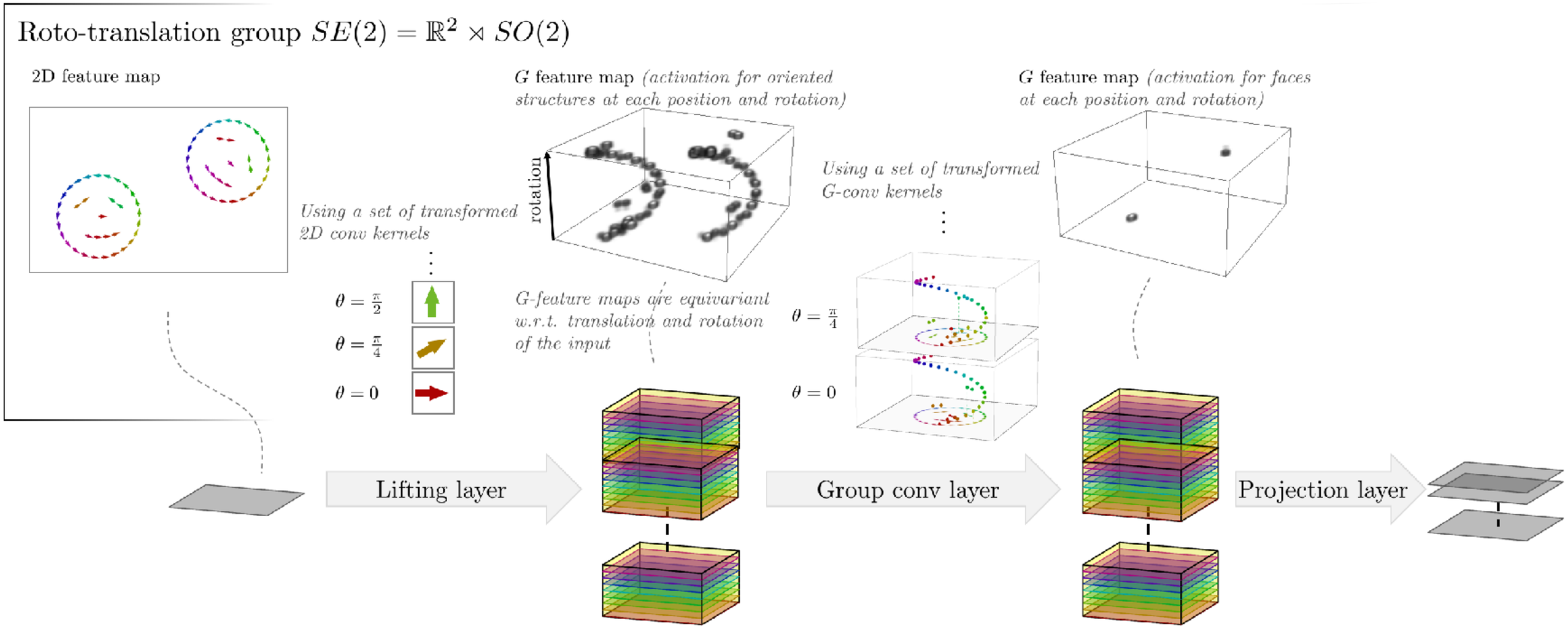
$$(k \tilde{\star} f)(\mathbf{x}, \theta) = (\mathscr{L}_g^{SE(2) \to \mathbb{L}_2(SE(2))} k \, , f)_{\mathbb{L}_2(SE(2)}$$

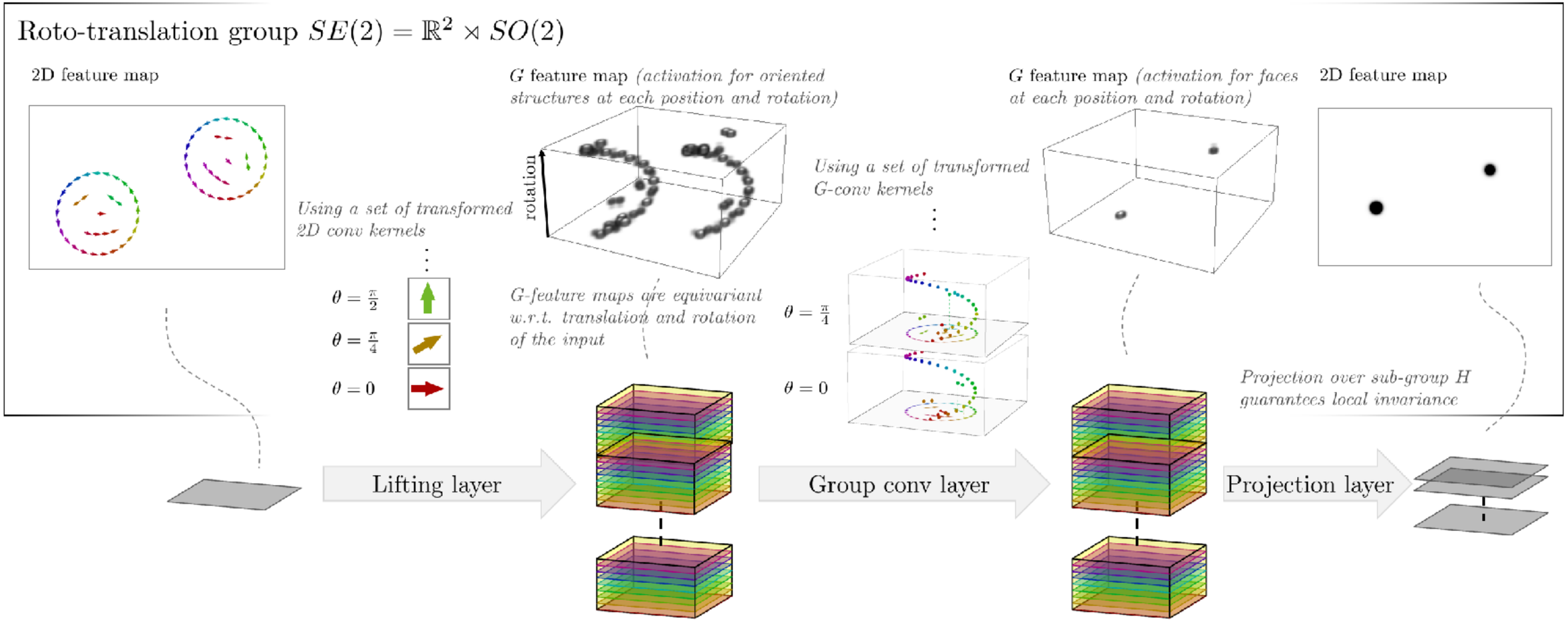
$$= \int_{\mathbb{R}^2} \int_{S^1} k(\mathbf{R}_\theta^{-1}(\mathbf{x}' - \mathbf{x}), \theta' - \theta \mod 2\pi) f(\mathbf{x}', \theta') \mathrm{d}\mathbf{x}' \mathrm{d}\theta'$$

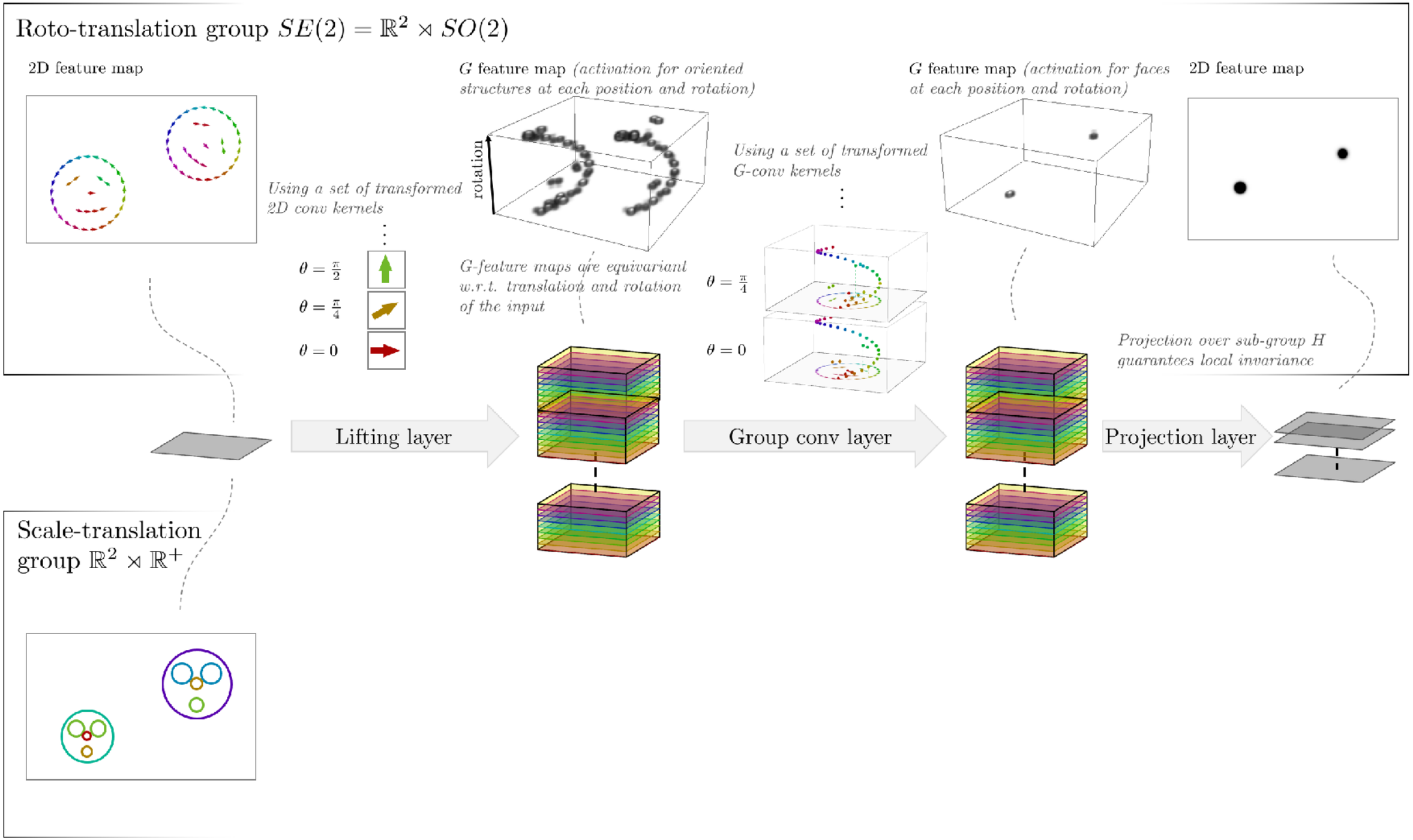

Lifting layer
Group conv layer
Projection layer

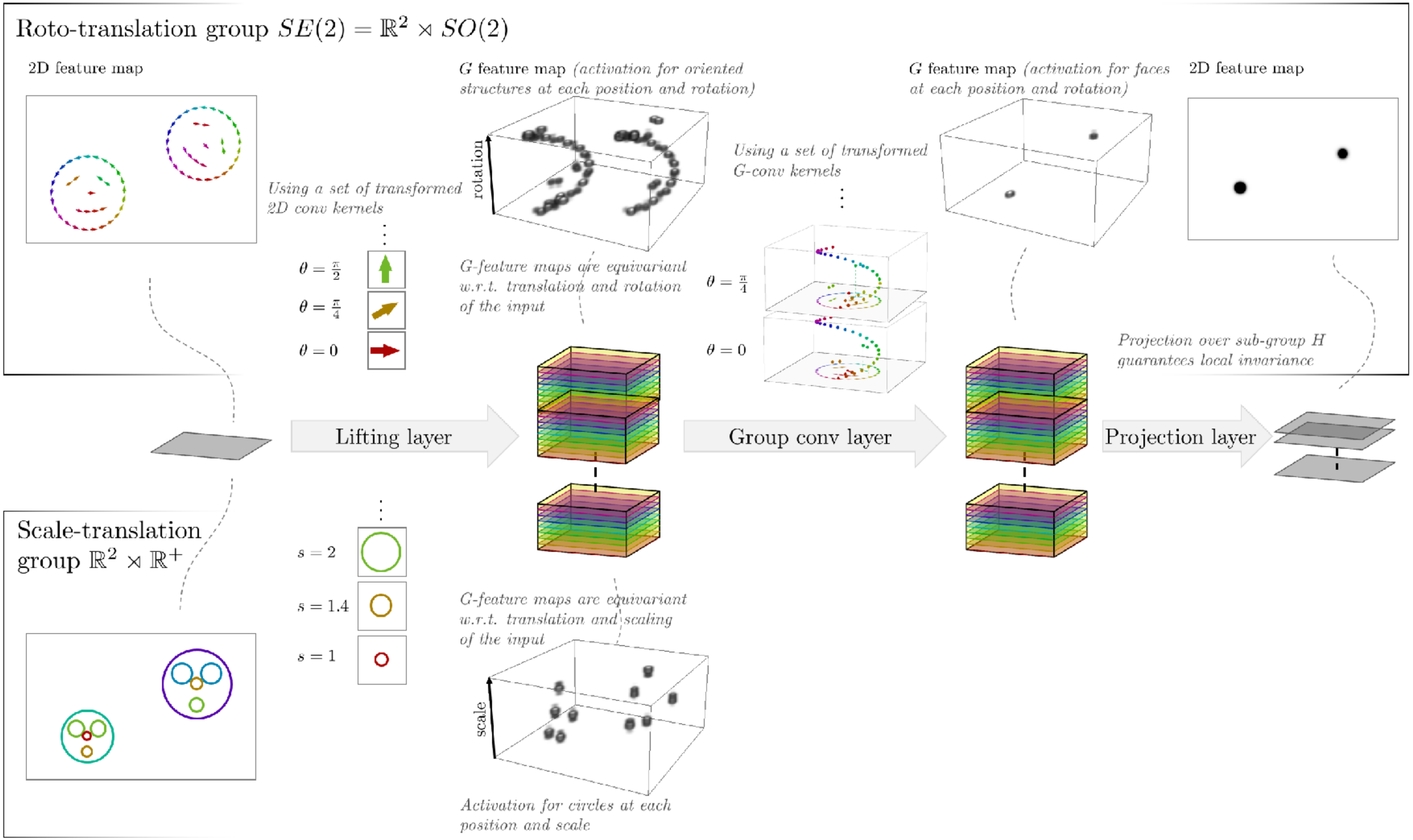

Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
Lifting layer
Group conv layer
Projection layer

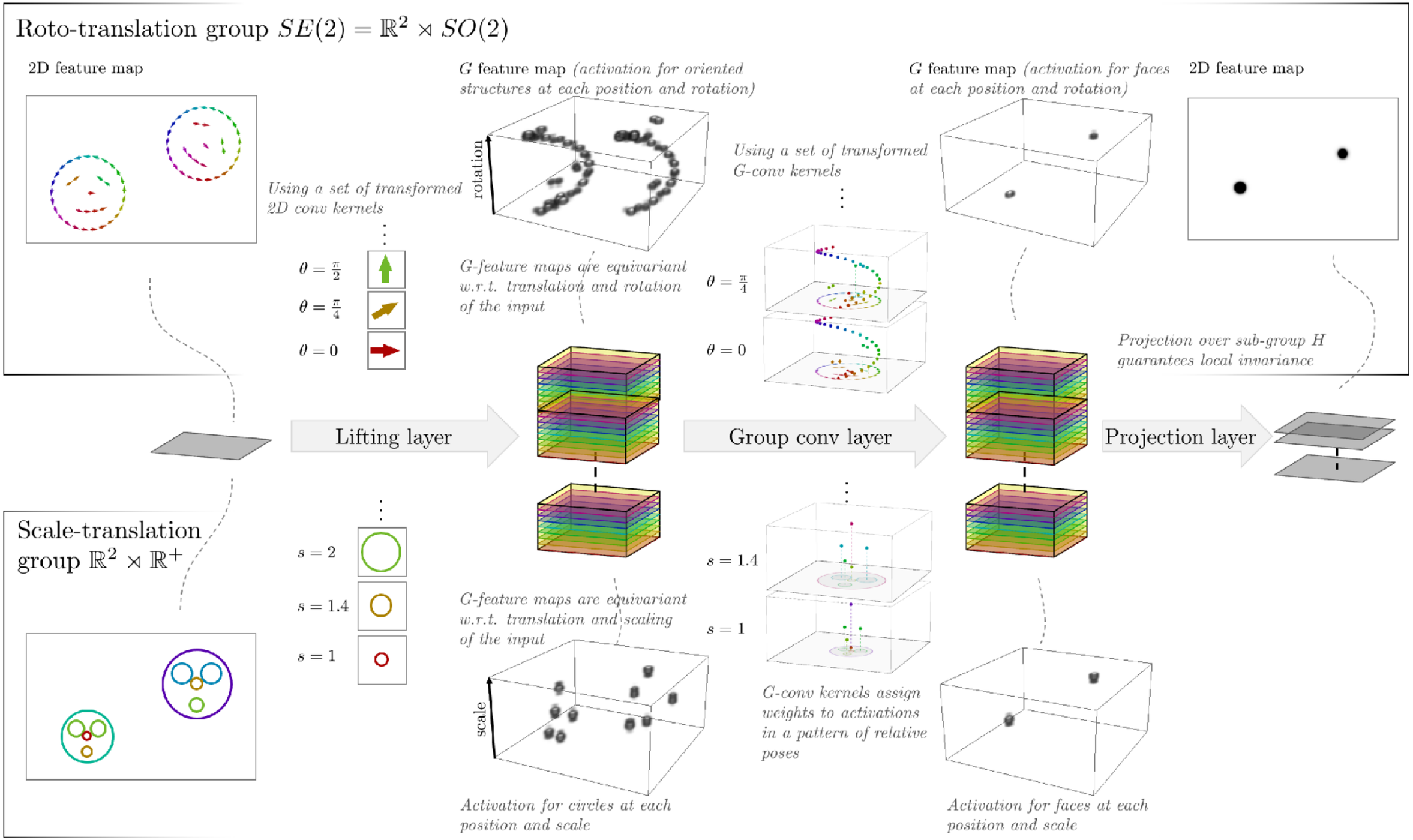

Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
G feature map (activation for oriented structures at each position and rotation)
rotation
Using a set of transformed 2D conv kernels
$\theta = \frac{\pi}{2}$
$\theta = \frac{\pi}{4}$
$\theta = 0$
G-feature maps are equivariant w.r.t. translation and rotation of the input
Lifting layer
Group conv layer
Projection layer

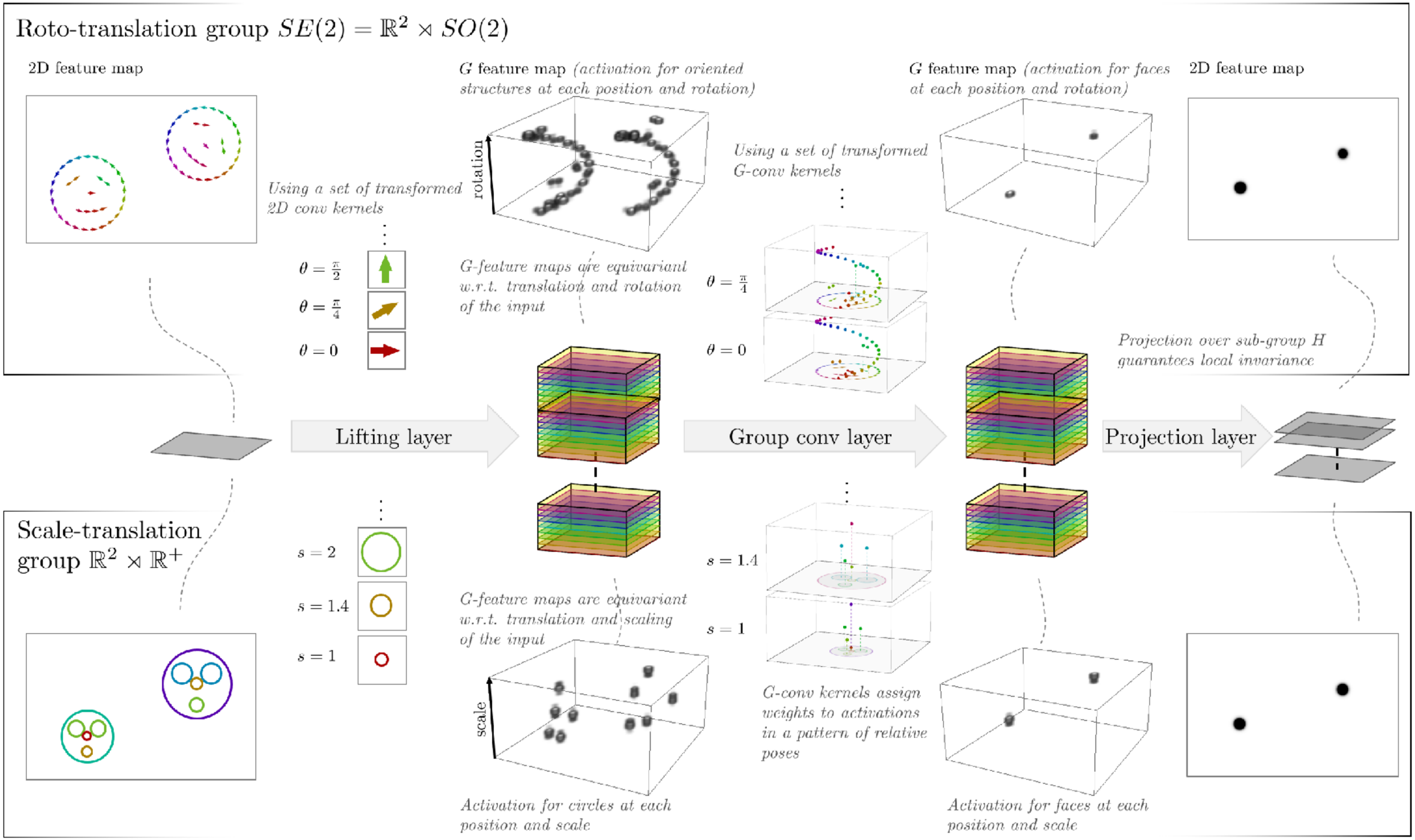

Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
Using a set of transformed 2D conv kernels
$\theta = \frac{\pi}{2}$
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for oriented structures at each position and rotation)
rotation
G-feature maps are equivariant w.r.t. translation and rotation of the input
Using a set of transformed G-conv kernels
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for faces at each position and rotation)
Lifting layer
Group conv layer
Projection layer


Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
Using a set of transformed 2D conv kernels
$\theta = \frac{\pi}{2}$
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for oriented structures at each position and rotation)
rotation
G-feature maps are equivariant w.r.t. translation and rotation of the input
Using a set of transformed G-conv kernels
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for faces at each position and rotation)
2D feature map
Projection over sub-group H guarantees local invariance
Lifting layer
Group conv layer
Projection layer


Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
Using a set of transformed 2D conv kernels
$\theta = \frac{\pi}{2}$
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for oriented structures at each position and rotation)
rotation
G-feature maps are equivariant w.r.t. translation and rotation of the input
Using a set of transformed G-conv kernels
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for faces at each position and rotation)
2D feature map
Projection over sub-group H guarantees local invariance
Lifting layer
Group conv layer
Projection layer
Scale-translation group $\mathbb{R}^2 \rtimes \mathbb{R}^+$

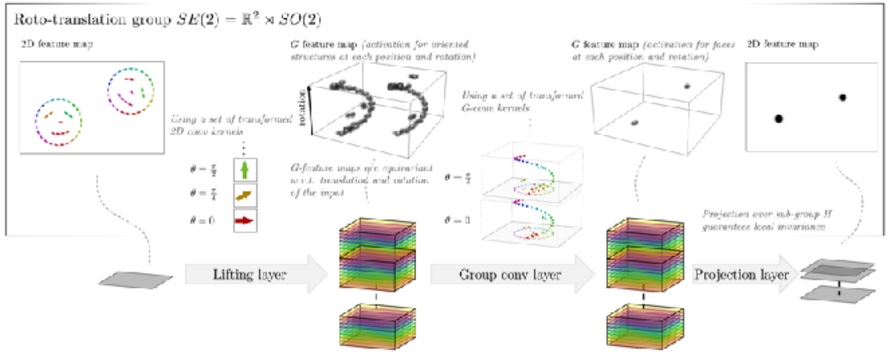

Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
Using a set of transformed 2D conv kernels
$\theta = \frac{\pi}{2}$
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for oriented structures at each position and rotation)
rotation
G-feature maps are equivariant w.r.t. translation and rotation of the input
Using a set of transformed G-conv kernels
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for faces at each position and rotation)
2D feature map
Projection over sub-group H guarantees local invariance
Lifting layer
Group conv layer
Projection layer
Scale-translation group $\mathbb{R}^2 \rtimes \mathbb{R}^+$
$s = 2$
$s = 1.4$
$s = 1$
G-feature maps are equivariant w.r.t. translation and scaling of the input
scale
Activation for circles at each position and scale


Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
Using a set of transformed 2D conv kernels
$\theta = \frac{\pi}{2}$
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for oriented structures at each position and rotation)
rotation
G-feature maps are equivariant w.r.t. translation and rotation of the input
Using a set of transformed G-conv kernels
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for faces at each position and rotation)
2D feature map
Projection over sub-group H guarantees local invariance
Lifting layer
Group conv layer
Projection layer
Scale-translation group $\mathbb{R}^2 \rtimes \mathbb{R}^+$
$s = 2$
$s = 1.4$
$s = 1$
G-feature maps are equivariant w.r.t. translation and scaling of the input
scale
Activation for circles at each position and scale
$s = 1.4$
$s = 1$
G-conv kernels assign weights to activations in a pattern of relative poses
Activation for faces at each position and scale

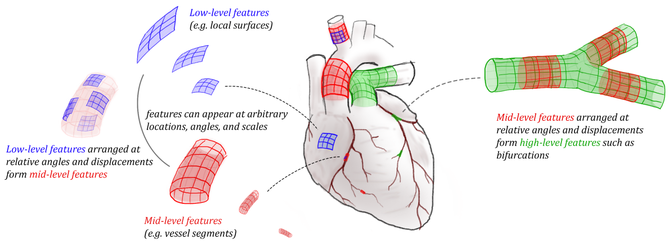

Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
Using a set of transformed 2D conv kernels
$\theta = \frac{\pi}{2}$
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for oriented structures at each position and rotation)
rotation
G-feature maps are equivariant w.r.t. translation and rotation of the input
Using a set of transformed G-conv kernels
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for faces at each position and rotation)
2D feature map
Projection over sub-group H guarantees local invariance
Lifting layer
Group conv layer
Projection layer
Scale-translation group $\mathbb{R}^2 \rtimes \mathbb{R}^+$
$s = 2$
$s = 1.4$
$s = 1$
G-feature maps are equivariant w.r.t. translation and scaling of the input
scale
Activation for circles at each position and scale
$s = 1.4$
$s = 1$
G-conv kernels assign weights to activations in a pattern of relative poses
Activation for faces at each position and scale

Summary

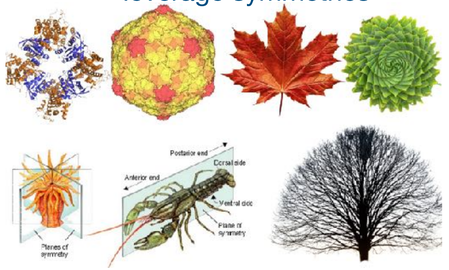
- Group convolutional neural networks intuitively perform template matching
- A template (kernel) is transformed and matched (inner-product) under all possible transformations in the group
- This creates higher-dimensional feature maps (functions on the group) on which we again define template matching via the group action
- In these higher dimensional feature maps we can detect advanced patterns in terms of features at relative poses!
- G-CNNs are based on equivariant layers (thus weight sharing) and guarantee invariance through pooling



recognition by components



leverage symmetries



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AMLAB Amsterdam Machine Learning Lab

Group Equivariant Deep Learning

Lecture 1 - Regular group convolutions

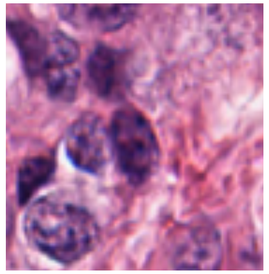
Lecture 1.4 - SE(2) Equivariant NN Example | With histopathology images

Visual example for roto-translation equivariance (SE(2))

Erik Bekkers, Amsterdam Machine Learning Lab, University of Amsterdam

This mini-course serves as a module with the UvA Master AI course Deep Learning 2 https://uvadl2c.github.io/

Architecture for rotation invariant mitotic cell detection



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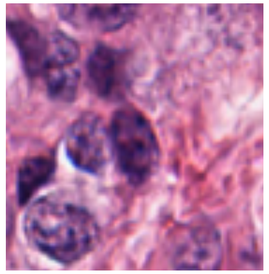

“normal” (0)
vs
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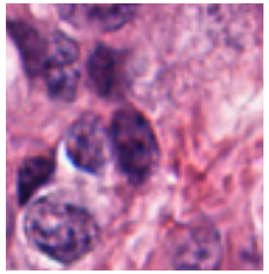

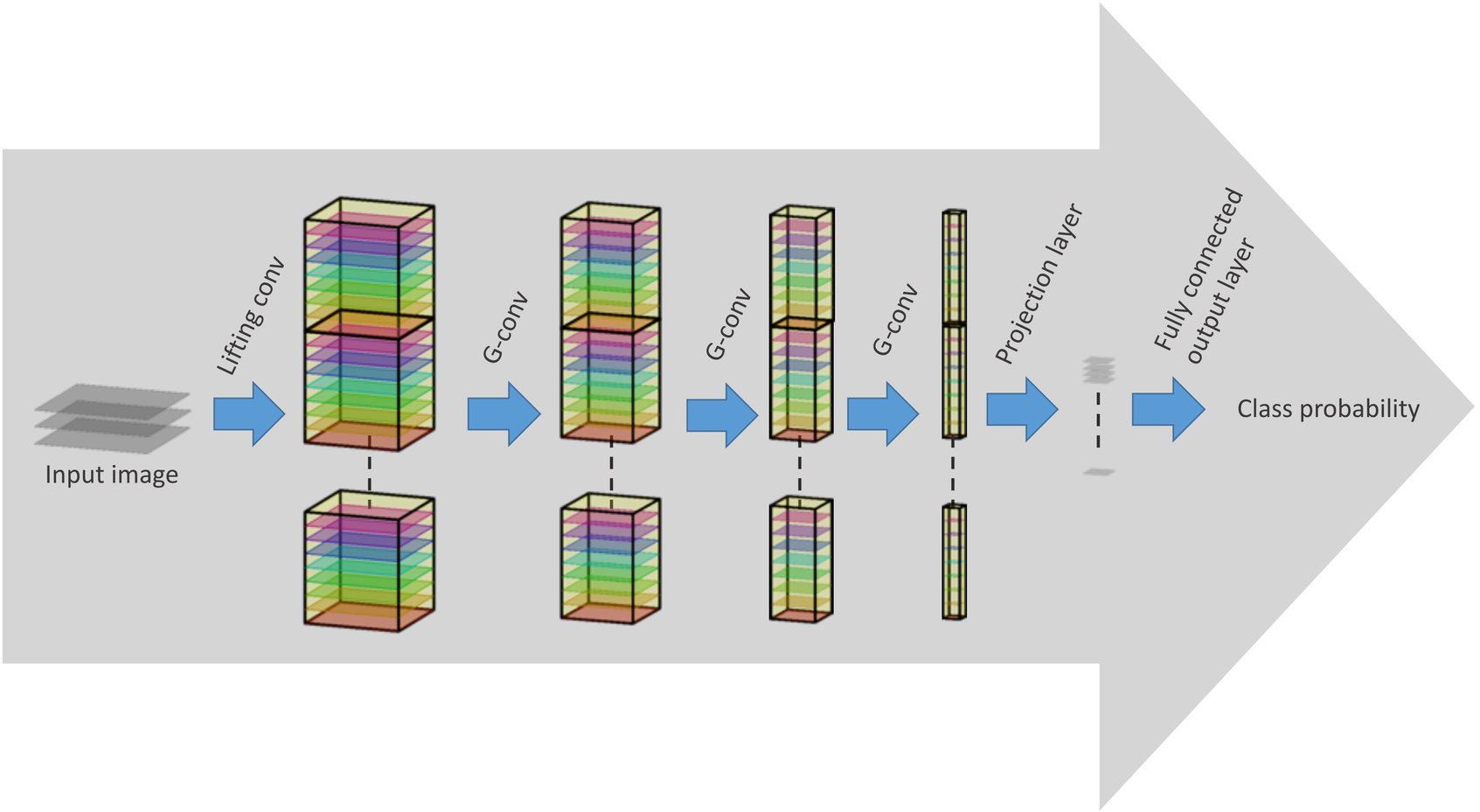

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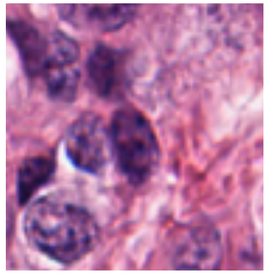

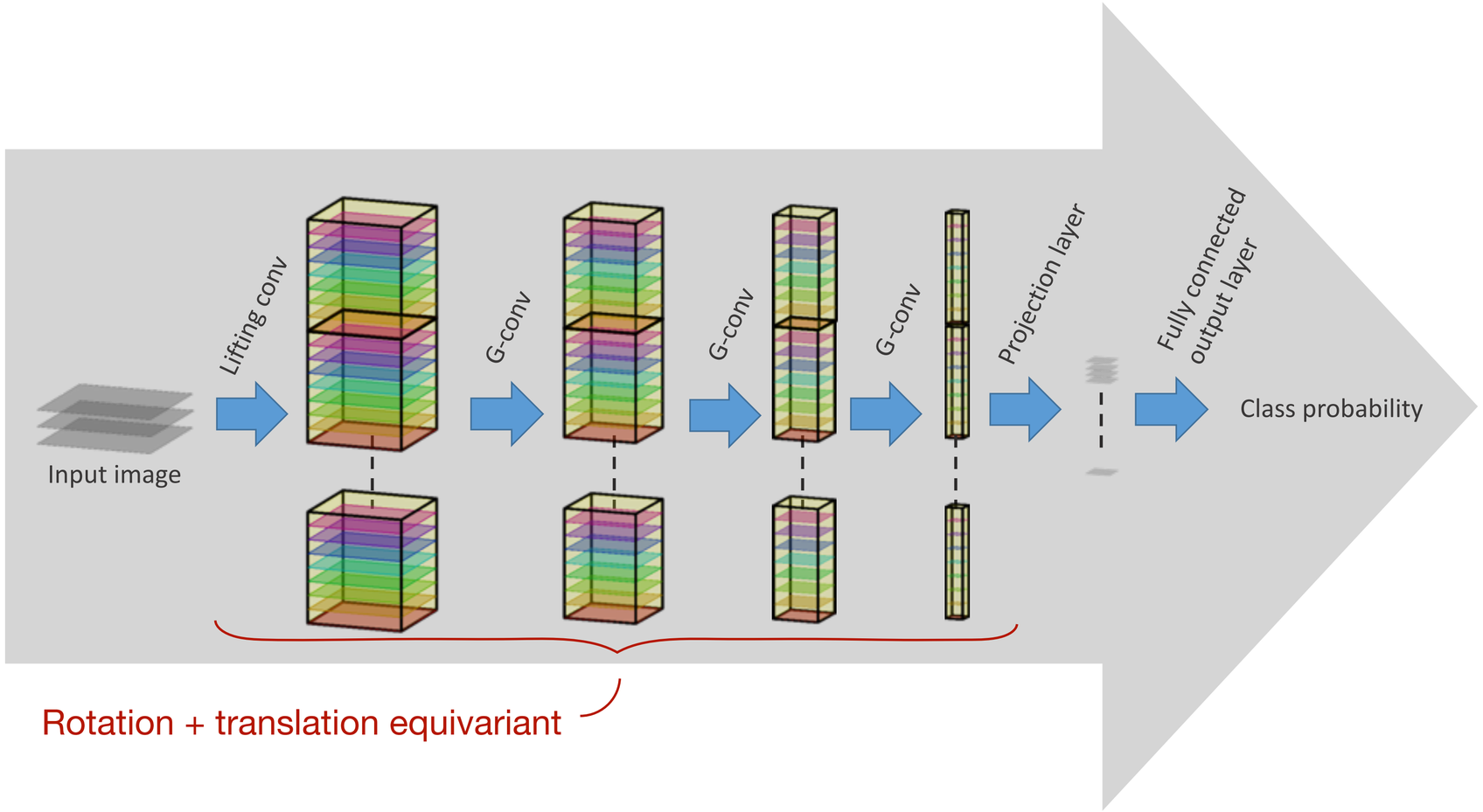

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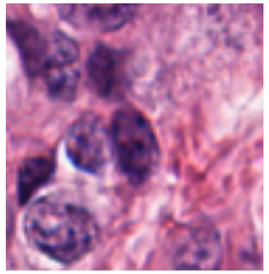

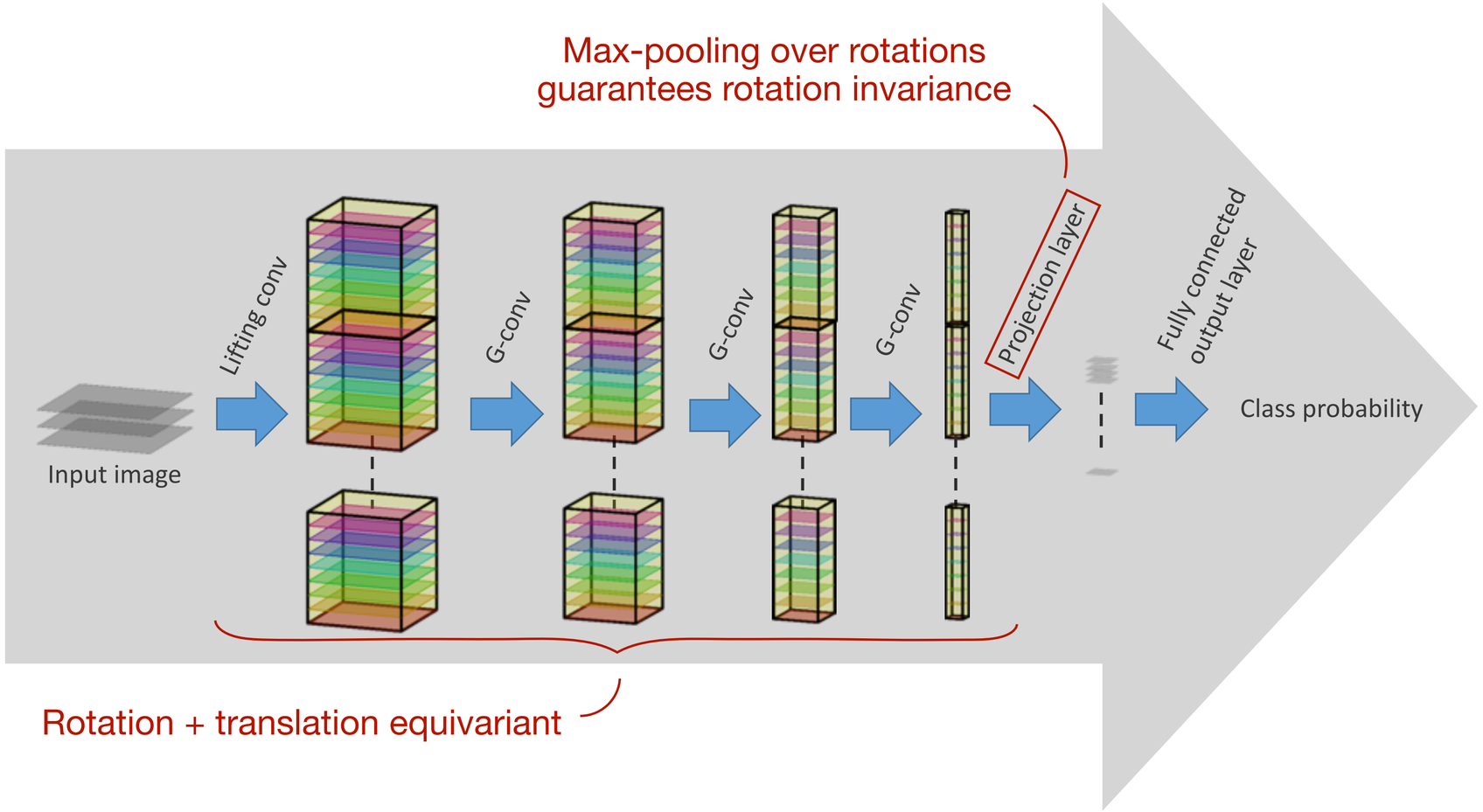

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Bekkers & Lafarge et al. MICCAI 2018

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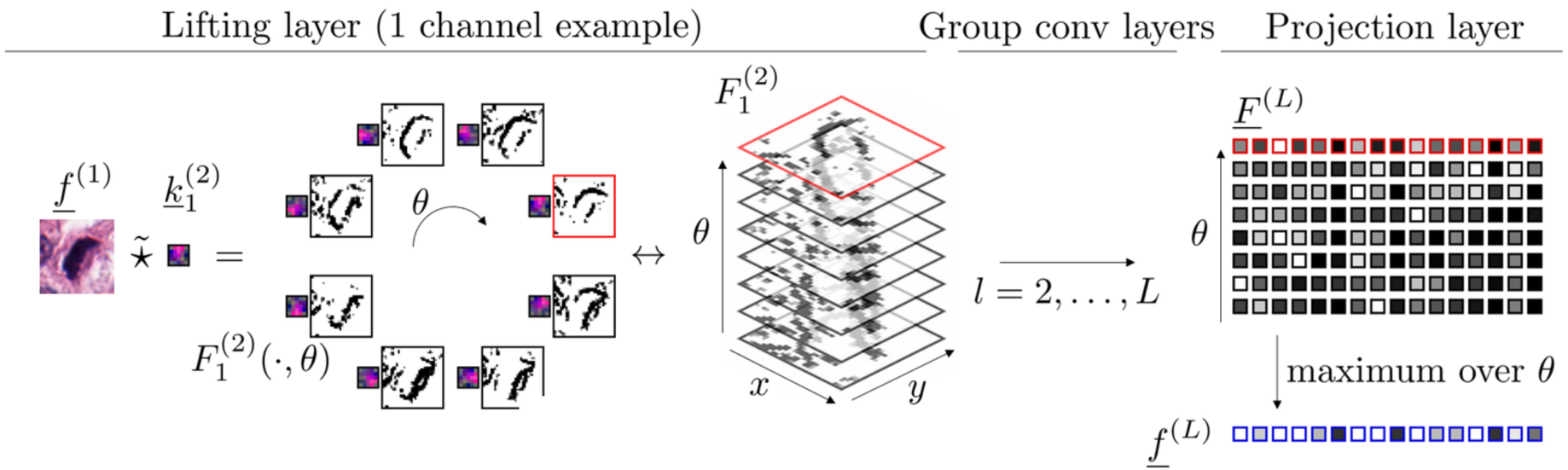

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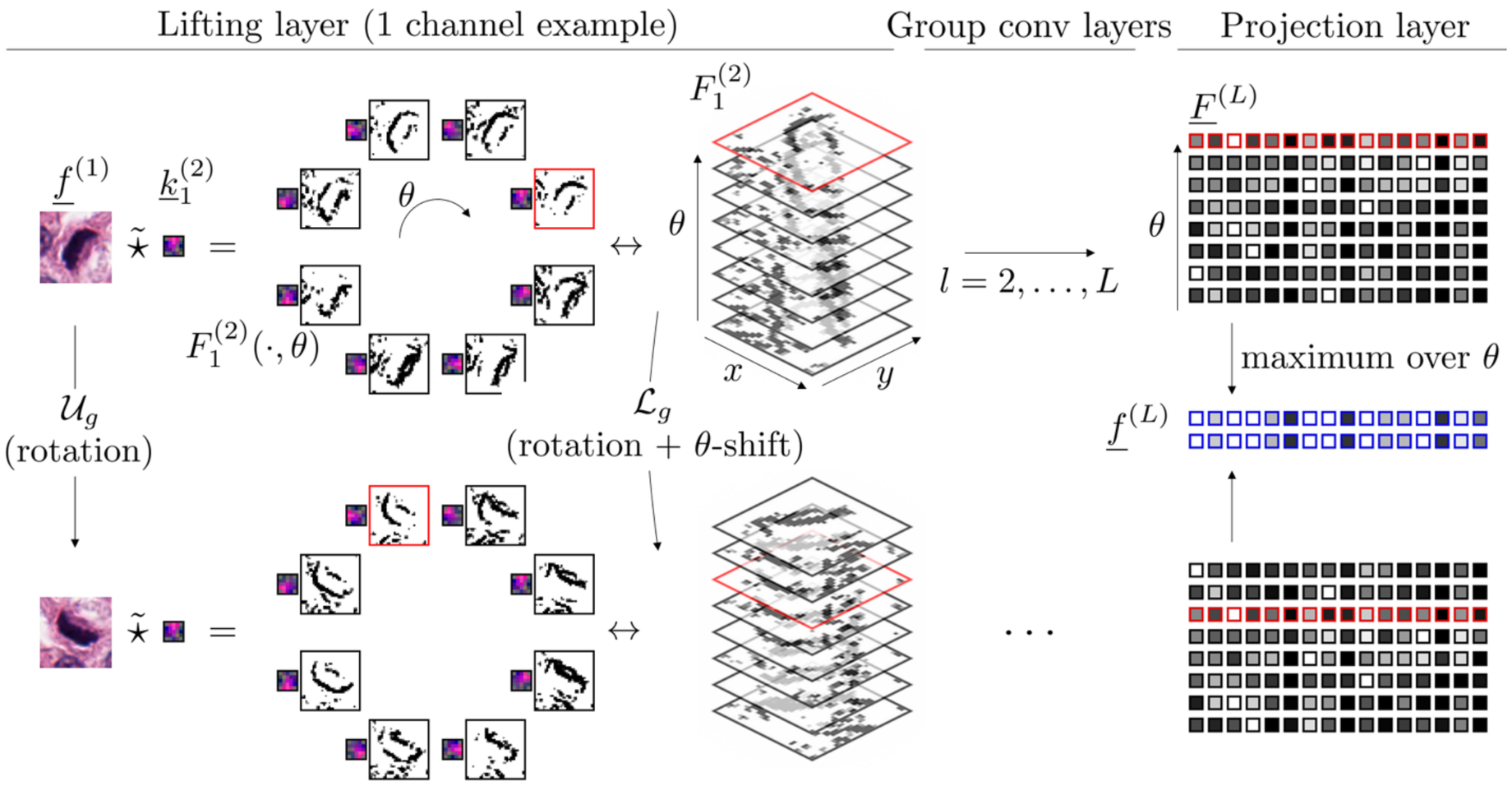

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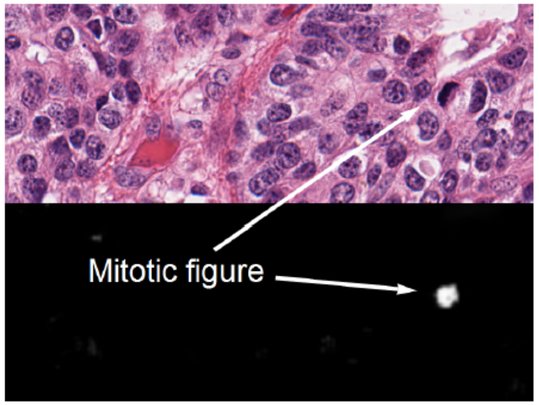

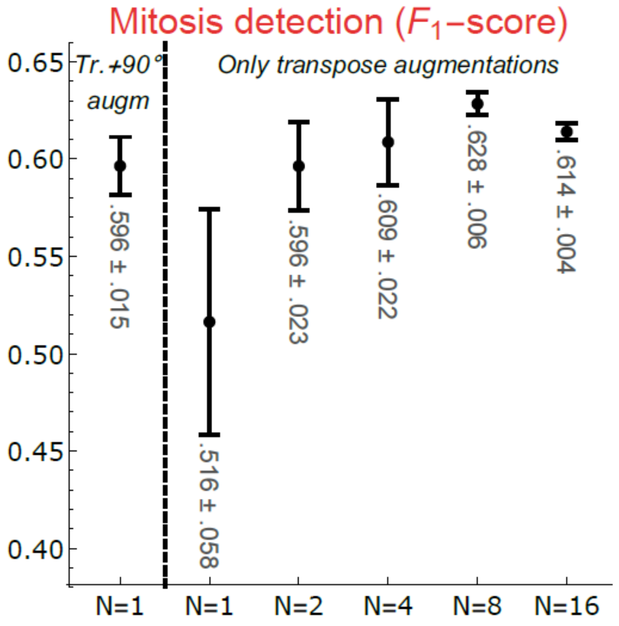

G-CNNs without data-augmentation
outperform
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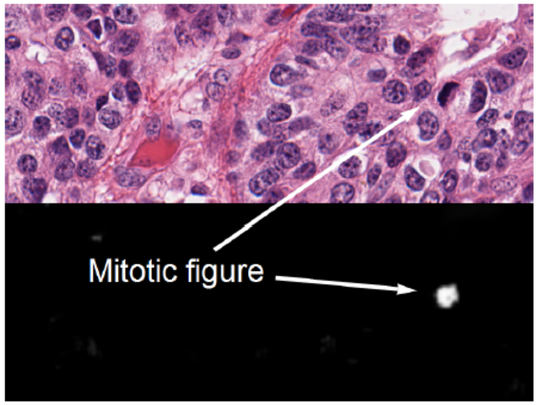
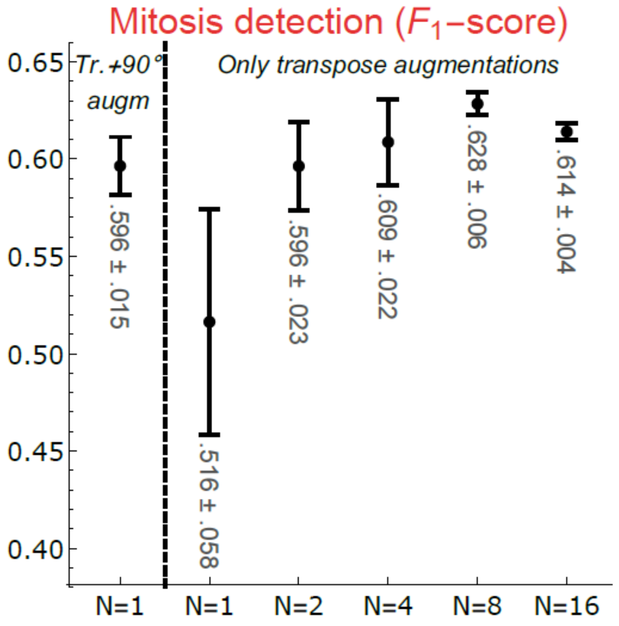
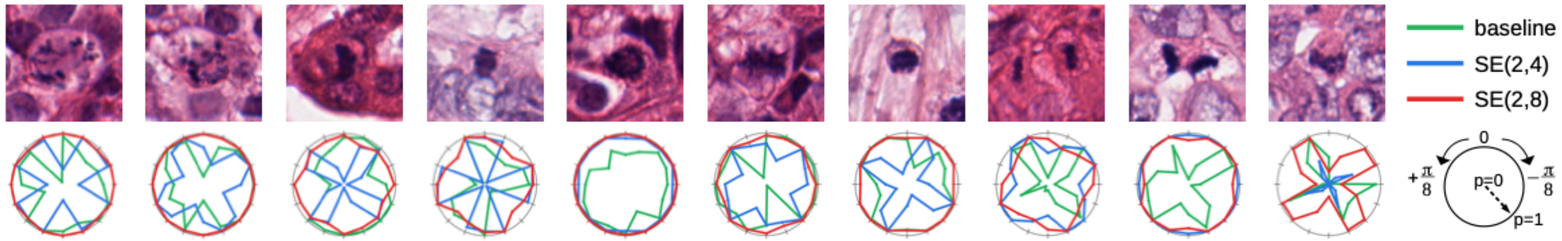




Lafarge et al. MedIA 2020



*G-CNNs guarantee geometric stability. They are **robust to input distortions**, regular CNNs aren't…*

***G-CNNs without data-augmentation** outperform CNNs with data-augmentation*

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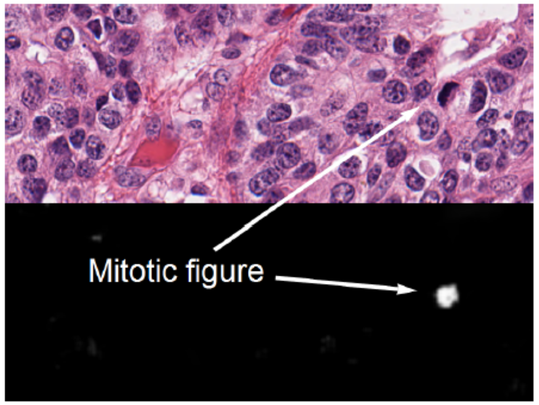

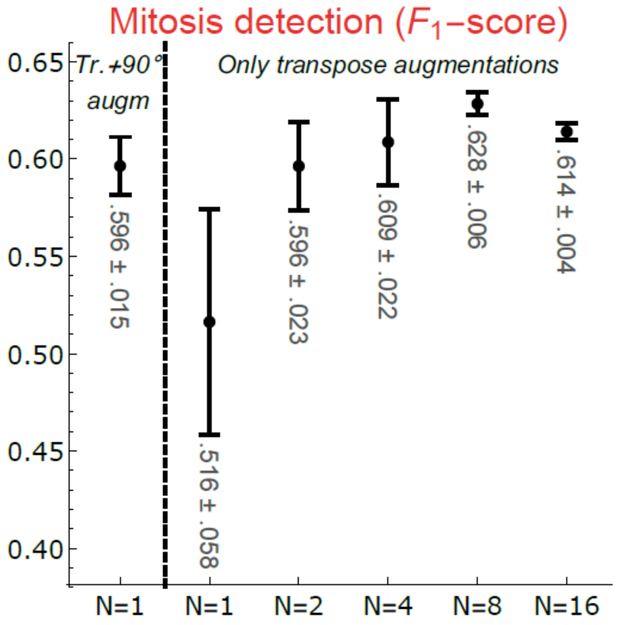

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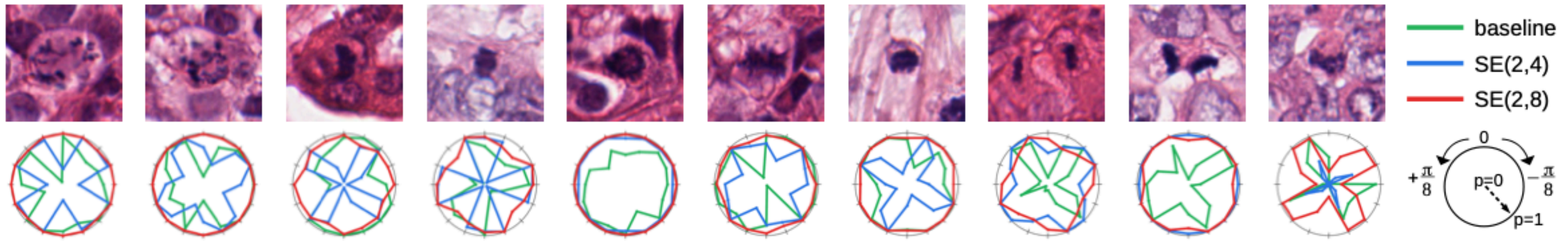

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*G-CNNs are more **sample efficient**!*
G-CNNs (25% data) > CNNs (100% data)

***G-CNNs without data-augmentation** outperform CNNs with data-augmentation*

Lafarge et al. ArXiv/MedIA 2020

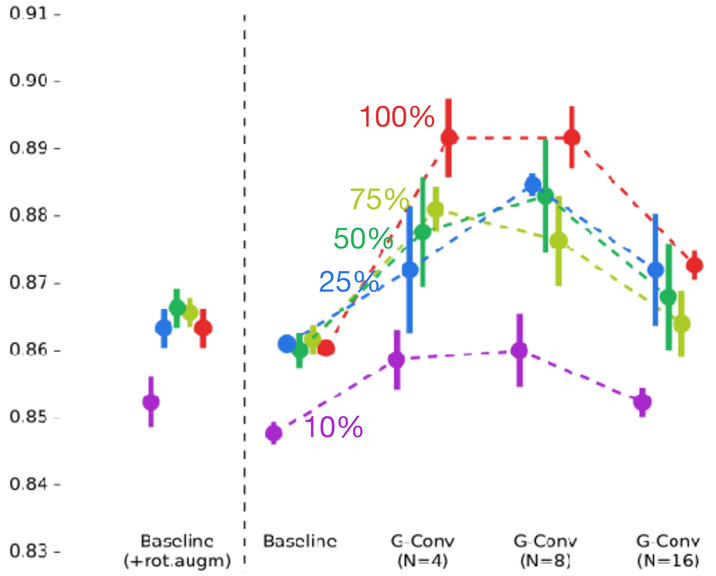
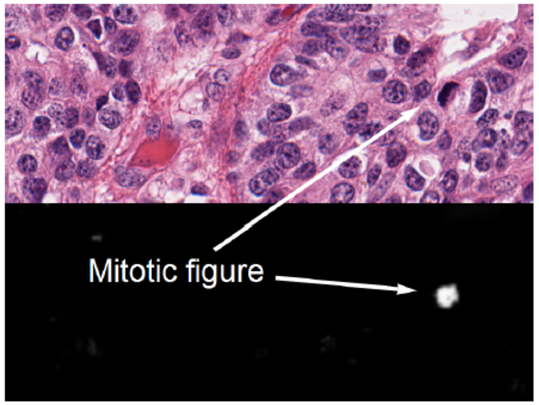
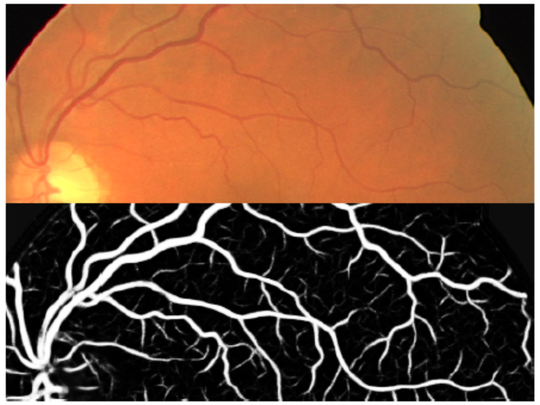


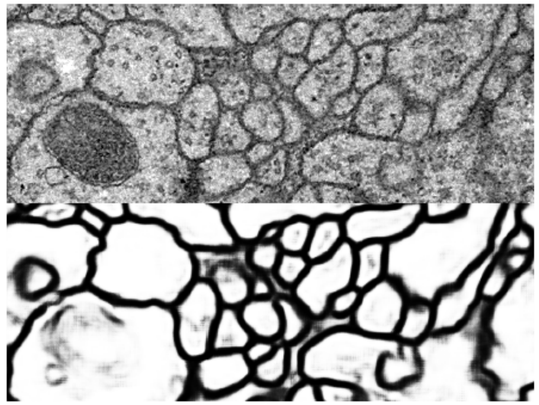
Figure 7: Mean and Standard Deviation plots summarizing the accuracy of the tumor classification models. Mean ± standard deviation is indicated. Color identifies the different data regime (red: 100%; lime: 75%; green: 50%; blue: 25%; purple: 10%).

Experiments in medical image analysis

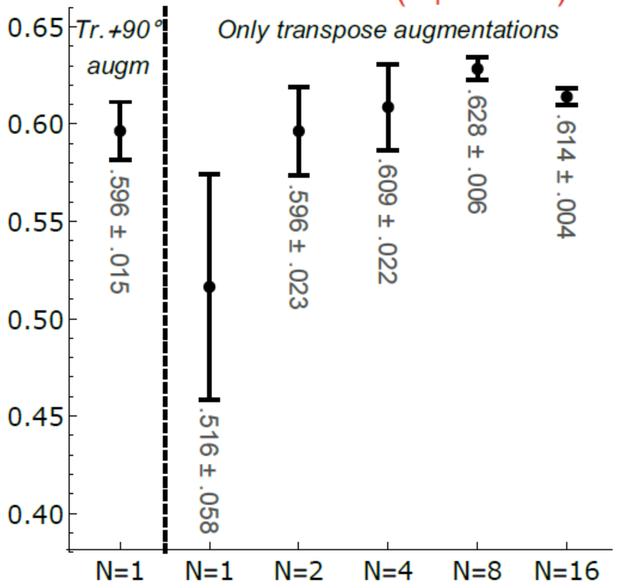
Bekkers & Lafarge et al. MICCAI 2018



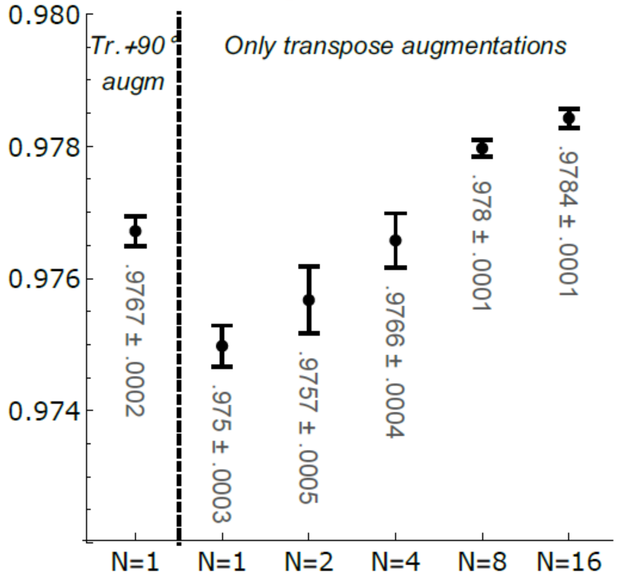




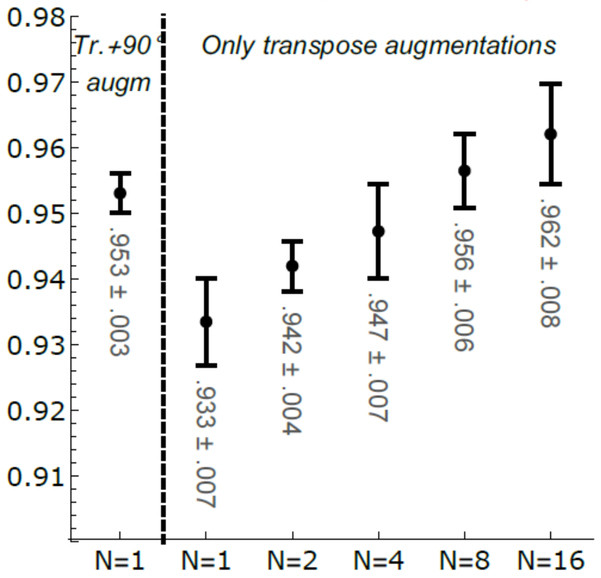
Mitosis detection (F_1–score)



Vessel segmentation (AUC)



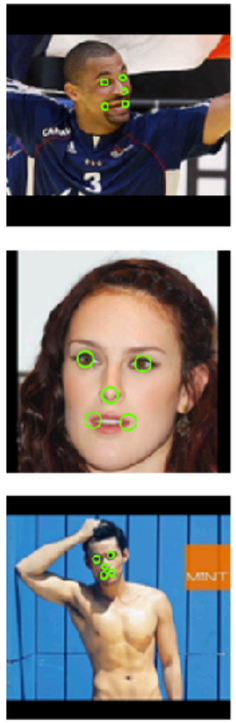
Cell boundary segmentation (Rand)

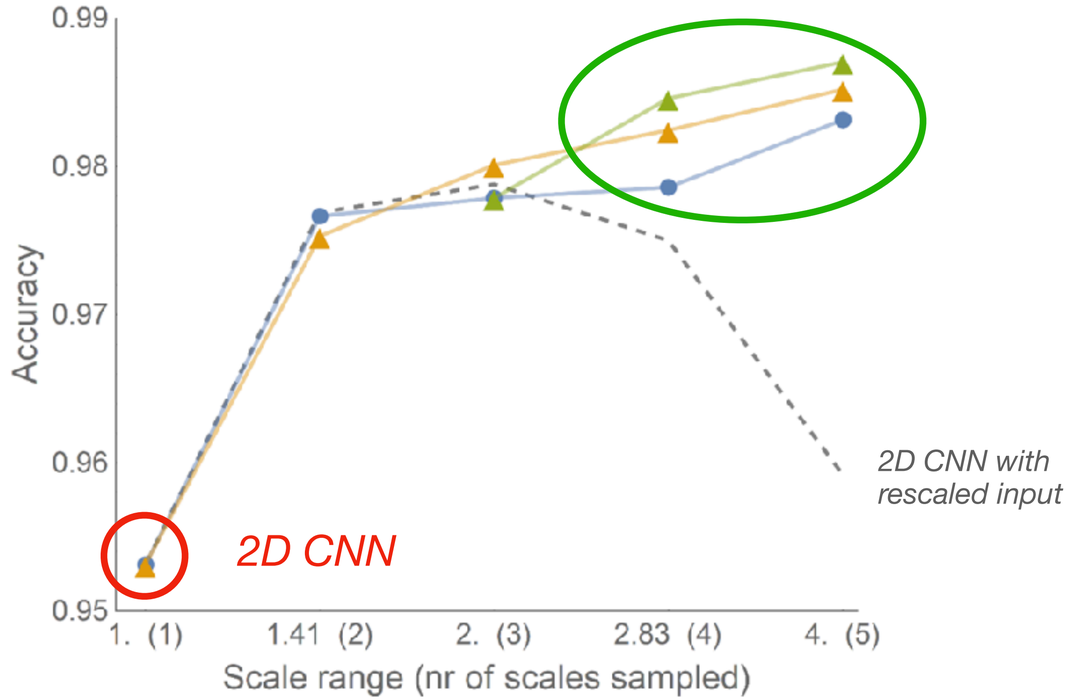


From rotation to scale equivariant CNNs

Bekkers ICLR 2020

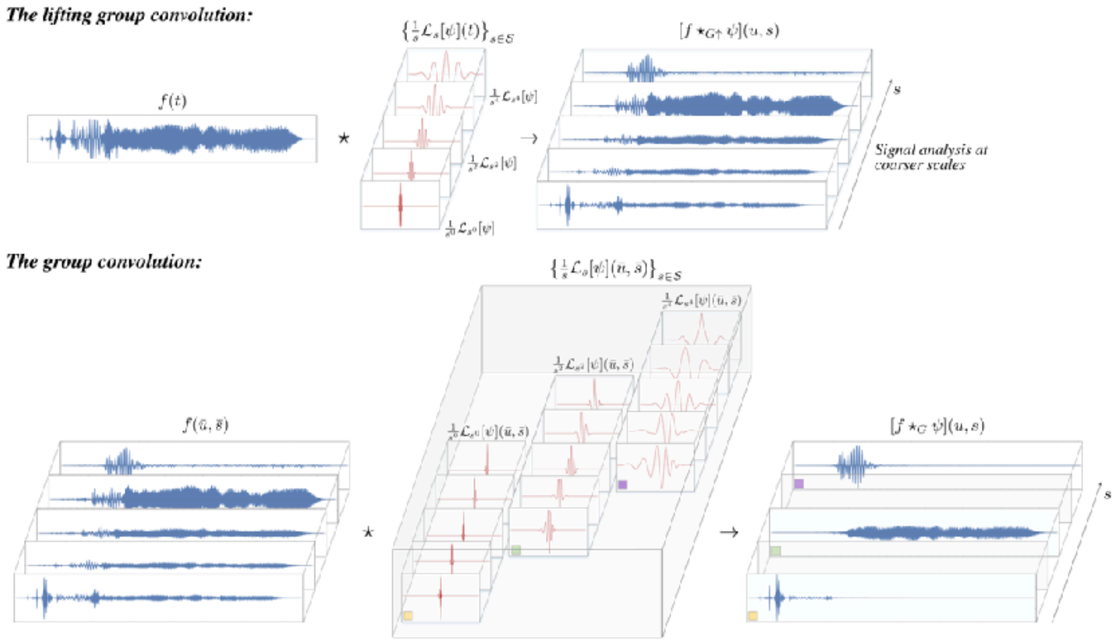
Translation + scale equivariant G-CNNs





From rotation to scale equivariant CNNs

Romero, Bekkers, Tomczak, Hoogeboom
Wavelet Networks: Scale Equivariant Learning From Raw Waveforms - arXiv:2006.05259



G-CNNs rule!

- The right inductive bias: guaranteed equivariance
  (no loss of information)
- Performance gains that can't be obtained by data-augmentation alone
  (both local and global equivariance/invariance)
- Increased sample efficiency
  (increased weight sharing, no geometric augmentation necessary)

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UNIVERSITY OF AMSTERDAM

AMLAB Amsterdam Machine Learning Lab

Group Equivariant Deep Learning

Lecture 1 - Regular group convolutions

Lecture 1.5 - A brief history of G-CNNs

Erik Bekkers, Amsterdam Machine Learning Lab, University of Amsterdam

This mini-course serves as a module with the UvA Master AI course Deep Learning 2 https://uvadl2c.github.io/

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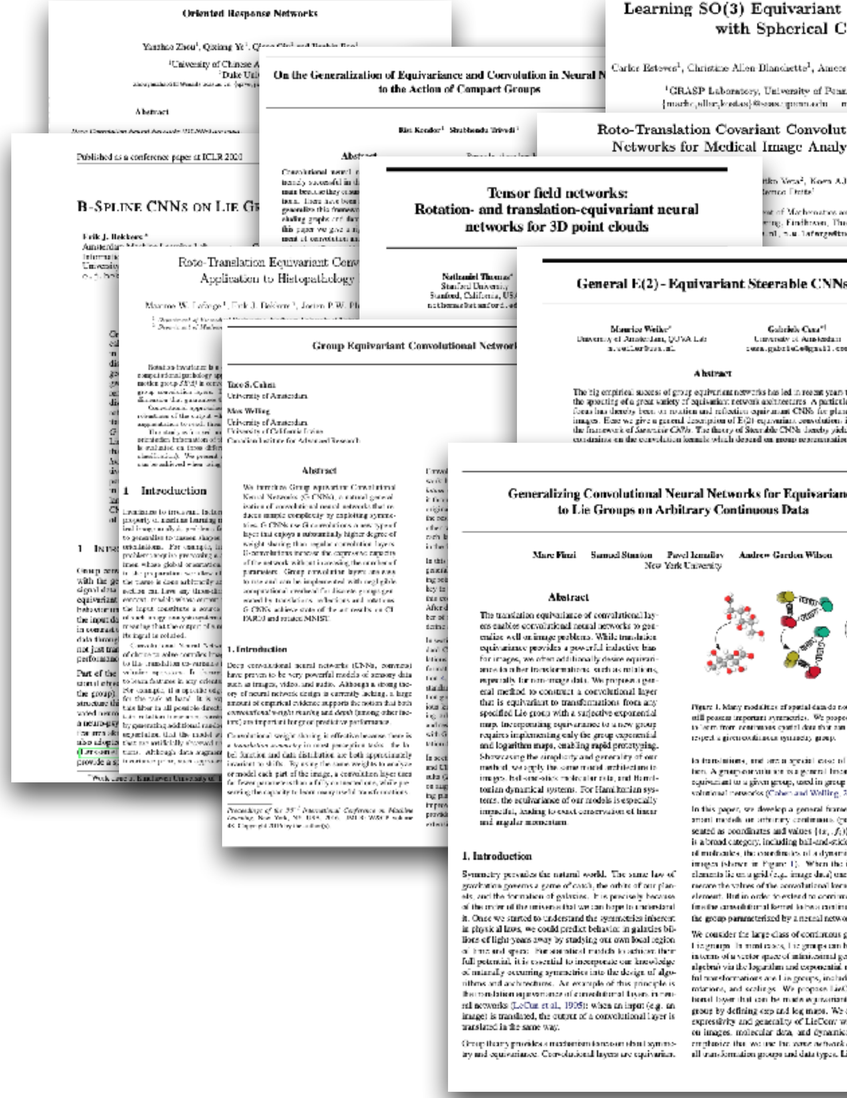

A brief history of G-CNNs

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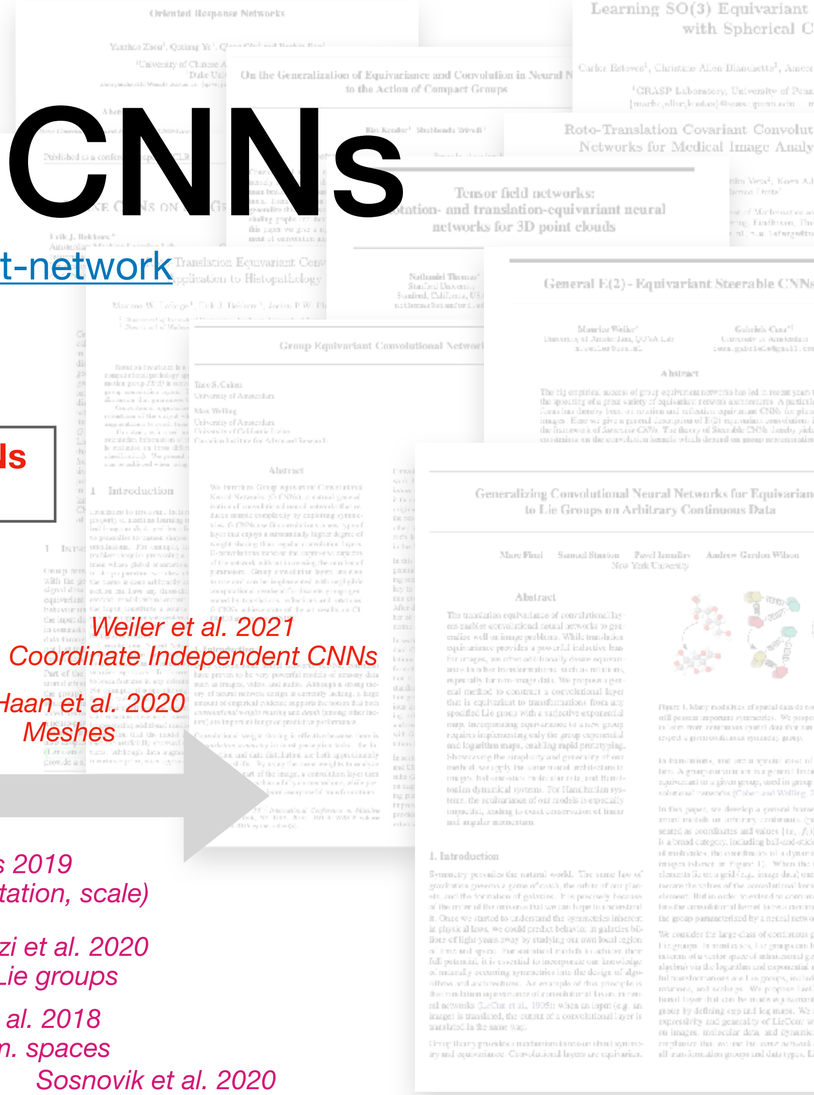

Discrete G-CNNs
(square/cube symmetries)

Gauge-equivariant CNNs
(manifolds)

NNs → CNNs → G-CNNs

LeCun et al. 1990

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p4m

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3D discrete roto-transl.

Hoogeboom et al. 2018
SE(2,6)

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Riemannian Hom. spaces

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Sosnovik et al. 2020
Scale-translation

Continuous rotation G-CNNs
(regular discretizations)

Continuous rotation G-CNNs
(steerable)

Continuous G-CNNs
(Lie groups)

Cesa-Lang-Weiler 2022
$G = \mathbb{R}^d \rtimes H$ with H compact

https://quva-lab.github.io/escnn/

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Cohen-Wellin
p4m

Die

NNs → CNNs → Mallat et al. 20 SE(2) → Continuous (regular → ous G-CNNs (groups)

LeCun et al. 1990

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iler et al. 2021
e Independent CNNs
2020

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translation

Group Equivariant Convolutional Networks

Taco S. Cohen T.S.COHEN@UVA.NL
University of Amsterdam

Max Welling M.WELLING@UVA.NL
University of Amsterdam
University of California Irvine
Canadian Institute for Advanced Research

Abstract

We introduce Group equivariant Convolutional Neural Networks (G-CNNs), a natural generalization of convolutional neural networks that reduces sample complexity by exploiting symmetries. G-CNNs use G-convolutions, a new type of layer that enjoys a substantially higher degree of weight sharing than regular convolution layers. G-convolutions increase the expressive capacity of the network without increasing the number of parameters. Group convolution layers are easy to use and can be implemented with negligible computational overhead for discrete groups generated by translations, reflections and rotations. G-CNNs achieve state of the art results on CIFAR10 and rotated MNIST.

1. Introduction

Deep convolutional neural networks (CNNs, convnets) have proven to be very powerful models of sensory data such as images, video, and audio. Although a strong theory of neural network design is currently lacking, a large amount of empirical evidence supports the notion that both *convolutional weight sharing* and *depth* (among other factors) are important for good predictive performance.

Convolutional weight sharing is effective because there is a *translation symmetry* in most perception tasks: the label function and data distribution are both approximately invariant to shifts. By using the same weights to analyze or model each part of the image, a convolution layer uses far fewer parameters than a fully connected one, while preserving the capacity to learn many useful transformations.

Proceedings of the 33rd International Conference on Machine Learning, New York, NY, USA, 2016. JMLR: W&CP volume 48.

Copyright 2016 by the author(s).

Convolution layers can be used effectively in a *deep* network because all the layers in such a network are *translation equivariant*: shifting the image and then feeding it through a number of layers is the same as feeding the original image through the same layers and then shifting the resulting feature maps (at least up to edge-effects). In other words, the symmetry (translation) is preserved by each layer, which makes it possible to exploit it not just in the first, but also in higher layers of the network.

In this paper we show how convolutional networks can be generalized to exploit larger groups of symmetries, including rotations and reflections. The notion of equivariance is key to this generalization, so in section 2 we will discuss this concept and its role in deep representation learning. After discussing related work in section 3, we recall a number of mathematical concepts in section 4 that allow us to define and analyze the G-convolution in a generic manner.

In section 5, we analyze the equivariance properties of standard CNNs, and show that they are equivariant to translations but may fail to equivary with more general transformations. Using the mathematical framework from section 4, we can define G-CNNs (section 6) by analogy to standard CNNs (the latter being the G-CNN for the translation group). We show that G-convolutions, as well as various kinds of layers used in modern CNNs, such as pooling, arbitrary pointwise nonlinearities, batch normalization and residual blocks are all equivariant, and thus compatible with G-CNNs. In section 7 we provide concrete implementation details for group convolutions.

In section 8 we report experimental results on MNIST-rot and CIFAR10, where G-CNNs achieve state of the art results (2.28% error on MNIST-rot, and 4.19% resp. 6.46% on augmented and plain CIFAR10). We show that replacing planar convolutions with G-convolutions consistently improves results without additional tuning. In section 9 we provide a discussion of these results and consider several extensions of the method, before concluding in section 10.

A brief history of G-CNNs

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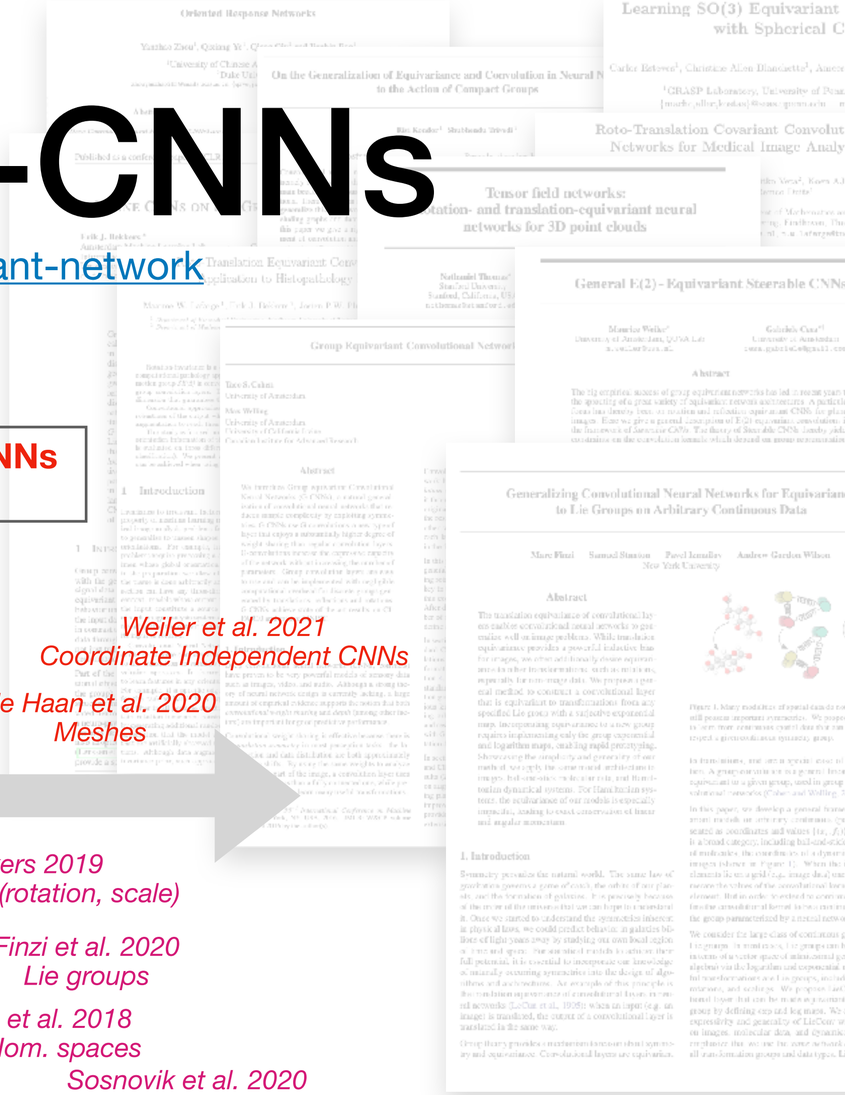

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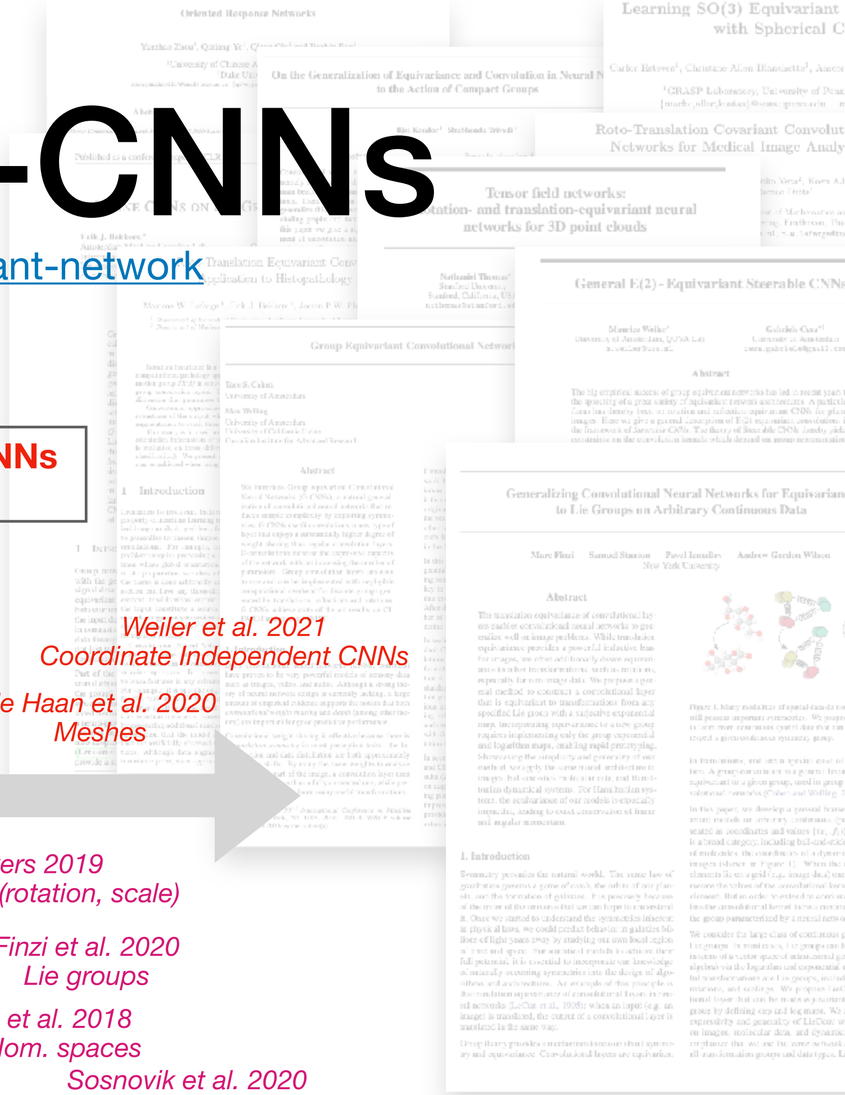

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Cesa-Lang-Weiler 2022
$G = \mathbb{R}^d \rtimes H$ with H compact

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A brief history of G-CNNs

https://github.com/Chen-Cai-OSU/awesome-equivariant-network

NNs

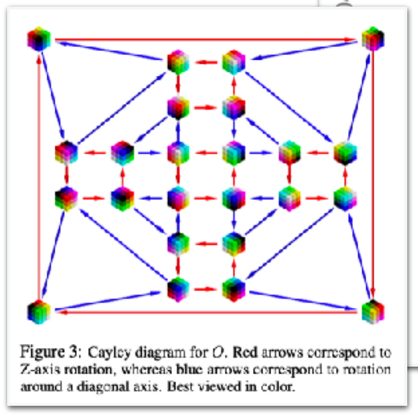
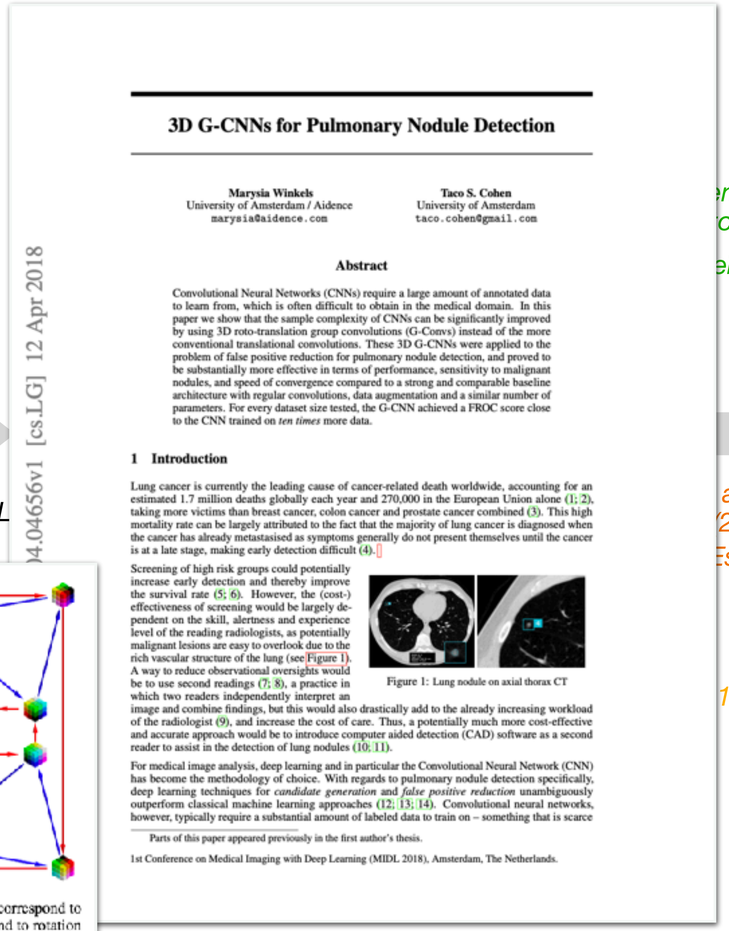


Figure 3: Cayley diagram for O. Red arrows correspond to Z-axis rotation, whereas blue arrows correspond to rotation around a diagonal axis. Best viewed in color.



3D G-CNNs for Pulmonary Nodule Detection

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Taco S. Cohen, University of Amsterdam, taco.cohen@gmail.com

Abstract

Convolutional Neural Networks (CNNs) require a large amount of annotated data to learn from, which is often difficult to obtain in the medical domain. In this paper we show that the sample complexity of CNNs can be significantly improved by using 3D roto-translation group convolutions (G-Convs) instead of the more conventional translational convolutions. These 3D G-CNNs were applied to the problem of false positive reduction for pulmonary nodule detection, and proved to be substantially more effective in terms of performance, sensitivity to malignant nodules, and speed of convergence compared to a strong and comparable baseline architecture with regular convolutions, data augmentation and a similar number of parameters. For every dataset size tested, the G-CNN achieved a FROC score close to the CNN trained on *ten times* more data.

1 Introduction

Lung cancer is currently the leading cause of cancer-related death worldwide, accounting for an estimated 1.7 million deaths globally each year and 270,000 in the European Union alone (1; 2), taking more victims than breast cancer, colon cancer and prostate cancer combined (3). This high mortality rate can be largely attributed to the fact that the majority of lung cancer is diagnosed when the cancer has already metastasised as symptoms generally do not present themselves until the cancer is at a late stage, making early detection difficult (4).

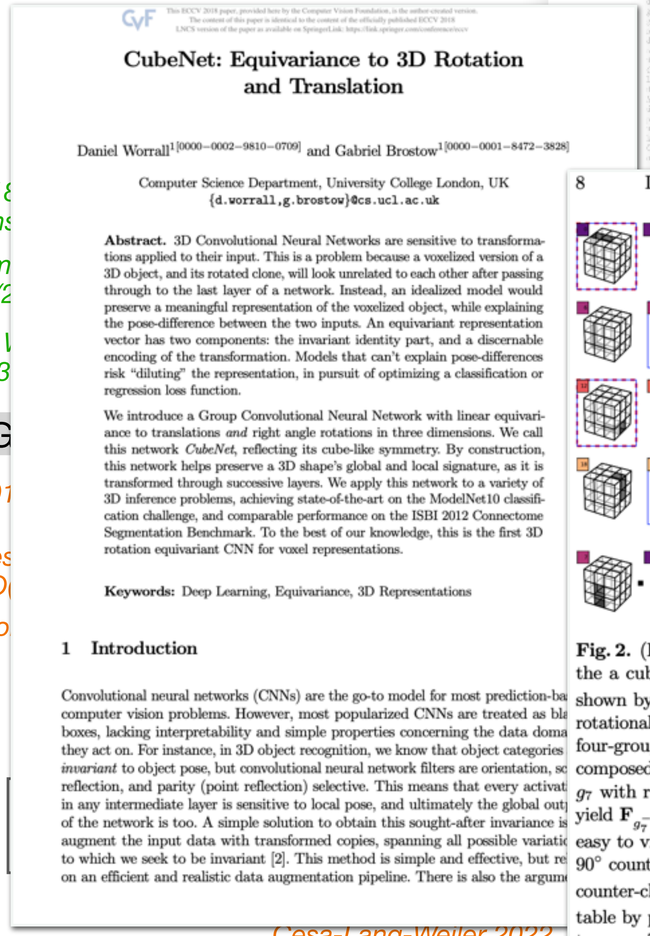
Screening of high risk groups could potentially increase early detection and thereby improve the survival rate (5; 6). However, the (cost-) effectiveness of screening would be largely dependent on the skill, alertness and experience level of the reading radiologists, as potentially malignant lesions are easy to overlook due to the rich vascular structure of the lung (see Figure 1). A way to reduce observational oversights would be to use second readings (7; 8), a practice in which two readers independently interpret an image and combine findings, but this would also drastically add to the already increasing workload of the radiologist (9), and increase the cost of care. Thus, a potentially much more cost-effective and accurate approach would be to introduce computer aided detection (CAD) software as a second reader to assist in the detection of lung nodules (10; 11).

Figure 1: Lung nodule on axial thorax CT

For medical image analysis, deep learning and in particular the Convolutional Neural Network (CNN) has become the methodology of choice. With regards to pulmonary nodule detection specifically, deep learning techniques for *candidate generation* and *false positive reduction* unambiguously outperform classical machine learning approaches (12; 13; 14). Convolutional neural networks, however, typically require a substantial amount of labeled data to train on – something that is scarce

Parts of this paper appeared previously in the first author's thesis.

1st Conference on Medical Imaging with Deep Learning (MIDL 2018), Amsterdam, The Netherlands.



CubeNet: Equivariance to 3D Rotation and Translation

Daniel Worrall[1][0000−0002−9810−0709] and Gabriel Brostow[1][0000−0001−8472−3828]

Computer Science Department, University College London, UK
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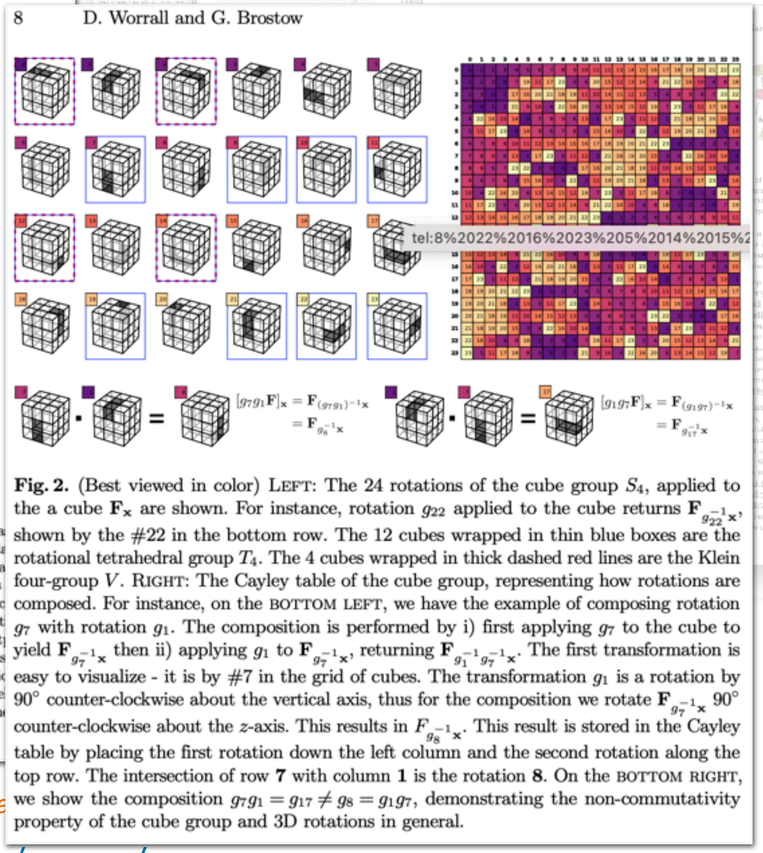
Abstract. 3D Convolutional Neural Networks are sensitive to transformations applied to their input. This is a problem because a voxelized version of a 3D object, and its rotated clone, will look unrelated to each other after passing through to the last layer of a network. Instead, an idealized model would preserve a meaningful representation of the voxelized object, while explaining the pose-difference between the two inputs. An equivariant representation vector has two components: the invariant identity part, and a discernable encoding of the transformation. Models that can't explain pose-differences risk "diluting" the representation, in pursuit of optimizing a classification or regression loss function.

We introduce a Group Convolutional Neural Network with linear equivariance to translations *and* right angle rotations in three dimensions. We call this network *CubeNet*, reflecting its cube-like symmetry. By construction, this network helps preserve a 3D shape's global and local signature, as it is transformed through successive layers. We apply this network to a variety of 3D inference problems, achieving state-of-the-art on the ModelNet10 classification challenge, and comparable performance on the ISBI 2012 Connectome Segmentation Benchmark. To the best of our knowledge, this is the first 3D rotation equivariant CNN for voxel representations.

Keywords: Deep Learning, Equivariance, 3D Representations

1 Introduction

Convolutional neural networks (CNNs) are the go-to model for most prediction-ba computer vision problems. However, most popularized CNNs are treated as bla boxes, lacking interpretability and simple properties concerning the data doma they act on. For instance, in 3D object recognition, we know that object categories *invariant* to object pose, but convolutional neural network filters are orientation, sc reflection, and parity (point reflection) selective. This means that every activat in any intermediate layer is sensitive to local pose, and ultimately the global out of the network is too. A simple solution to obtain this sought-after invariance is augment the input data with transformed copies, spanning all possible variatio to which we seek to be invariant [2]. This method is simple and effective, but re on an efficient and realistic data augmentation pipeline. There is also the argume



8 D. Worrall and G. Brostow

Fig. 2. (Best viewed in color) LEFT: The 24 rotations of the cube group S_4, applied to the a cube $\mathbf{F_x}$ are shown. For instance, rotation g_{22} applied to the cube returns $\mathbf{F}_{g_{22}^{-1}\mathbf{x}}$, shown by the #22 in the bottom row. The 12 cubes wrapped in thin blue boxes are the rotational tetrahedral group T_4. The 4 cubes wrapped in thick dashed red lines are the Klein four-group V. RIGHT: The Cayley table of the cube group, representing how rotations are composed. For instance, on the BOTTOM LEFT, we have the example of composing rotation g_7 with rotation g_1. The composition is performed by i) first applying g_7 to the cube to yield $\mathbf{F}_{g_7^{-1}\mathbf{x}}$ then ii) applying g_1 to $\mathbf{F}_{g_7^{-1}\mathbf{x}}$, returning $\mathbf{F}_{g_1^{-1}g_7^{-1}\mathbf{x}}$. The first transformation is easy to visualize - it is by #7 in the grid of cubes. The transformation g_1 is a rotation by 90° counter-clockwise about the vertical axis, thus for the composition we rotate $\mathbf{F}_{g_7^{-1}\mathbf{x}}$ 90° counter-clockwise about the z-axis. This results in $F_{g_8^{-1}\mathbf{x}}$. This result is stored in the Cayley table by placing the first rotation down the left column and the second rotation along the top row. The intersection of row **7** with column **1** is the rotation **8**. On the BOTTOM RIGHT, we show the composition $g_7 g_1 = g_{17} \neq g_8 = g_1 g_7$, demonstrating the non-commutativity property of the cube group and 3D rotations in general.

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NNs

Published as a conference paper at ICLR 2018

HEXACONV

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arXiv:1803.02108v1 [cs.LG] 6 Mar 2018

ABSTRACT

The effectiveness of convolutional neural networks stems in large part from their ability to exploit the translation invariance that is inherent in many learning problems. Recently, it was shown that CNNs can exploit other sources of invariance, such as rotation invariance, by using *group convolutions* instead of planar convolutions. However, for reasons of performance and ease of implementation, it has been necessary to limit the group convolution to transformations that can be applied to the filters without interpolation. Thus, for images with square pixels, only integer translations, rotations by multiples of 90 degrees, and reflections are admissible.

Whereas the square tiling provides a 4-fold rotational symmetry, a hexagonal tiling of the plane has a 6-fold rotational symmetry. In this paper we show how one can efficiently implement planar convolution and group convolution over hexagonal lattices, by re-using existing highly optimized convolution routines. We find that, due to the reduced anisotropy of hexagonal filters, planar HexaConv provides better accuracy than planar convolution with square filters, given a fixed parameter budget. Furthermore, we find that the increased degree of symmetry of the hexagonal grid increases the effectiveness of group convolutions, by allowing for more parameter sharing. We show that our method significantly outperforms conventional CNNs on the AID aerial scene classification dataset, even outperforming ImageNet pretrained models.

1 INTRODUCTION

For sensory perception tasks, neural networks have mostly replaced handcrafted features. Instead of defining features by hand using domain knowledge, it is now possible to learn them, resulting in improved accuracy and saving a considerable amount of work. However, successful generalization is still critically dependent on the inductive bias encoded in the network architecture, whether this bias is understood by the network architect or not.

The canonical example of a successful network architecture is the Convolutional Neural Network (CNN, ConvNet). Through convolutional weight sharing, these networks exploit the fact that a given visual pattern may appear in different locations in the image with approximately equal likelihood. Furthermore, this translation symmetry is preserved throughout the network, because a translation of the input image leads to a translation of the feature maps at each layer: convolution is translation equivariant.

Very often, the true label function (the mapping from image to label that we wish to learn) is invariant to more transformations than just translations. Rotations are an obvious example, but standard translational convolutions cannot exploit this symmetry, because they are not rotation equivariant. As it turns out, a convolution operation can be defined for almost any group of transformation — not just translations. By simply replacing convolutions with group convolutions (wherein filters are not

*Equal contribution

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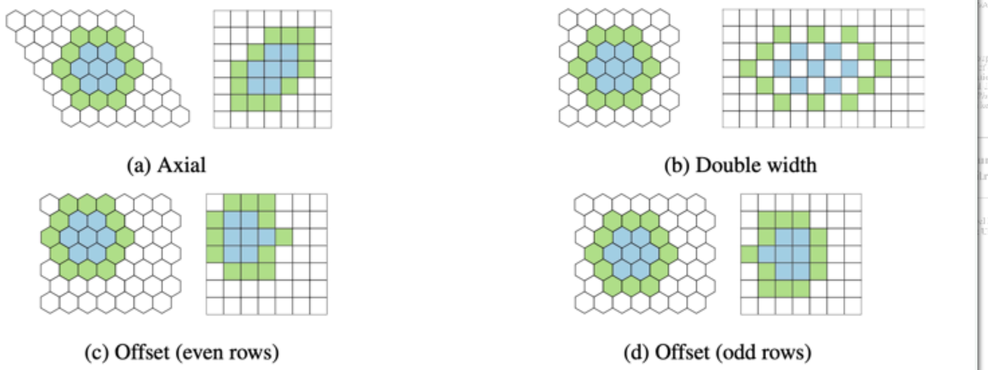

(a) Axial (b) Double width (c) Offset (even rows) (d) Offset (odd rows)

Figure 4: Hexagonal convolution filters (left) represented in 2D memory (right) for filters of size three (blue) and five (blue and green). Standard 2D convolution using both feature map and filter stored according to the coordinate system is equivalent to convolution on the hexagonal lattice. Note that for the offset coordinate system two separate planar convolution are required — one for even and one for odd rows.

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Kondor-Trivedi 2018
SE(3)

Bekkers 2019
Lie groups (rotation, scale)

Finzi et al. 2020

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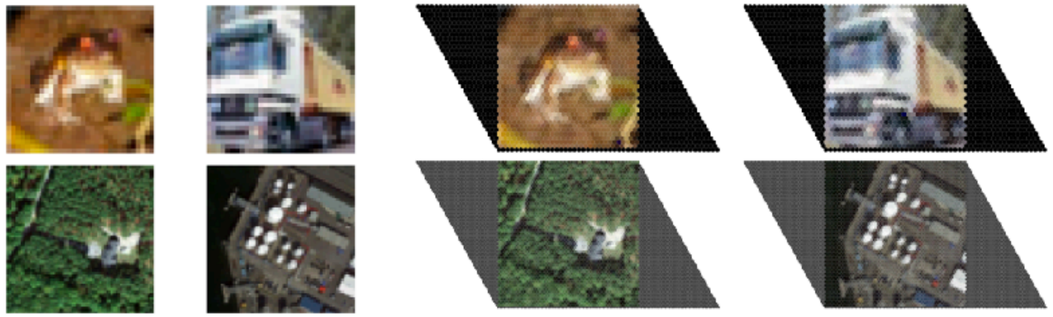

(a) Original example images (b) Hexagonal sampled images

Figure 6: CIFAR-10 (top) and AID (bottom) examples sampled from Cartesian to hexagonal axial coordinates. Zero padding enlarges the images in axial systems.

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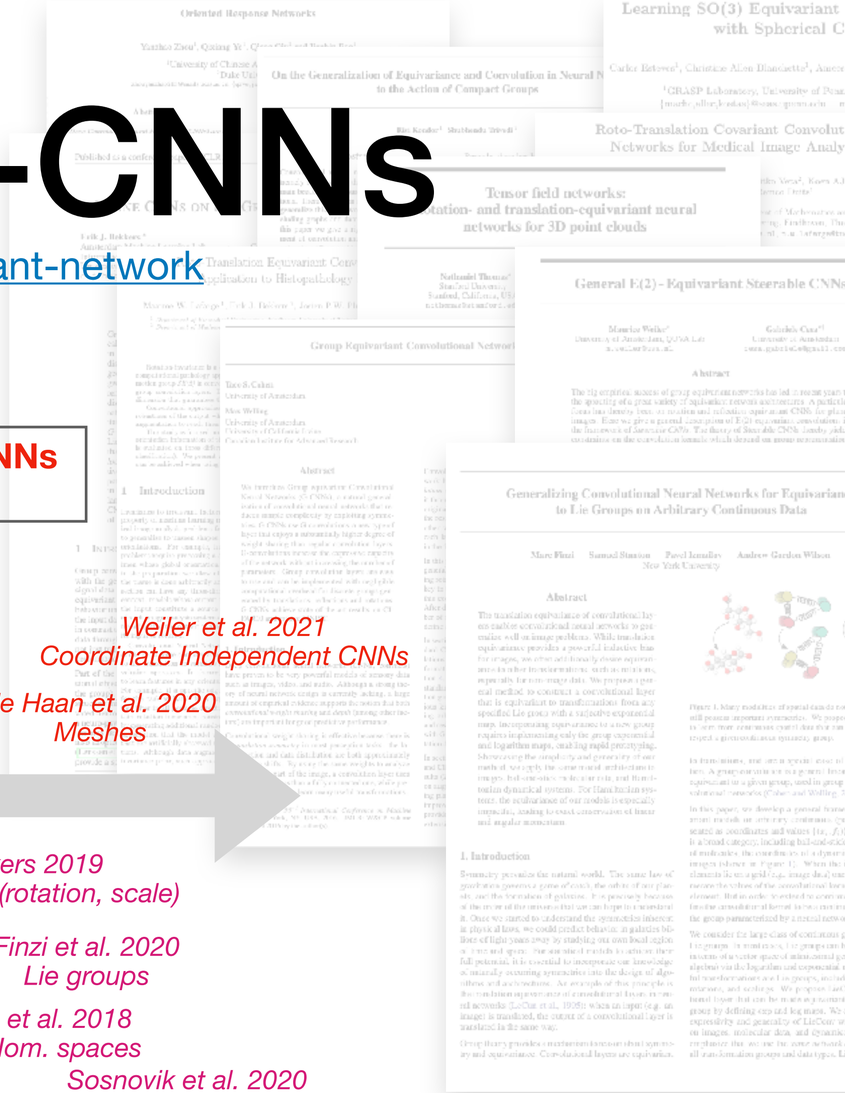

Discrete G-CNNs
(square/cube symmetries)

Gauge-equivariant CNNs
(manifolds)

NNs → CNNs → G-CNNs

LeCun et al. 1990

Cohen-Welling 2016
p4m

Dieleman et al. 2016
p4m

Winkels-Cohen 2018
3D discrete roto-transl.

Hoogeboom et al. 2018
SE(2,6)

Worrall-Brostow 2018
3D discrete roto-transl.

Cohen et al. 2019
Icosahedron

Weiler et al. 2021
Coordinate Independent CNNs

de Haan et al. 2020
Meshes

Mallat et al. 2013, 2015
SE(2)

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SE(2)

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SO(3)

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SE(3)

Bekkers 2019
Lie groups (rotation, scale)

Finzi et al. 2020
Lie groups

Chakraborty et al. 2018
Riemannian Hom. spaces

Weiler-Cesa 2019
SE(2)

Sosnovik et al. 2020
Scale-translation

Continuous rotation G-CNNs
(regular discretizations)

Continuous rotation G-CNNs
(steerable)

Continuous G-CNNs
(Lie groups)

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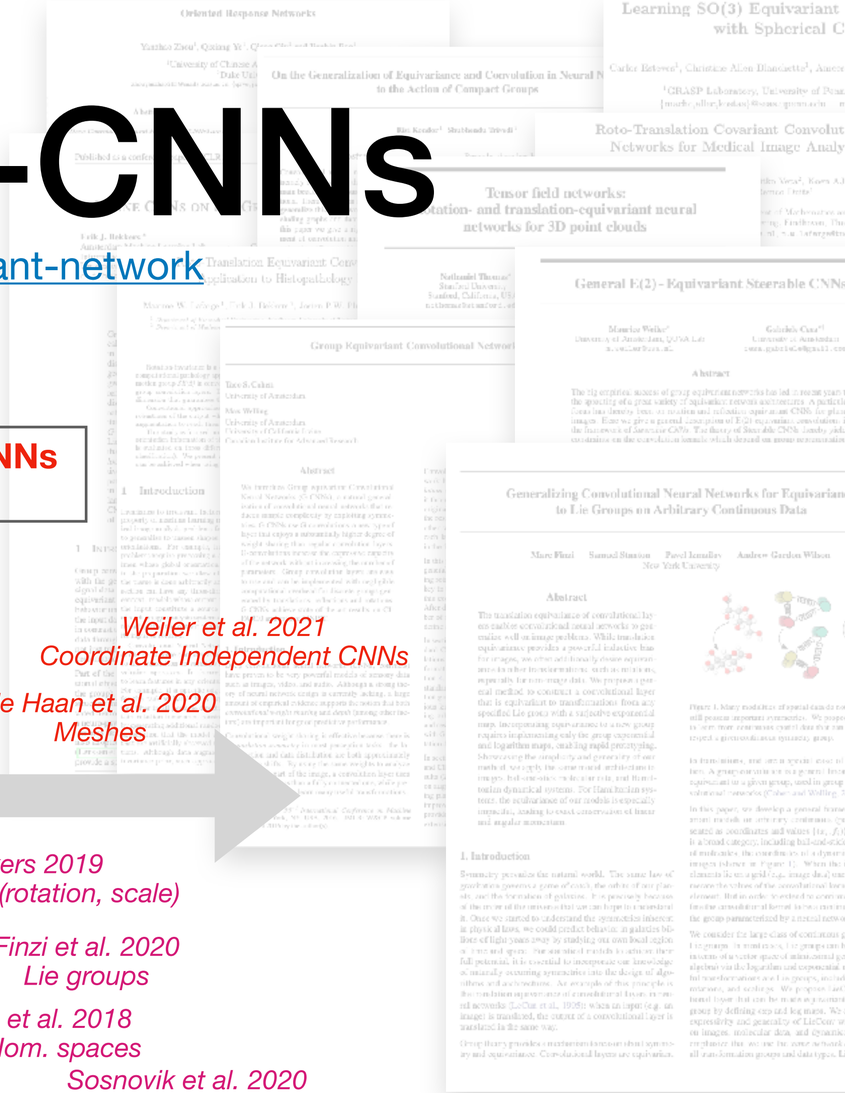

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arXiv:1804.03393v3 [cs.CV] 11 Jun 2018

Roto-Translation Covariant Convolutional Networks for Medical Image Analysis

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Eindhoven University of Technology, [1]Department of Mathematics and Computer Science and [2]Department of Biomedical Engineering, Eindhoven, The Netherlands
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Abstract. We propose a framework for rotation and translation covariant deep learning using $SE(2)$ group convolutions. The group product of the special Euclidean motion group $SE(2)$ describes how a concatenation of two roto-translations results in a net roto-translation. We encode this geometric structure into convolutional neural networks (CNNs) via $SE(2)$ group convolutional layers, which fit into the standard 2D CNN framework, and which allow to generically deal with rotated input samples without the need for data augmentation.
We introduce three layers: a *lifting layer* which lifts a 2D (vector valued) image to an $SE(2)$-image, i.e., 3D (vector valued) data whose domain is $SE(2)$; a *group convolution layer* from and to an $SE(2)$-image; and a *projection layer* from an $SE(2)$-image to a 2D image. The lifting and group convolution layers are $SE(2)$ *covariant* (the output roto-translates with the input). The final projection layer, a maximum intensity projection over rotations, makes the full CNN rotation *invariant*.
We show with three different problems in histopathology, retinal imaging, and electron microscopy that with the proposed group CNNs, state-of-the-art performance can be achieved, without the need for data augmentation by rotation and with increased performance compared to standard CNNs that do rely on augmentation.

Keywords: Group convolutional network, roto-translation group, mitosis detection, vessel segmentation, cell boundary segmentation

1 Introduction

In this work we generalize $\mathbb{R}^2$ convolutional neural networks (CNNs) to $SE(2)$ group CNNs (G-CNNs) in which the data lives on position orientation space, and in which the convolution layers are defined in terms of representations of the special Euclidean motion group $SE(2)$. In essence this means that we replace the convolutions (with translations of a kernel) by $SE(2)$ group convolutions (with roto-translations of a kernel). The advantage of the proposed approach compared to standard $\mathbb{R}^2$ CNNs is that rotation covariance is encoded in the network design and does not have to be learned by the convolution kernels. E.g., a feature that may appear in the data under several orientations does not have

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Roto-translation equivariant convolutional networks: Application to histopathology image analysis

Maxime W. Lafarge[a,*], Erik J. Bekkers[b], Josien P.W. Pluim[a], Remco Duits[b], Mitko Veta[a]

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Tumor detection
Nuclei segmentation

ABSTRACT

Rotation-invariance is a desired property of machine-learning models for medical image analysis and in particular for computational pathology applications. We propose a framework to encode the geometric structure of the special Euclidean motion group $SE(2)$ in convolutional networks to yield translation and rotation equivariance via the introduction of $SE(2)$-group convolution layers. This structure enables models to learn feature representations with a discretized orientation dimension that guarantees that their outputs are invariant under a discrete set of rotations.

Conventional approaches for rotation invariance rely mostly on data augmentation, but this does not guarantee the robustness of the output when the input is rotated. At that, trained conventional CNNs may require test-time rotation augmentation to reach their full capability.

This study is focused on histopathology image analysis applications for which it is desirable that the arbitrary global orientation information of the imaged tissues is not captured by the machine learning models. The proposed framework is evaluated on three different histopathology image analysis tasks (mitosis

omparative analysis for each problem
when using the proposed framework.
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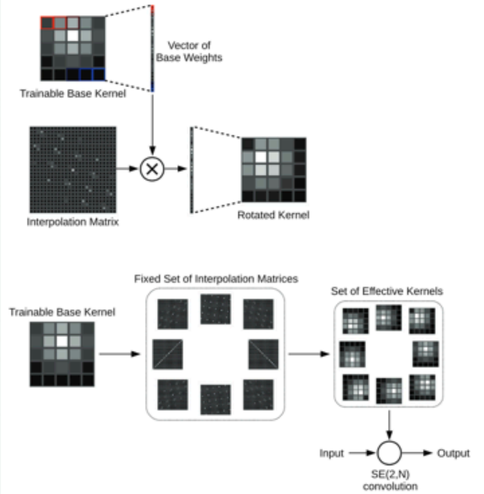

Fig. 2. Illustration of the process generating a rotated set of effective kernels from a trainable vector of base weights via the introduction of fixed interpolation matrix in the computational pipeline.

experiments that we used to analyze and validate them. In the construction of the G-CNNs we adhere to the following principle of group equivariant architecture design.

G-CNN design principle A sequence of layers starting with a lifting layer (Eq. (7)) and followed by one or more group convolution layers (Eq. (9)), possibly intertwined with point-wise nonlinearities, results in the encoding of roto-translation equivariant feature maps. If such a block is followed by a projection layer (Eq. (10)) then the entire block results in a encoding of features that is guaranteed to be rotationally invariant. Our implementation of the G-CNN layers is available at https://github.com/tueimage/se2cnn.

4.1. Applications and model architectures

For each task introduced in Section 3.1 we conducted two experiments: first, we trained a set of variations of a baseline CNN, by changing the orientation sampling level N of their $SE(2,N)$ layers, while keeping the total number of weights of each model approximately the same. Second, we trained each model with the reduced data regime counterparts of the training sets introduced in Section 3.1. For each task we opted for versions of straight-forward architectures with a low number of parameters that were in-line with methods reported in the literature. This way, we propose new G-CNN baselines that facilitate comparative experiments and that can be extended to more sophisticated architectures.

Mitosis detection We used the mitosis classification model orig-

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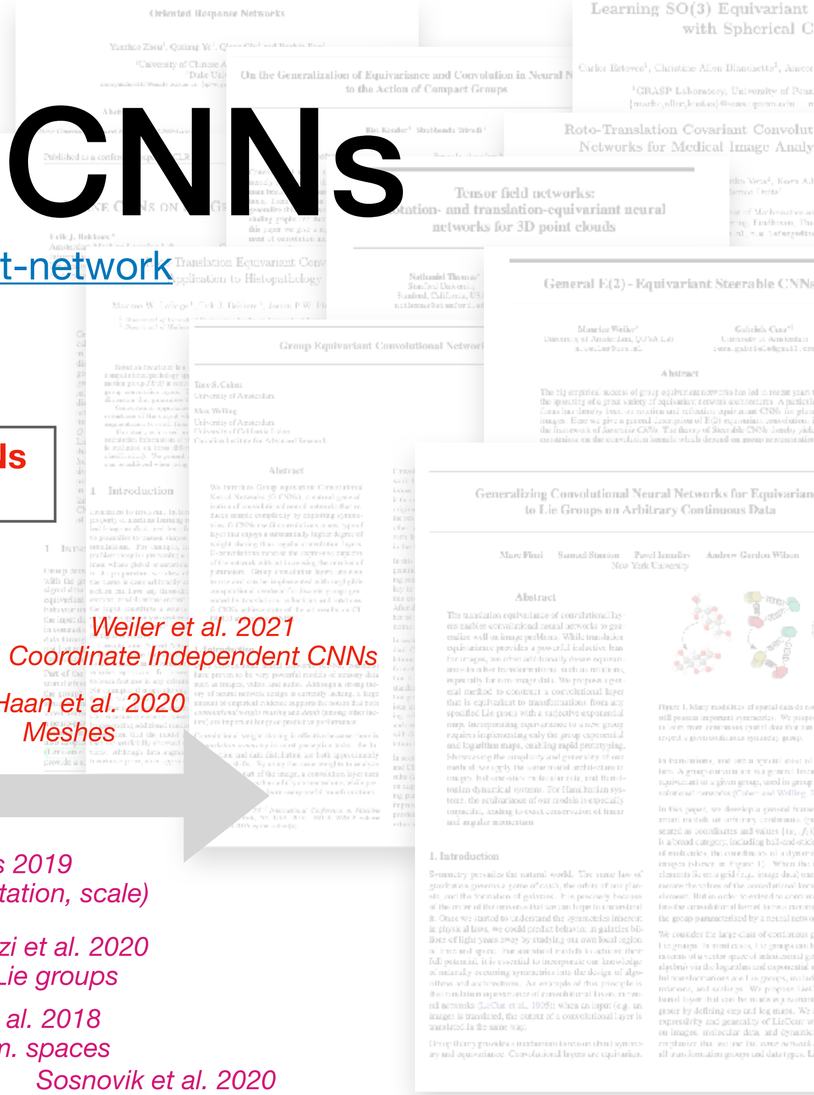

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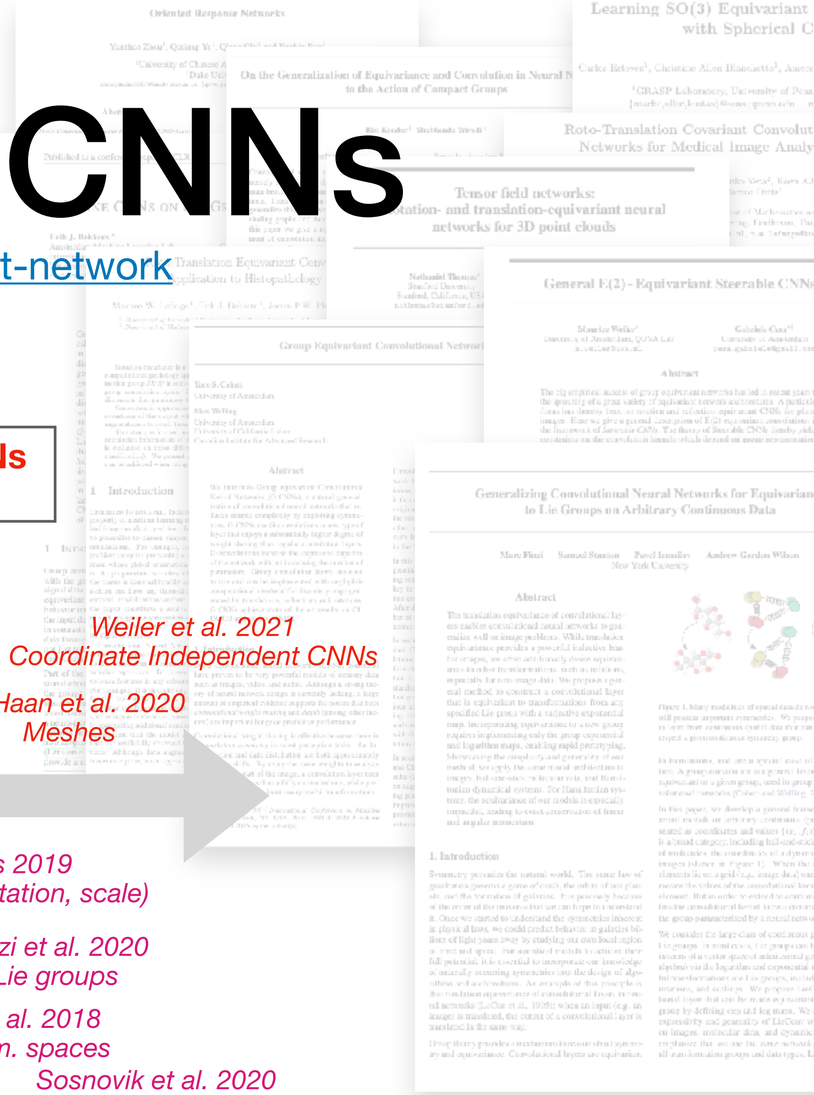

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Continuous G-CNNs
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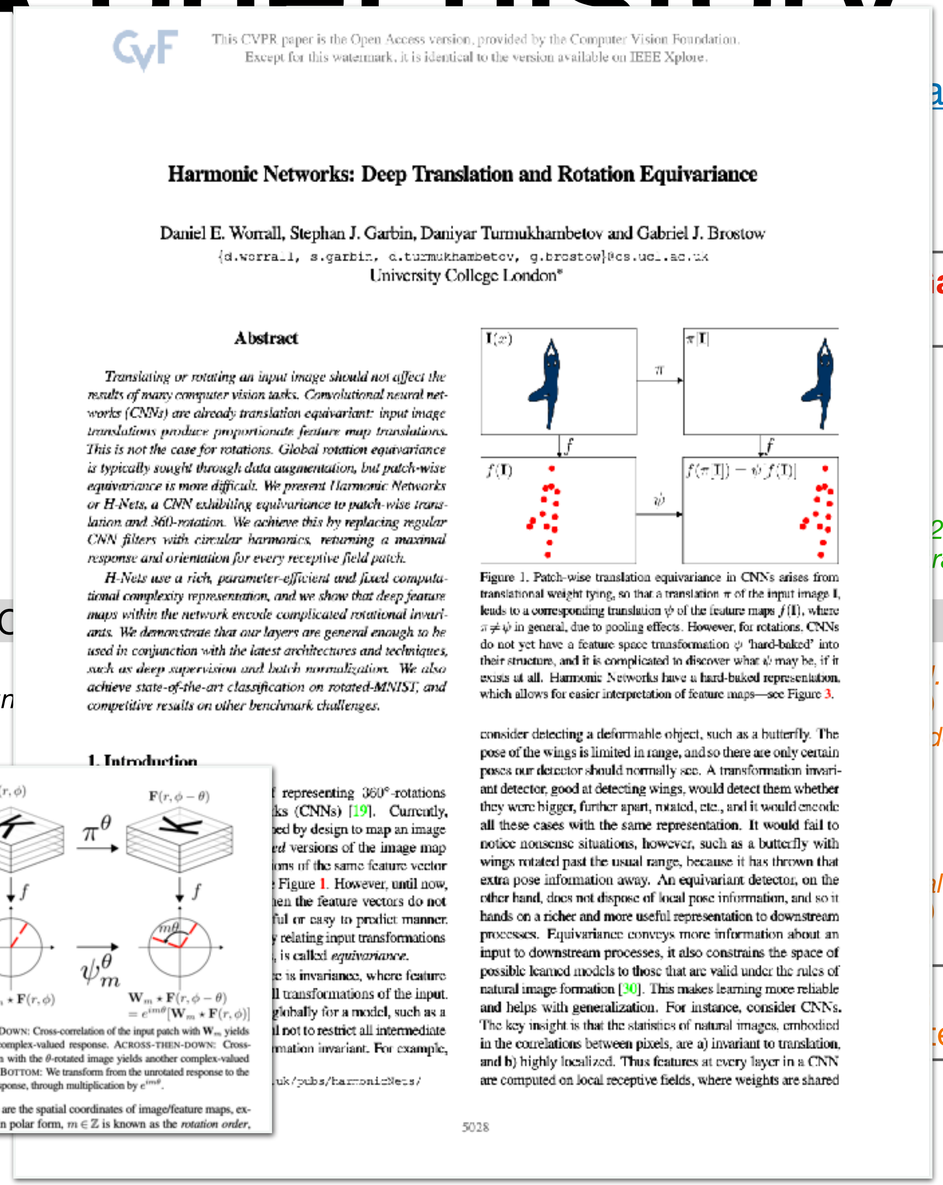
A brief history of G-CNNs

awesome-equivariant-network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Harmonic Networks: Deep Translation and Rotation Equivariance

Daniel E. Worrall, Stephan J. Garbin, Daniyar Turmukhambetov and Gabriel J. Brostow
{d.worrall, s.garbin, d.turmukhambetov, g.brostow}@cs.ucl.ac.uk
University College London*

Abstract

Translating or rotating an input image should not affect the results of many computer vision tasks. Convolutional neural networks (CNNs) are already translation equivariant: input image translations produce proportionate feature map translations. This is not the case for rotations. Global rotation equivariance is typically sought through data augmentation, but patch-wise equivariance is more difficult. We present Harmonic Networks or H-Nets, a CNN exhibiting equivariance to patch-wise translation and 360-rotation. We achieve this by replacing regular CNN filters with circular harmonics, returning a maximal response and orientation for every receptive field patch.

H-Nets use a rich, parameter-efficient and fixed computational complexity representation, and we show that deep feature maps within the network encode complicated rotational invariants. We demonstrate that our layers are general enough to be used in conjunction with the latest architectures and techniques, such as deep supervision and batch normalization. We also achieve state-of-the-art classification on rotated-MNIST, and competitive results on other benchmark challenges.

auge-equivariant CNNs
(manifolds)

Cohen et al. 2019
Icosahedron

Weiler et al. 2021
Coordinate Independent CNNs

de Haan et al. 2020
Meshes

2018
ransl.

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SE(2)

Sosnovik et al. 2020
Scale-translation

NNs

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rotation G-CNNs
eerable)

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Cesa-Lang-Weiler 2022
$G = \mathbb{R}^d \rtimes H$ with H compact

https://quva-lab.github.io/escnn/

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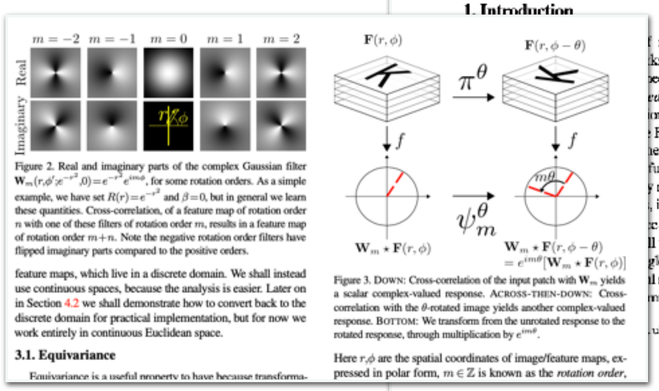

Figure 2. Real and imaginary parts of the complex Gaussian filter $\mathbf{W}_m(r,\phi|\sigma,\beta)=e^{-r^2}e^{im\phi}$, for some rotation orders. As a simple example, we have set $R(r)=e^{-r^2}$ and $\beta=0$, but in general we learn these quantities. Cross-correlation, of a feature map of rotation order n with one of these filters of rotation order m, results in a feature map of rotation order $m+n$. Note the negative rotation order filters have flipped imaginary parts compared to the positive orders.

feature maps, which live in a discrete domain. We shall instead use continuous spaces, because the analysis is easier. Later on in Section 4.2 we shall demonstrate how to convert back to the discrete domain for practical implementation, but for now we work entirely in continuous Euclidean space.

3.1. Equivariance

Equivariance is a useful property to have because transforma-

Figure 3. DOWN: Cross-correlation of the input patch with $\mathbf{W}_m$ yields a scalar complex-valued response. ACROSS-THEN-DOWN: Cross-correlation with the θ-rotated image yields another complex-valued response. BOTTOM: We transform from the unrotated response to the rotated response, through multiplication by $e^{im\theta}$.

Here r,ϕ are the spatial coordinates of image/feature maps, expressed in polar form, $m \in \mathbb{Z}$ is known as the *rotation order*,

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H-Nets use a rich, parameter-efficient and fixed computational complexity representation, and we show that deep feature maps within the network encode complicated rotational invariants. We demonstrate that our layers are general enough to be used in conjunction with the latest architectures and techniques, such as deep supervision and batch normalization. We also achieve state-of-the-art classification on rotated-MNIST, and competitive results on other benchmark challenges.

1. Introduction

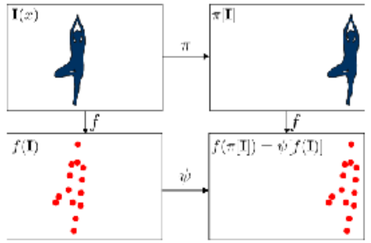

Figure 1. Patch-wise translation equivariance in CNNs arises from translational weight tying, so that a translation π of the input image $\mathbf{I}$, leads to a corresponding translation ψ of the feature maps $f(\mathbf{I})$, where $\pi \neq \psi$ in general, due to pooling effects. However, for rotations, CNNs do not yet have a feature space transformation ψ 'hard-baked' into their structure, and it is complicated to discover what ψ may be, if it exists at all. Harmonic Networks have a hard-baked representation, which allows for easier interpretation of feature maps—see Figure 3.

representing 360°-rotations
ks (CNNs) [19]. Currently,
ed by design to map an image
rd versions of the image map
ions of the same feature vector
Figure 1. However, until now,
hen the feature vectors do not
ful or easy to predict manner.
relating input transformations
, is called *equivariance*.
e is invariance, where feature
ll transformations of the input.
globally for a model, such as a
ll not to restrict all intermediate
rmation invariant. For example,

uk/pubs/harmonicNets/

consider detecting a deformable object, such as a butterfly. The pose of the wings is limited in range, and so there are only certain poses our detector should normally see. A transformation invariant detector, good at detecting wings, would detect them whether they were bigger, further apart, rotated, etc., and it would encode all these cases with the same representation. It would fail to notice nonsense situations, however, such as a butterfly with wings rotated past the usual range, because it has thrown that extra pose information away. An equivariant detector, on the other hand, does not dispose of local pose information, and so it hands on a richer and more useful representation to downstream processes. Equivariance conveys more information about an input to downstream processes, it also constrains the space of possible learned models to those that are valid under the rules of natural image formation [30]. This makes learning more reliable and helps with generalization. For instance, consider CNNs. The key insight is that the statistics of natural images, embodied in the correlations between pixels, are a) invariant to translation, and b) highly localized. Thus features at every layer in a CNN are computed on local receptive fields, where weights are shared

3D Steerable CNNs: Learning Rotationally Equivariant Features in Volumetric Data

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Abstract

We present a convolutional network that is equivariant to rigid body motions. The model uses scalar, vector, and tensor fields over 3D Euclidean space to represent data, and equivariant convolutions to map between such representations. These SE(3)-equivariant convolutions utilize kernels which are parameterized as a linear combination of a complete steerable kernel basis, which is derived analytically in this paper. We prove that equivariant convolutions are the most general equivariant linear maps between fields over $\mathbb{R}^3$. Our experimental results confirm the effectiveness of 3D Steerable CNNs for the problem of amino acid propensity prediction and protein structure classification, both of which have inherent SE(3) symmetry.

1 Introduction

Increasingly, machine learning techniques are being applied in the natural sciences. Many problems in this domain, such as the analysis of protein structure, exhibit exact or approximate symmetries. It has long been understood that the equations that define a model or natural law should respect the symmetries of the system under study, and that knowledge of symmetries provides a powerful constraint on the space of admissible models. Indeed, in theoretical physics, this idea is enshrined as a fundamental principle, known as Einstein's principle of general covariance. Machine learning, which is, like physics, concerned with the induction of predictive models, is no different: our models must respect known symmetries in order to produce physically meaningful results.

A lot of recent work, reviewed in Sec. 2, has focused on the problem of developing equivariant networks, which respect some known symmetry. In this paper, we develop the theory of SE(3)-equivariant networks. This is far from trivial, because SE(3) is both non-commutative and non-compact. Nevertheless, at run-time, all that is required to make a 3D convolution equivariant using our method, is to parameterize the convolution kernel as a linear combination of pre-computed steerable basis kernels. Hence, the 3D Steerable CNN incorporates equivariance to symmetry transformations without deviating far from current engineering best practices.

The architectures presented here fall within the framework of Steerable G-CNNs [8, 10, 40, 45], which represent their input as fields over a homogeneous space ($\mathbb{R}^3$ in this case), and use steerable

* Equal Contribution. MG initiated the project, derived the kernel space constraint, wrote the first network implementation and ran the Shrec17 experiment. MW solved the kernel constraint analytically, designed the anti-aliased kernel sampling in discrete space and coded / run many of the CATH experiments.
Source code is available at https://github.com/mariogeiger/se3cnn

32nd Conference on Neural Information Processing Systems (NeurIPS 2018), Montréal, Canada.

https://quva-lab.github.io/escnn/

Published as a conference paper at ICLR 2022

A Program to Build E(n)-Equivariant Steerable CNNs

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Leon Lang
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Maurice Weiler
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m.weiler.ml@gmail.com

Abstract

Equivariance is becoming an increasingly popular design choice to build data efficient neural networks by exploiting prior knowledge about the symmetries of the problem at hand. Euclidean steerable CNNs are one of the most common classes of equivariant networks. While the constraints these architectures need to satisfy are understood, existing approaches are tailored to specific (classes of) groups. No generally applicable method that is *practical* for implementation has been described so far. In this work, we generalize the Wigner-Eckart theorem proposed in Lang & Weiler (2020), which characterizes general G-steerable kernel spaces for compact groups G over their homogeneous spaces, to arbitrary G-spaces. This enables us to directly parameterize filters in terms of a band-limited basis on the whole space rather than on G's orbits, but also to easily implement steerable CNNs equivariant to a large number of groups. To demonstrate its generality, we instantiate our method on a variety of isometry groups acting on the Euclidean space $\mathbb{R}^3$. Our framework allows us to build E(3) and SE(3)-steerable CNNs like previous works, but also CNNs with arbitrary $G \leq \mathrm{O}(3)$-steerable kernels. For example, we build 3D CNNs equivariant to the symmetries of platonic solids or choose $G = \mathrm{SO}(2)$ when working with 3D data having only azimuthal symmetries. We compare these models on 3D shapes and molecular datasets, observing improved performance by matching the model's symmetries to the ones of the data.

1 Introduction

In machine learning, it is common for learning tasks to present a number of *symmetries*. A symmetry in the data occurs, for example, when some property (e.g., the label) does not change if a set of transformations is applied to the data itself, e.g. translations or rotations of images. Symmetries are algebraically described by *groups*. If prior knowledge about the symmetries of a task is available, it is usually beneficial to encode them in the models used (Shawe-Taylor, 1989; Cohen & Welling, 2016a). The property of such models is referred to as *equivariance* and is obtained by introducing some *equivariance constraints* in the architecture (see Eq. 2). A classical example are convolutional neural networks (CNNs), which achieve translation equivariance by constraining linear layers to be convolution operators. A wider class of equivariant models are Euclidean steerable CNNs (Cohen & Welling, 2016b; Weiler et al., 2018a; Weiler & Cesa, 2019; Jenner & Weiler, 2022), which guarantee equivariance to isometries $\mathbb{R}^n \rtimes G$ of a Euclidean space $\mathbb{R}^n$, i.e., to translations and a group G of origin-preserving transformations, such as rotations and reflections. As proven in Weiler et al. (2018a; 2021); Jenner & Weiler (2022), this requires convolutions with *G-steerable* (equivariant) kernels.

Our goal is developing a program to parameterize with minimal requirements arbitrary G-steerable kernel spaces, with compact G, which are required to implement $\mathbb{R}^n \rtimes G$ equivariant CNNs. Lang & Weiler (2020) provides a first step in this direction by generalizing the *Wigner-Eckart theorem* from quantum mechanics to obtain a general technique to parametrize G-steerable kernel spaces over *orbits* of a compact G. The theorem reduces the task of building steerable kernel bases to that of finding some pure representation theoretic ingredients. Since the equivariance constraint only relates points $g.x \in \mathbb{R}^n$ in the same *orbit* $G.x \subset \mathbb{R}^n$, a kernel can take independent values on different orbits. Fig. 1 shows

*Qualcomm AI Research is an initiative of Qualcomm Technologies, Inc.

README.md

General E(2)-Equivariant Steerable CNNs

Documentation | Experiments | Paper | Thesis

e2cnn is a PyTorch extension for equivariant deep learning.

Equivariant neural networks guarantee a specified transformation behavior of their feature spaces under transformations of their input. For instance, classical convolutional neural networks (*CNNs*) are by design equivariant to translations of their input. This means that a translation of an image leads to a corresponding translation of the network's feature maps. This package provides implementations of neural network modules which are equivariant under all *isometries* E(2) of the image plane $\mathbb{R}^2$, that is, under *translations*, *rotations* and *reflections*. In contrast to conventional CNNs, E(2)-equivariant models are guaranteed to generalize over such transformations, and are therefore more data efficient.

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Getting Started

e2cnn is easy to use since it provides a high level user interface which abstracts most intricacies of group and representation theory away. The following code snippet shows how to perform an equivariant convolution from an RGB-image to 10 *regular* feature fields (corresponding to a group convolution).

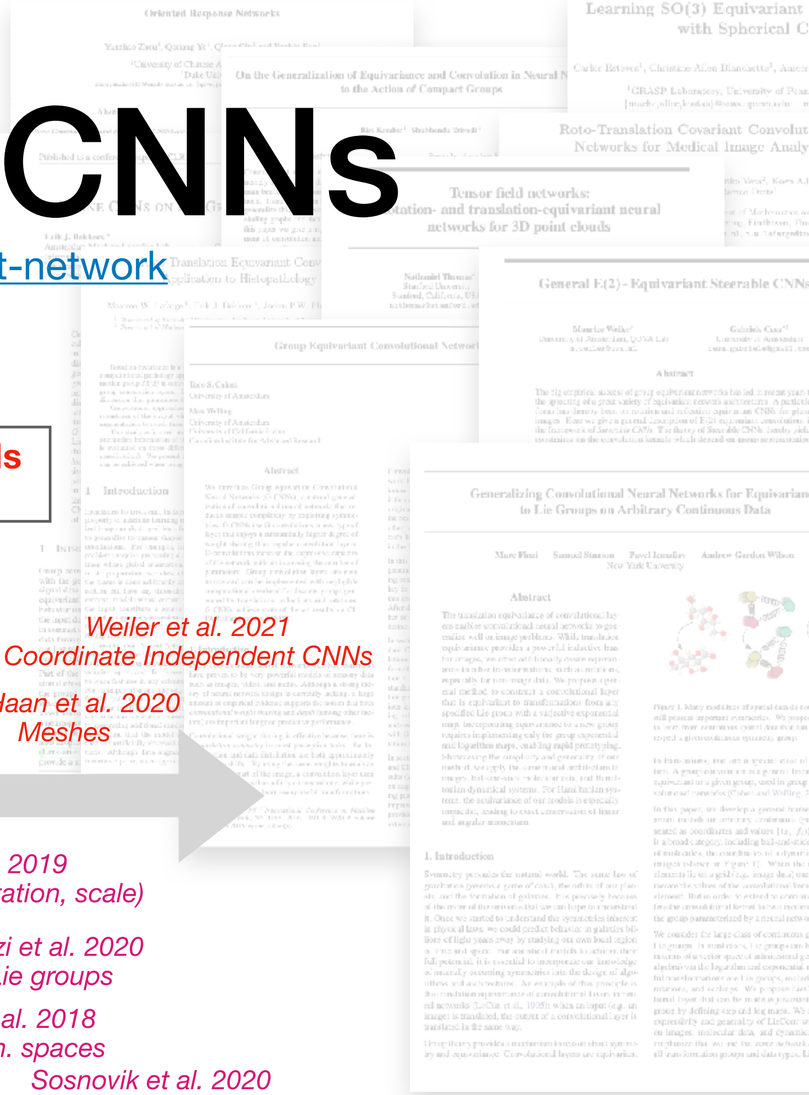
```
from e2cnn import gspaces                                  #  1
from e2cnn import nn                                       #  2
import torch                                               #  3
                                                           #  4
r2_act = gspaces.Rot2dOnR2(N=8)                            #  5
feat_type_in  = nn.FieldType(r2_act,  3*[r2_act.trivial_repr])   #  6
feat_type_out = nn.FieldType(r2_act, 10*[r2_act.regular_repr])   #  7
                                                           #  8
conv = nn.R2Conv(feat_type_in, feat_type_out, kernel_size=5)     #  9
relu = nn.ReLU(feat_type_out)                              # 10
                                                           # 11
x = torch.randn(16, 3, 32, 32)                             # 12
x = nn.GeometricTensor(x, feat_type_in)                    # 13
                                                           # 14
y = relu(conv(x))                                          # 15
```

Line 5 specifies the symmetry group action on the image plane $\mathbb{R}^2$ under which the network should be equivariant. We choose the *cyclic group* C_8, which describes discrete rotations by multiples of $2\pi/8$. Line 6 specifies the input feature field types. The three color channels of an RGB image are thereby to be identified as three independent scalar fields, which transform under the *trivial representation* of C_8. Similarly, the output feature space is in line 7

https://quva-lab.github.io/escnn/

A brief history of G-CNNs

https://github.com/Chen-Cai-OSU/awesome-equivariant-network



Discrete G-CNNs
(square/cube symmetries)

Gauge-equivariant CNNs
(manifolds)

NNs → CNNs → G-CNNs

LeCun et al. 1990

Cohen-Welling 2016
p4m

Dieleman et al. 2016
p4m

Winkels-Cohen 2018
3D discrete roto-transl.

Hoogeboom et al. 2018
SE(2,6)

Worrall-Brostow 2018
3D discrete roto-transl.

Cohen et al. 2019
Icosahedron

Weiler et al. 2021
Coordinate Independent CNNs

de Haan et al. 2020
Meshes

Mallat et al. 2013, 2015
SE(2)

Bekkers et al. 2014-2018
SE(2)

Weiler et al. 2017
SE(2)

Zhou et al. 2017
SE(2)

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SE(2)

Esteves 2017
SO(3)

Kondor 2018
SE(3)

Cohen et al. 2018
SE(3)

Kondor-Trivedi 2018
SE(3)

Weiler et al. 2018
SE(3)

Thomas et al. 2018
SE(3)

Weiler-Cesa 2019
SE(2)

Bekkers 2019
Lie groups (rotation, scale)

Finzi et al. 2020
Lie groups

Chakraborty et al. 2018
Riemannian Hom. spaces

Sosnovik et al. 2020
Scale-translation

Continuous rotation G-CNNs
(regular discretizations)

Continuous rotation G-CNNs
(steerable)

Continuous G-CNNs
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Cesa-Lang-Weiler 2022
$G = \mathbb{R}^d \rtimes H$ with H compact

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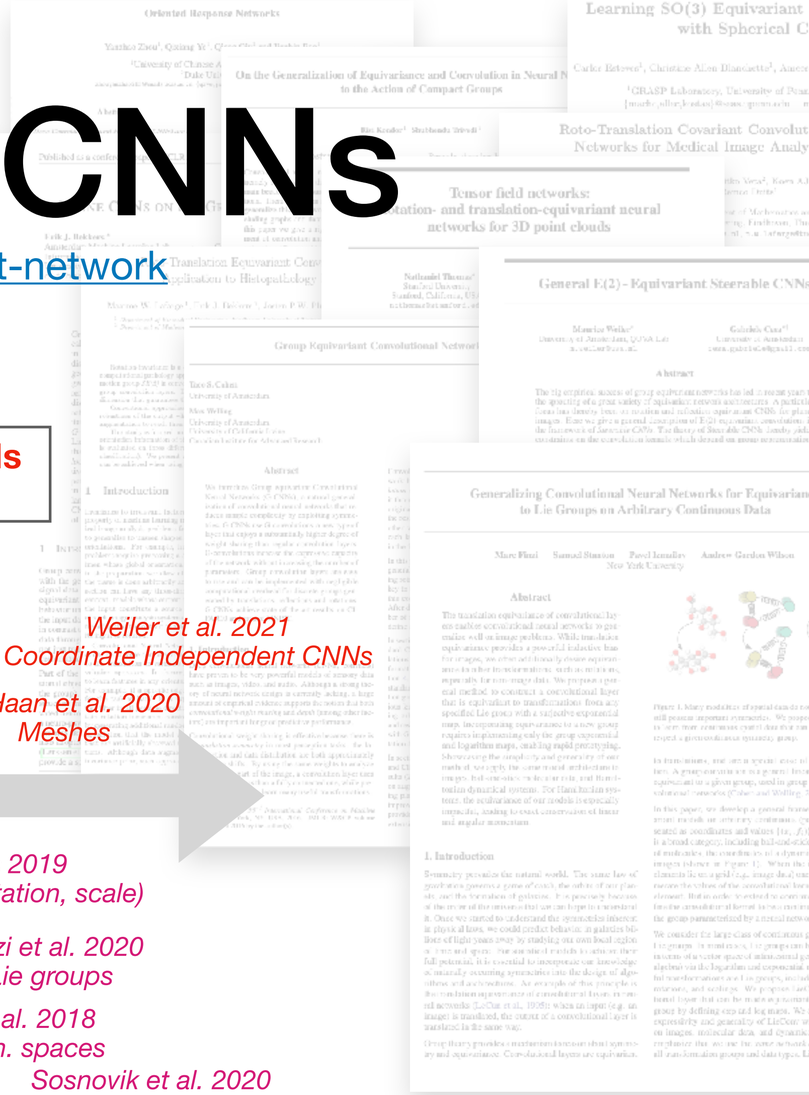

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Published as a conference paper at ICLR 2020

B-SPLINE CNNS ON LIE GROUPS

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ABSTRACT

Group convolutional neural networks (G-CNNs) can be used to improve classical CNNs by equipping them with the geometric structure of groups. Central in the success of G-CNNs is the lifting of feature maps to higher dimensional disentangled representations in which data characteristics are effectively learned, geometric data-augmentations are made obsolete, and predictable behavior under geometric transformations (equivariance) is guaranteed via group theory. Currently, however, the practical implementations of G-CNNs are limited to either discrete groups (that leave the grid intact) or continuous compact groups such as rotations (that enable the use of Fourier theory). In this paper we lift these limitations and propose a modular framework for the design and implementation of *G-CNNs for arbitrary Lie groups*. In our approach the differential structure of Lie groups is used to expand convolution kernels in a generic basis of B-splines that is defined on the Lie algebra. This leads to a flexible framework that enables *localized, atrous, and deformable convolutions* in G-CNNs by means of respectively *localized, sparse* and *non-uniform B-spline* expansions. The impact and potential of our approach is studied on two benchmark datasets: cancer detection in histopathology slides in which rotation equivariance plays a key role and facial landmark localization in which scale equivariance is important. In both cases, G-CNN architectures outperform their classical 2D counterparts and the added value of atrous and localized group convolutions is studied in detail.

1 INTRODUCTION

Group convolutional neural networks (G-CNNs) are a class of neural networks that are equipped with the geometry of groups. This enables them to profit from the structure and symmetries in signal data such as images (Cohen & Welling, 2016). A key feature of G-CNNs is that they are equivariant with respect to transformations described by the group, i.e., they guarantee predictable behavior under such transformations and are insensitive to both local and global transformations on the input data. Classical CNNs are a special case of G-CNNs that are equivariant to translations and, in contrast to unconstrained NNs, they make advantage of (and preserve) the basic structure of signal data throughout the network (LeCun et al., 1990). By considering larger groups (i.e. considering not just translation equivariance) additional geometric structure can be utilized in order to improve performance and data efficiency (see G-CNN literature in Sec. 2).

Part of the success of G-CNNs can be attributed to the lifting of feature maps to higher dimensional objects that are generated by matching kernels under a range of poses (transformations in the group). This leads to a disentanglement with respect to the pose and together with the group structure this enables a flexible way of learning high level representations in terms of low-level activated neurons observed in specific configurations, which we conceptually illustrate in Fig. 1. From a neuro-psychological viewpoint, this resembles a hierarchical composition from low- to high-level features akin to the recognition-by-components model by Biederman (1987), a viewpoint which is also adopted in work on capsule networks (Hinton et al., 2011; Sabour et al., 2017). In particular in (Lenssen et al., 2018) the group theoretical connection is made explicit with equivariant capsules that provide a sparse index/value representation of feature maps on groups (Gens & Domingos, 2014).

1

arXiv:1909.12057v4 [cs.LG] 22 Mar 2021

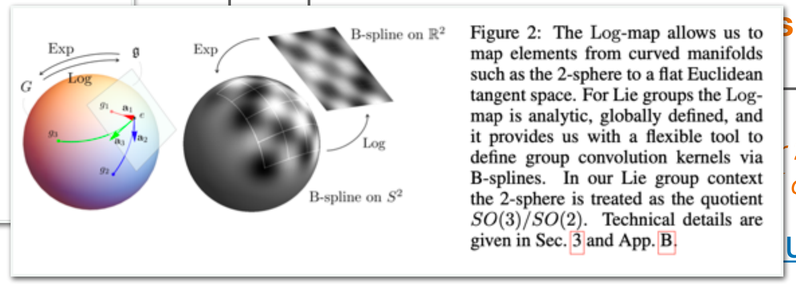

Figure 2: The Log-map allows us to map elements from curved manifolds such as the 2-sphere to a flat Euclidean tangent space. For Lie groups the Log-map is analytic, globally defined, and it provides us with a flexible tool to define group convolution kernels via B-splines. In our Lie group context the 2-sphere is treated as the quotient $SO(3)/SO(2)$. Technical details are given in Sec. 3 and App. B.

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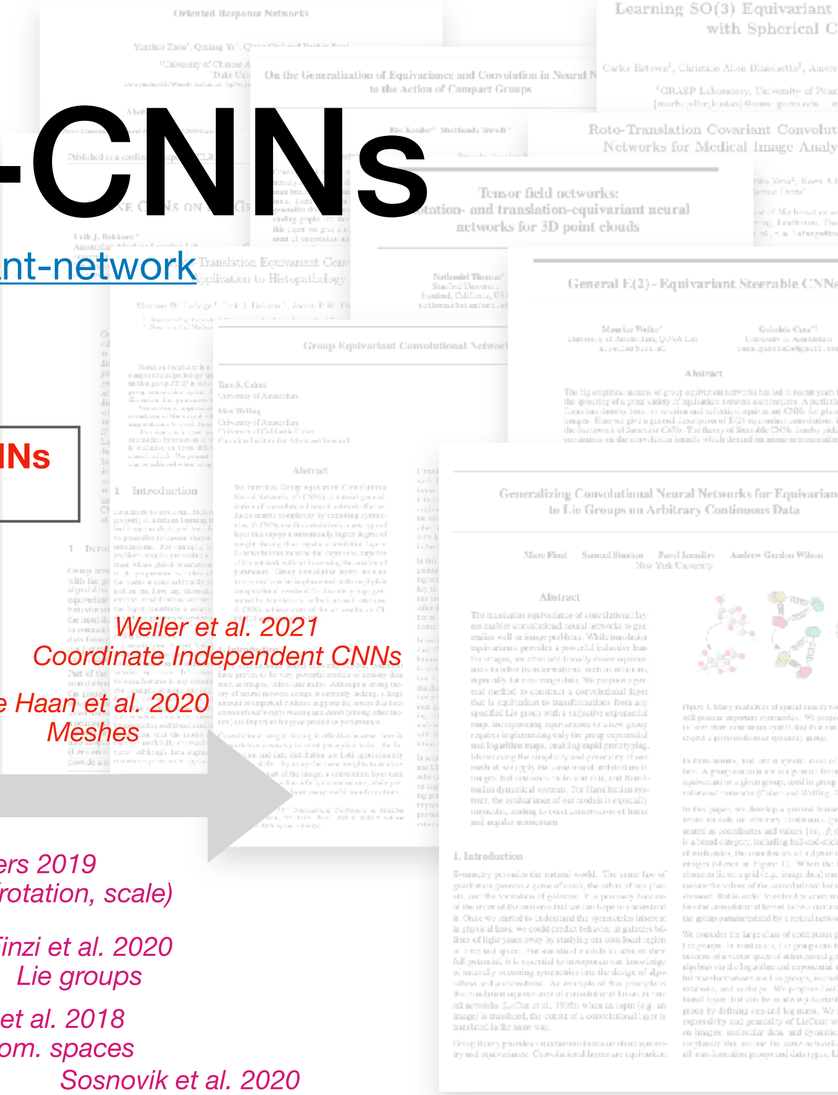

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$G = \mathbb{R}^d \rtimes H$ with H compact

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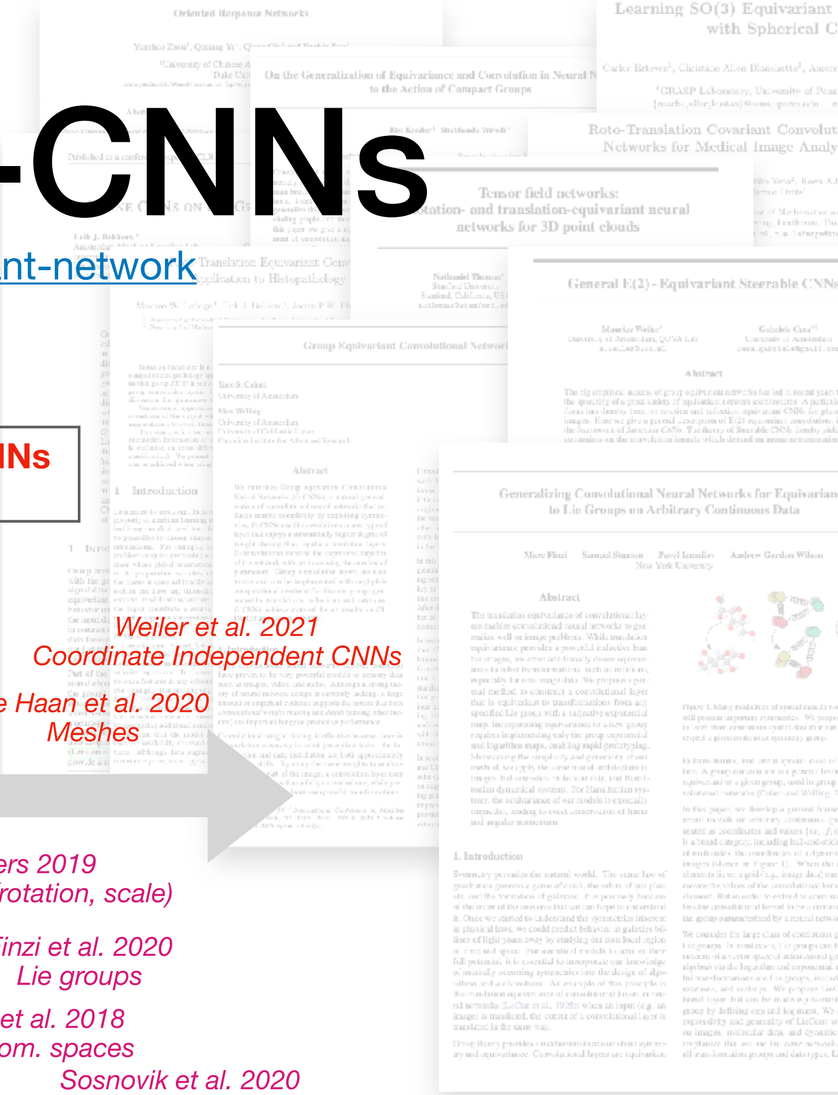

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Coordinate Independent Convolutional Networks

Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds

Maurice Weiler
University of Amsterdam
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Patrick Forré
University of Amsterdam
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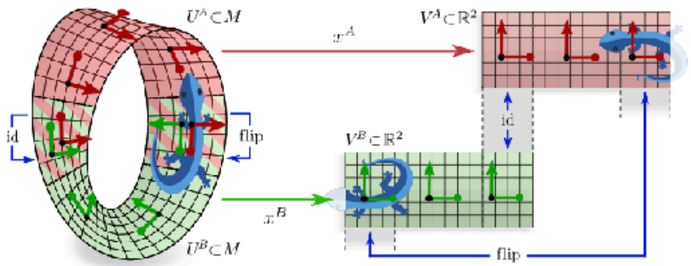
Erik Verlinde
University of Amsterdam
e.p.verlinde@uva.nl

Max Welling
University of Amsterdam,
Qualcomm AI Research
m.welling@uva.nl

Abstract

Motivated by the vast success of deep convolutional networks, there is a great interest in generalizing convolutions to non-Euclidean manifolds. A major complication in comparison to flat spaces is that it is unclear in which alignment a convolution kernel should be applied on a manifold. The underlying reason for this ambiguity is that general manifolds do not come with a canonical choice of reference frames (gauge). Kernels and features therefore have to be expressed relative to *arbitrary coordinates*. We argue that the particular choice of coordinatization should not affect a network's inference – it should be *coordinate independent*. A simultaneous demand for coordinate independence and weight sharing is shown to result in a requirement on the network to be *equivariant under local gauge transformations* (changes of local reference frames). The ambiguity of reference frames depends thereby on the *G-structure* of the manifold, such that the necessary level of gauge equivariance is prescribed by the corresponding *structure group* G. Coordinate independent convolutions are proven to be equivariant w.r.t. those *isometries* that are symmetries of the G-structure. The resulting theory is formulated in a coordinate free fashion in terms of fiber bundles. To exemplify the design of coordinate independent convolutions, we implement a convolutional network on the Möbius strip. The generality of our differential geometric formulation of convolutional networks is demonstrated by an extensive literature review which explains a large number of Euclidean CNNs, spherical CNNs and CNNs on general surfaces as specific instances of coordinate independent convolutions.



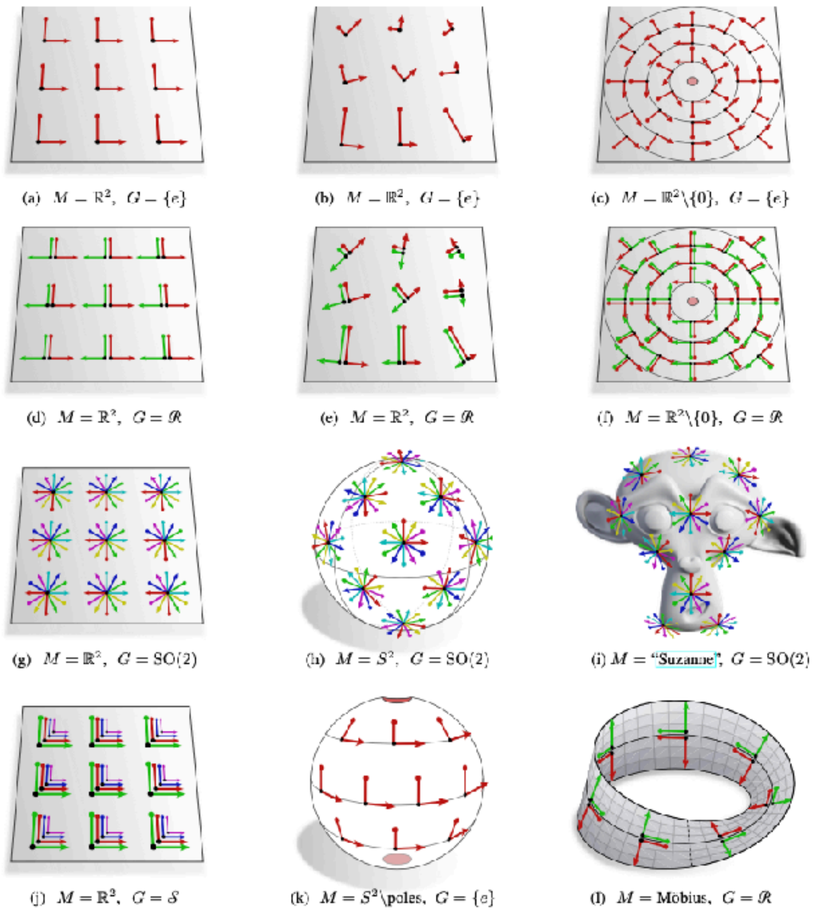


Figure 5: Exemplary G-structures GM for different structure groups G and on different manifolds M. The structure group G signals which values gauge transformations can take, and therefore how "big" the subset of distinguished frames at each point p is. Fig. 5a shows the canonical $\{e\}$-structure (frame field) of $\mathbb{R}^2$, which corresponds to conventional Euclidean CNNs. The G-structures in Figs. 5d, 5g and 5j are constructed by adding reflected ($G = \mathcal{R}$), rotated ($G = \mathrm{SO}(2)$) and scaled ($G = \mathcal{S}$) frames, respectively. The corresponding GM-convolutions are not only translation equivariant but equivariant under the action of affine groups $\mathrm{Aff}(G)$. G structures are usually not unique. Figs. 5b and 5e show alternative G structures on $\mathbb{R}^2$ (corresponding to an alternative metric relative to which their frames are orthonormal). They might not be practically relevant but demonstrate the flexibility of our framework. The $\{e\}$-structure in Fig. 5c corresponds to polar coordinates. As G-structures are required to be continuous, we removed the origin 0 where polar coordinates are singular. One can once again define an $\mathcal{R}$-structure by adding reflected frames as shown in Fig. 5f. These G structures model convolutions on $\mathbb{R}^2 \backslash \{0\}$ which are $\mathrm{SO}(2)$ and $\mathrm{O}(2)$ equivariant but not translation equivariant. Fig. 5h shows the usual $\mathrm{SO}(2)$-structure on the embedded 2-sphere S^2, which is underlying $\mathrm{SO}(3)$-equivariant spherical CNNs. Another popular choice is the $\{e\}$-structure in Fig. 5k, which is induced by spherical coordinates. Note that this $\{e\}$-structure would be singular at the poles, which are therefore cut out. Continuous (i.e. non-singular) reductions of the structure group beyond $\mathrm{SO}(2)$ are on the sphere topologically obstructed. G steerable kernels with $G \geq \mathrm{SO}(2)$ are therefore strictly necessary for continuous convolutions on topological spheres like the mesh in Fig. 5i. Fig. 5l shows an $\mathcal{R}$-structure on the Möbius strip. As the Möbius strip is non-orientable, it does not admit a continuous reduction of the structure group beyond the reflection group $G = \mathcal{R}$.

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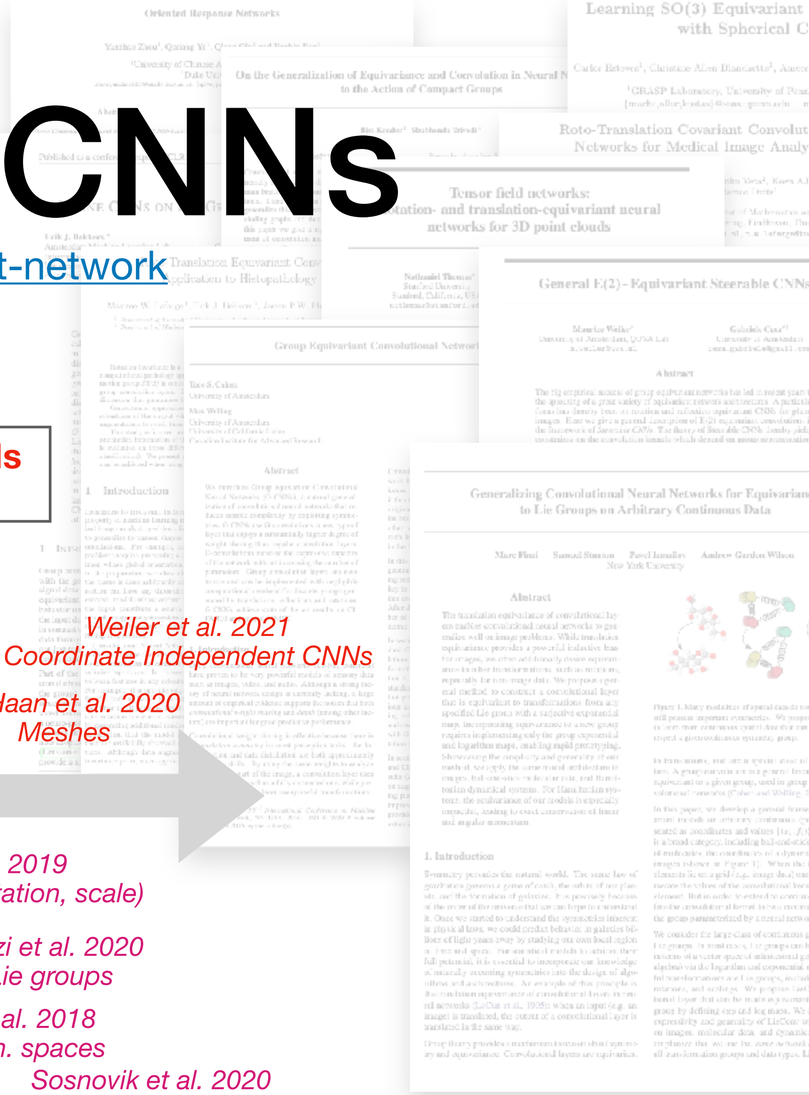

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"Inductive bias"

Reduce the search space for NNs

to only the sensible ones!

2022
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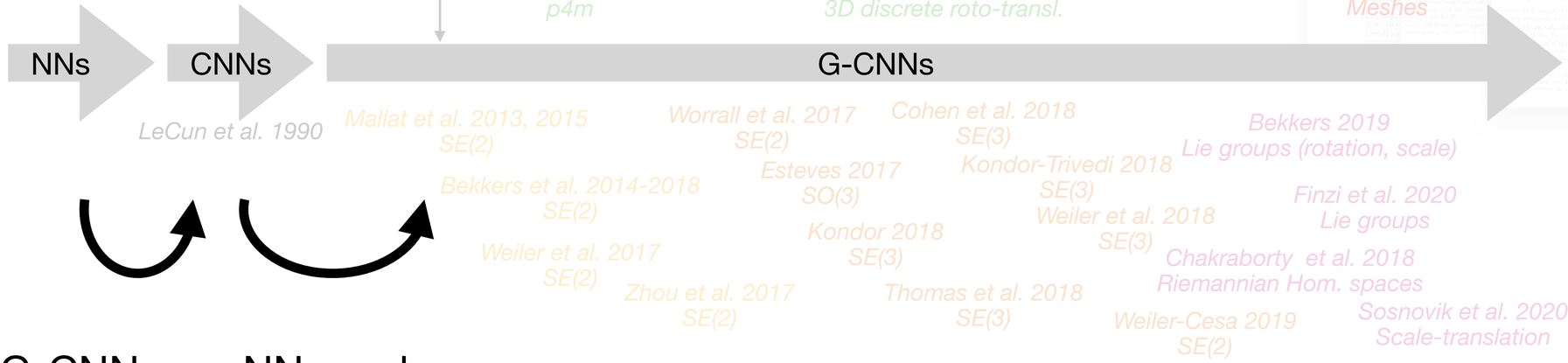
Up next:
A linear map is equivariant
if and only if it is a group convolution



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UNIVERSITY OF AMSTERDAM

AMLAB Amsterdam Machine Learning Lab

Group Equivariant Deep Learning

Lecture 1 - Regular group convolutions

Lecture 1.6 - Group Theory | Homogeneous/quotient spaces

Preliminaries for "group convolutions are all you need"

Transitive action, homogeneous space, quotient space, examples

Erik Bekkers, Amsterdam Machine Learning Lab, University of Amsterdam

This mini-course serves as a module with the UvA Master AI course Deep Learning 2 https://uvadl2c.github.io/

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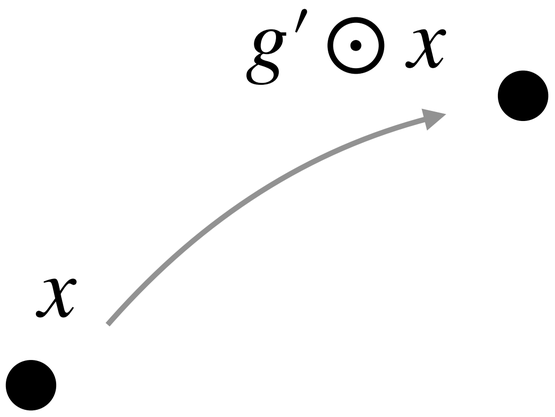
$$\forall_{g,g' \in G, x \in X} : \; g \odot (g' \odot x) = (gg') \odot x$$



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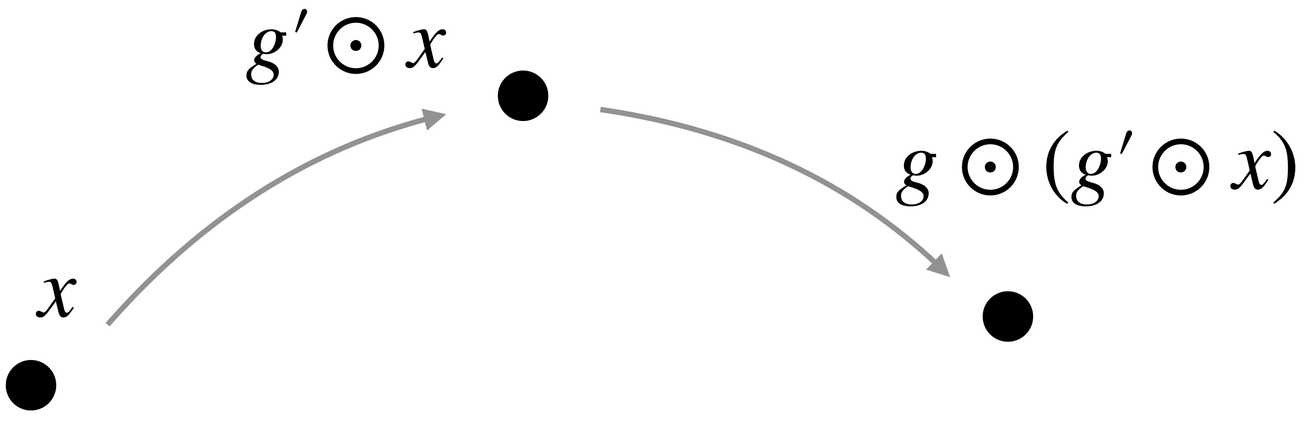

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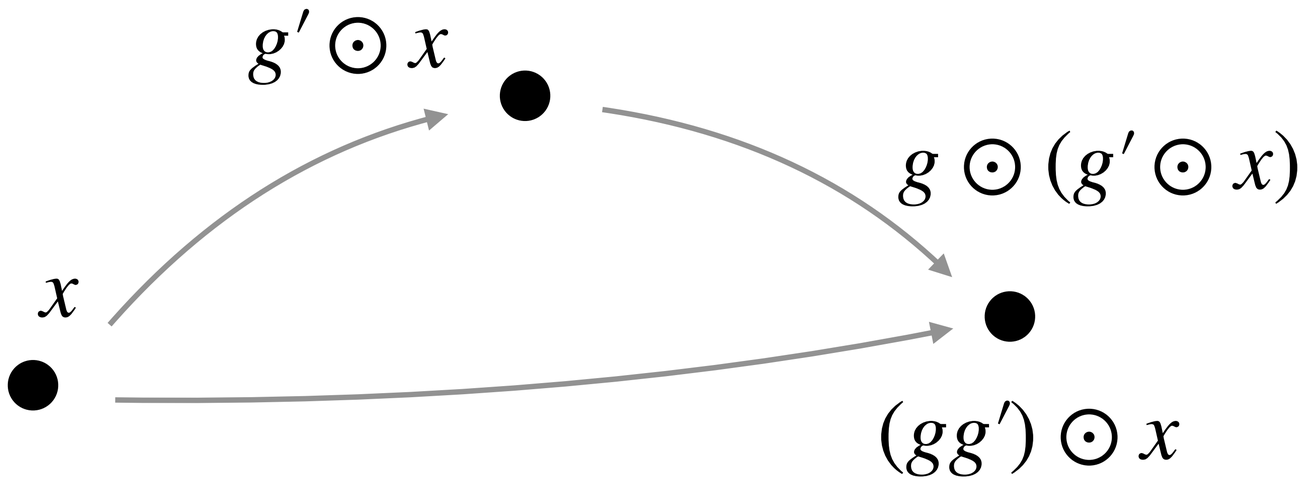

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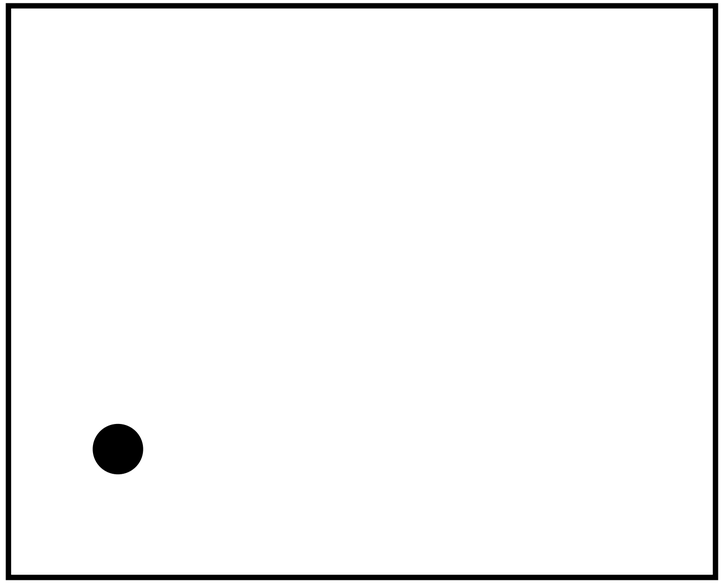

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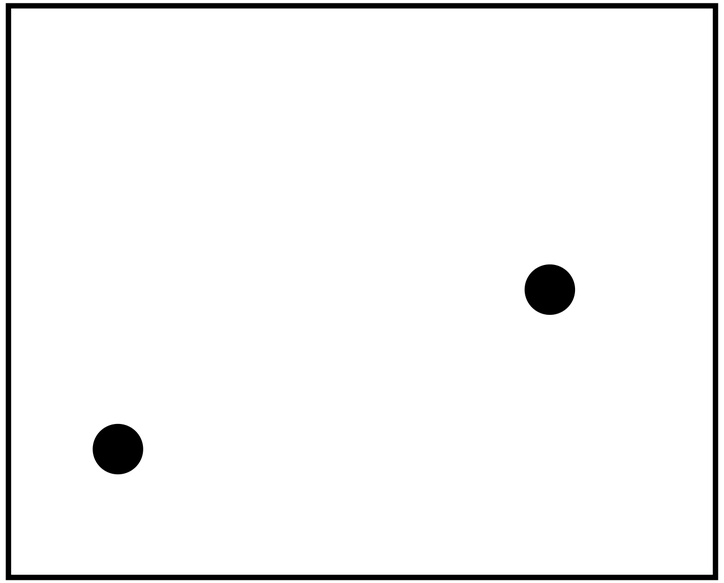

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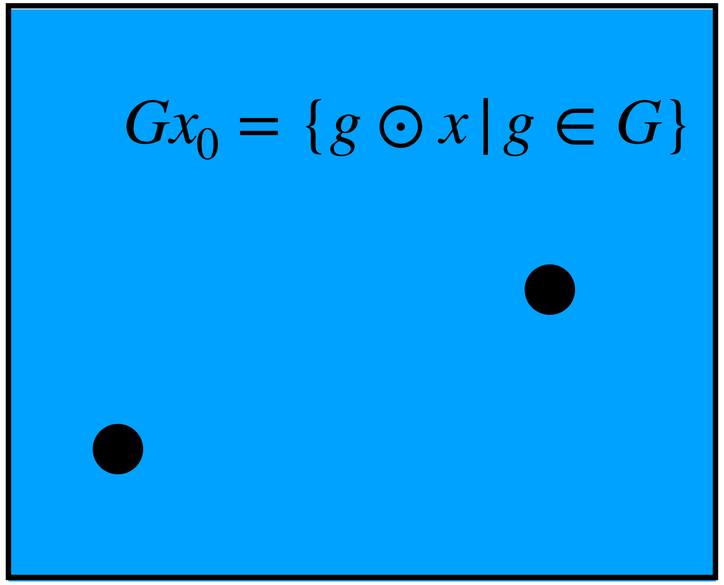

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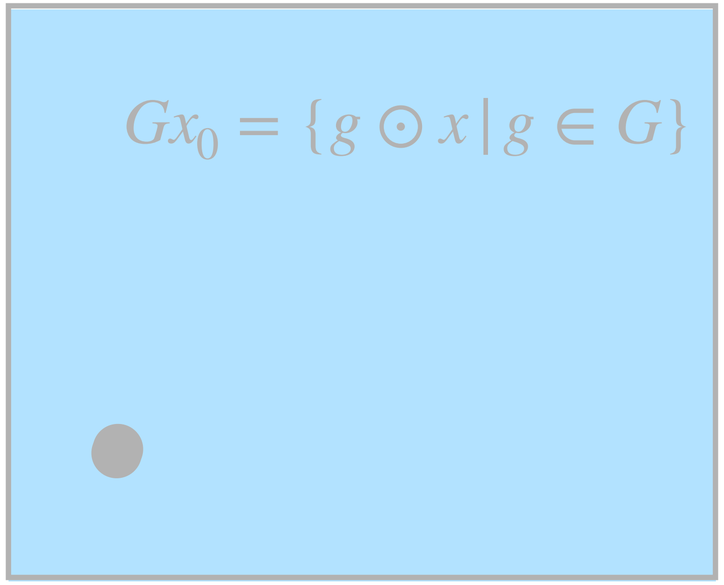

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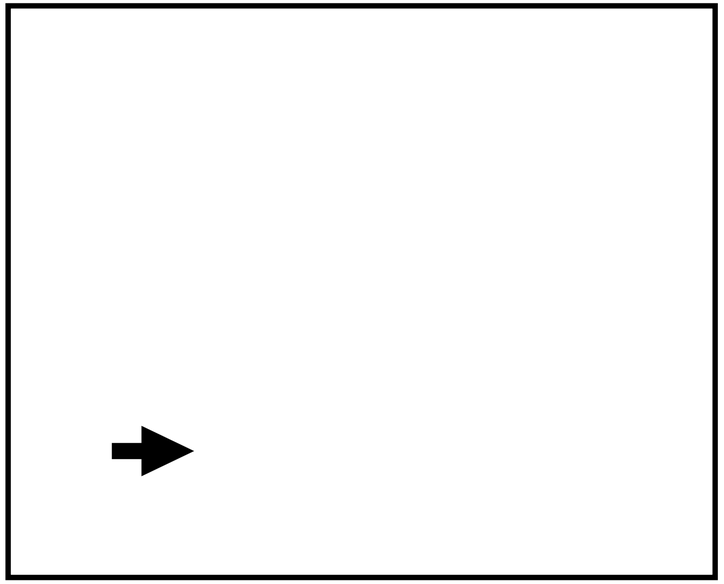

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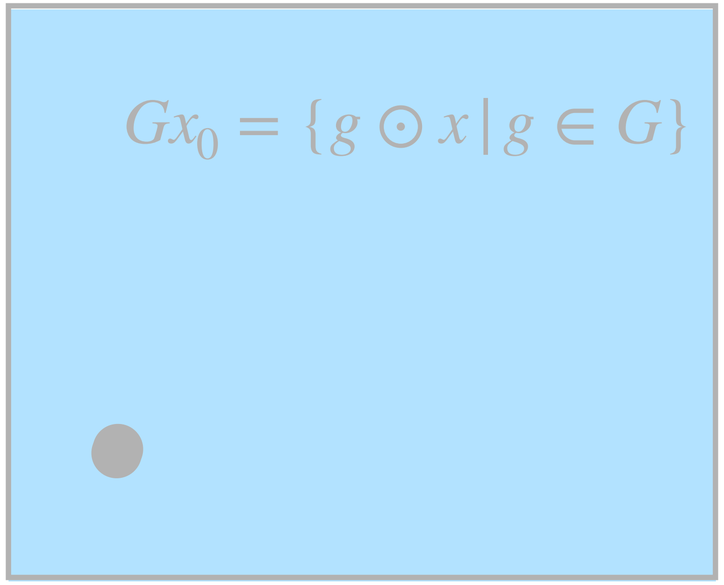

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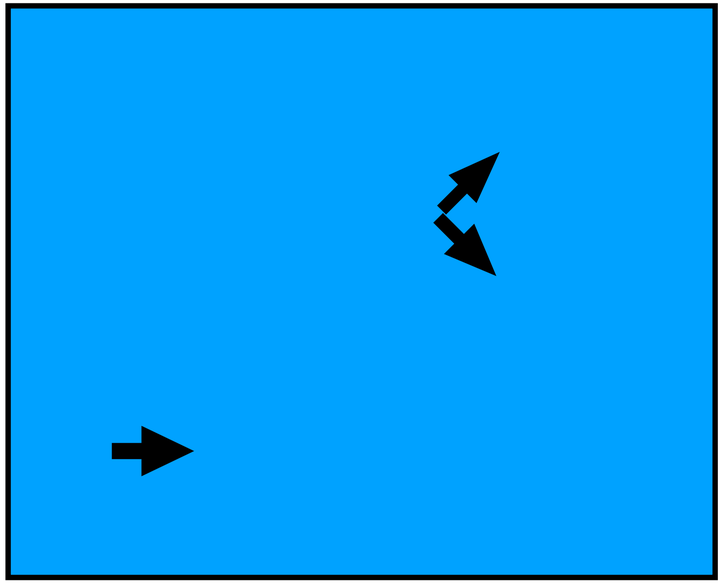

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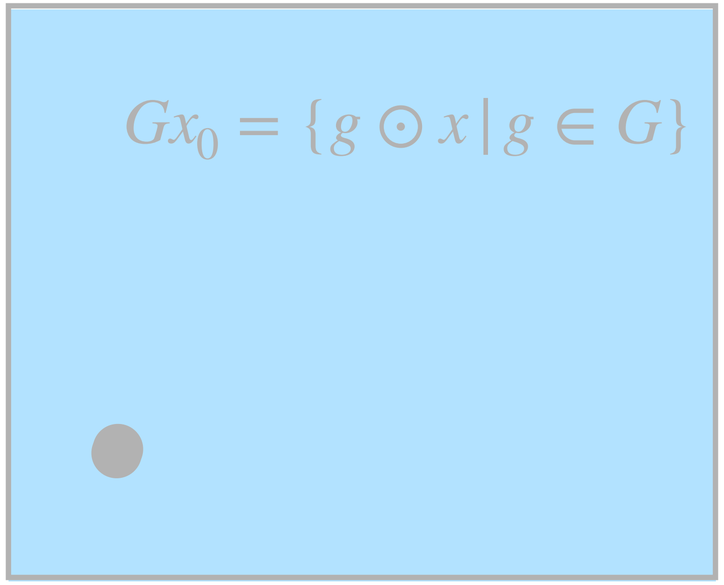

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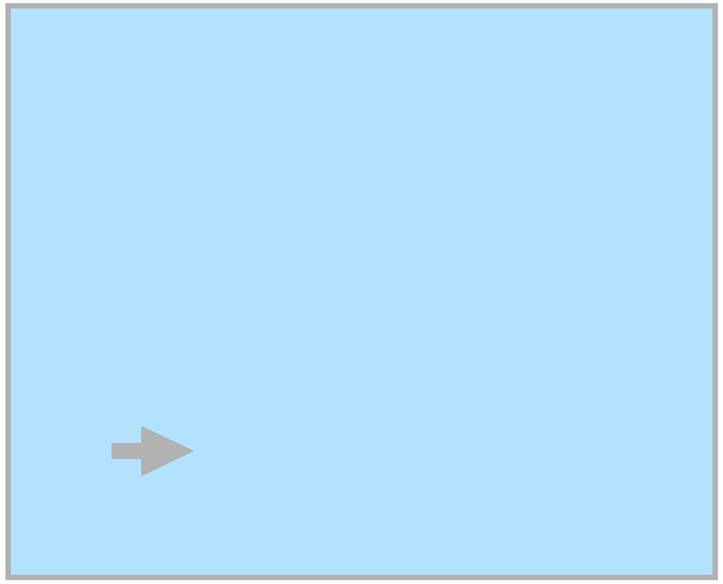

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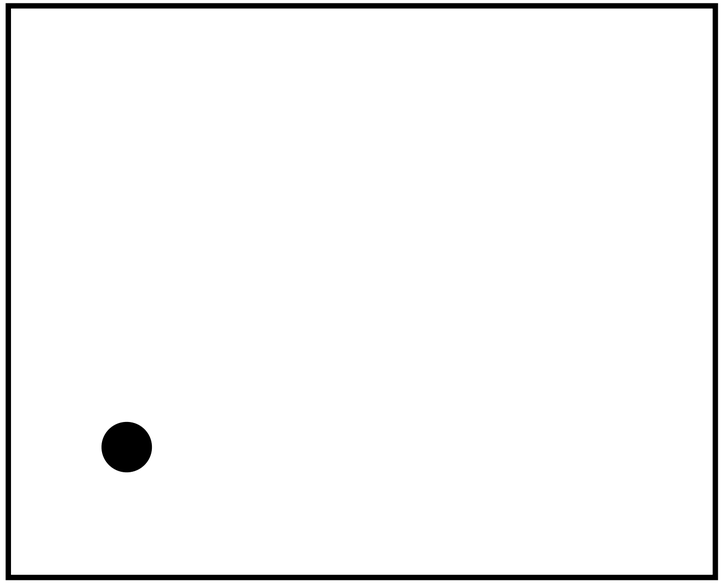

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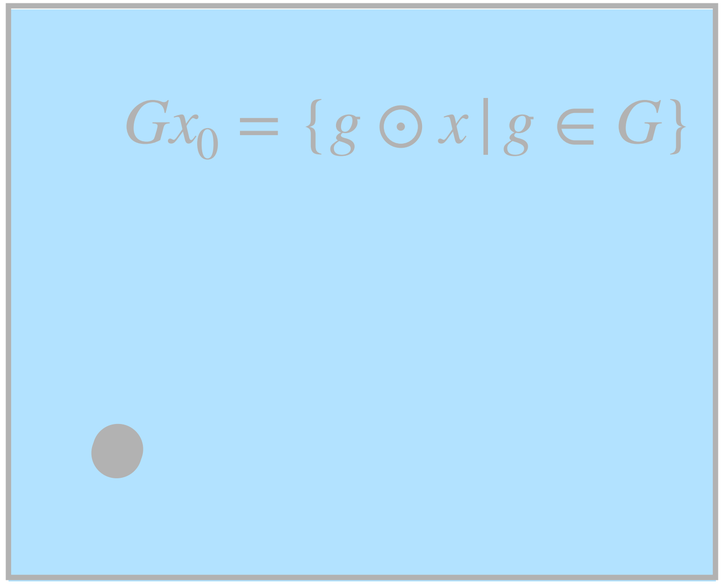

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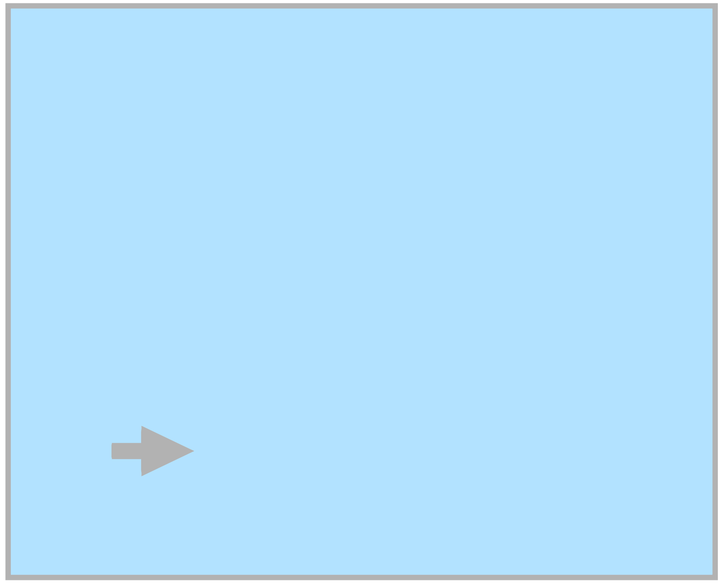

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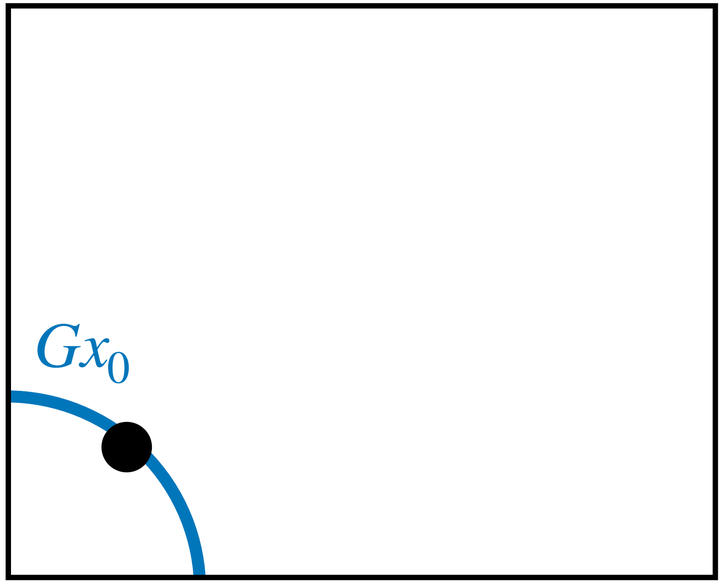

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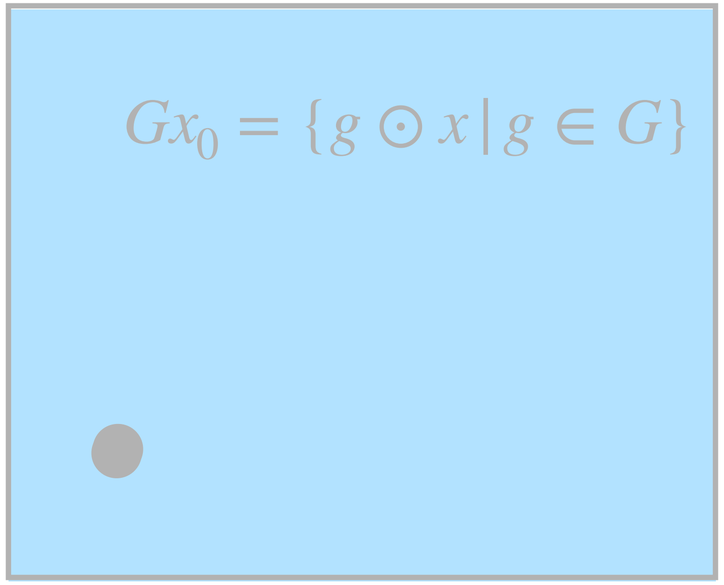

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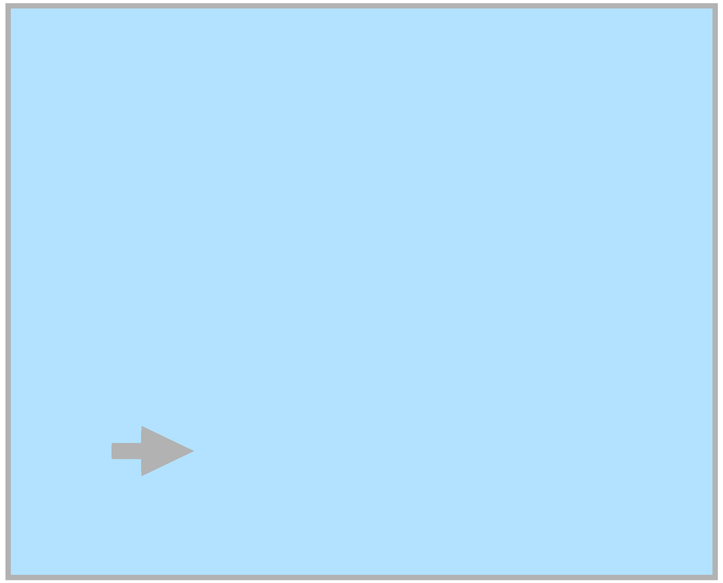

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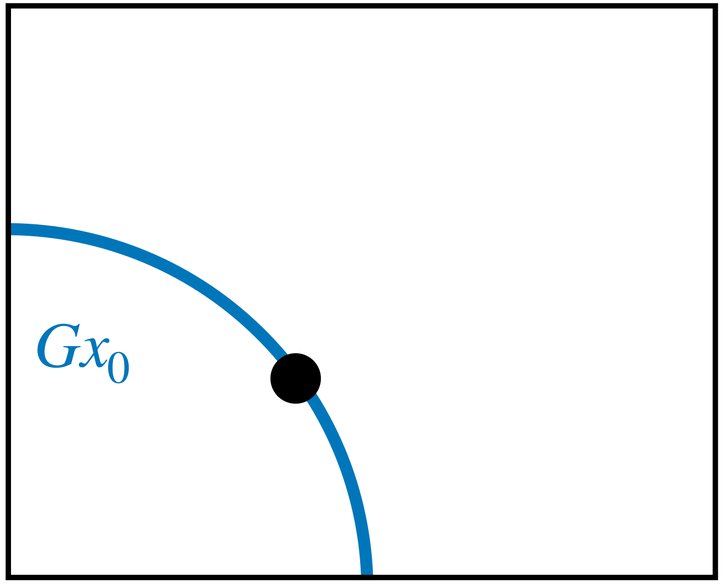

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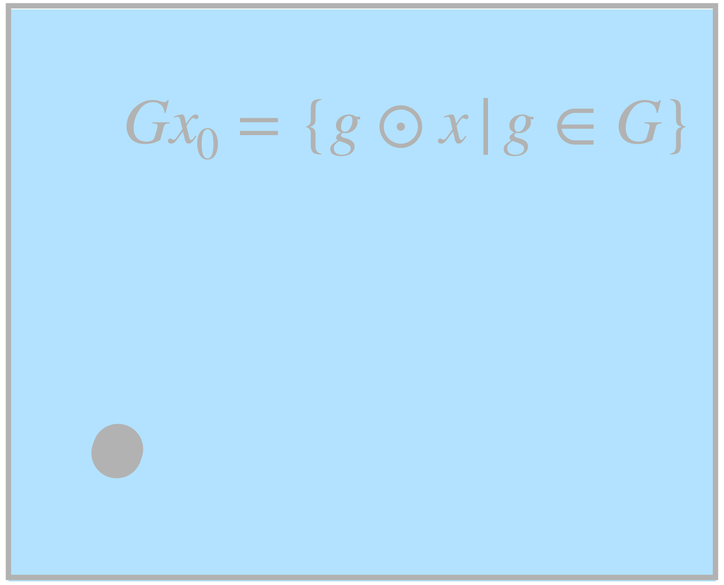

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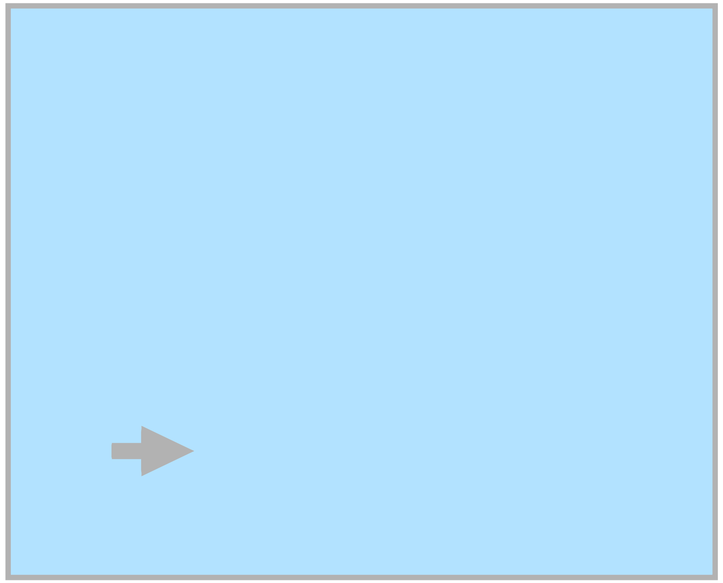
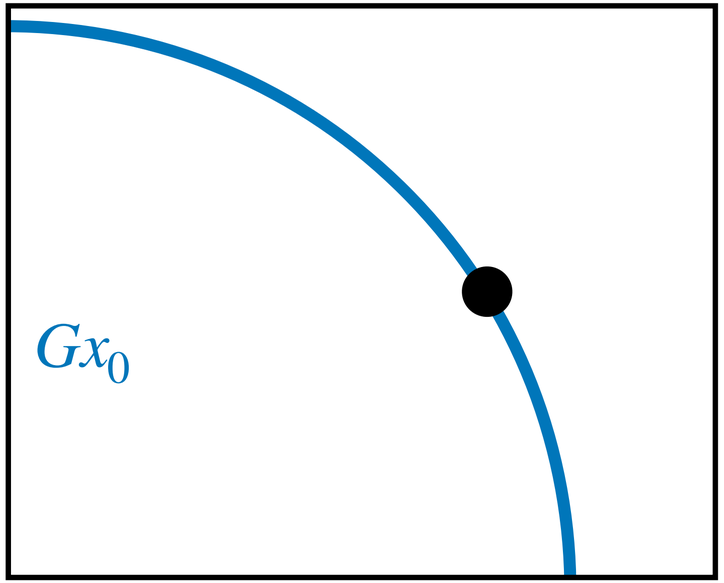


SO(2) does not …



Homogeneous space

Homogeneous space: A space X on which G acts transitively.

This is important as then we can guarantee that every part of the signal can be "seen" (probed by the convolution kernel)

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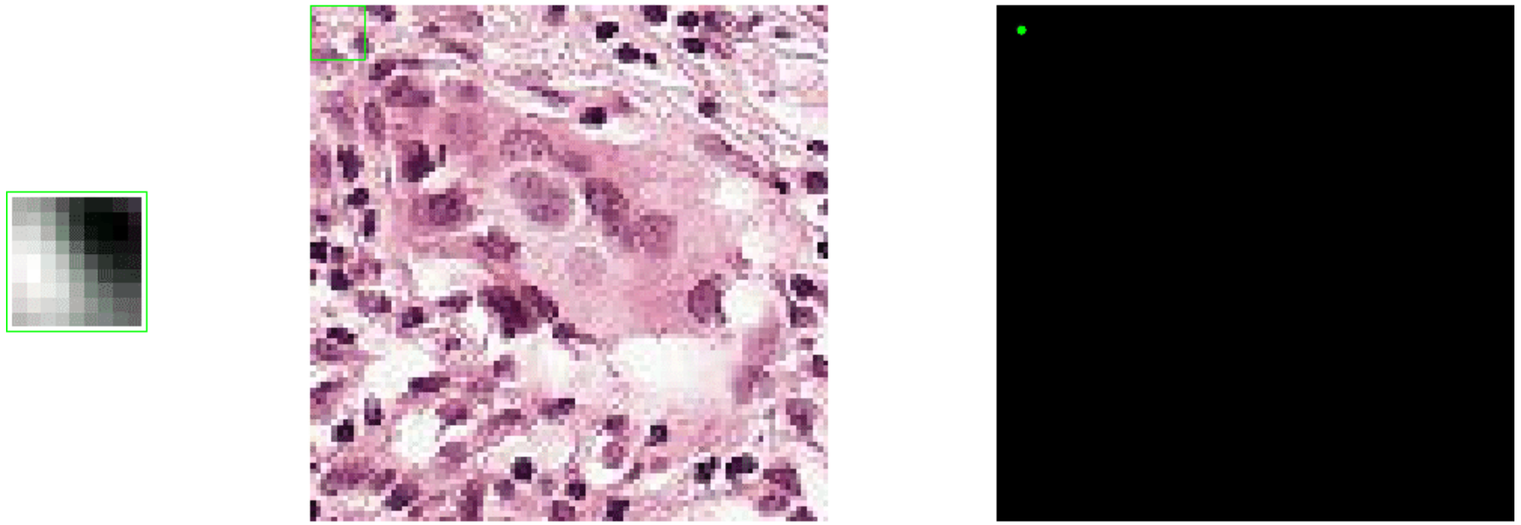


Homogeneous space: the sphere S^2

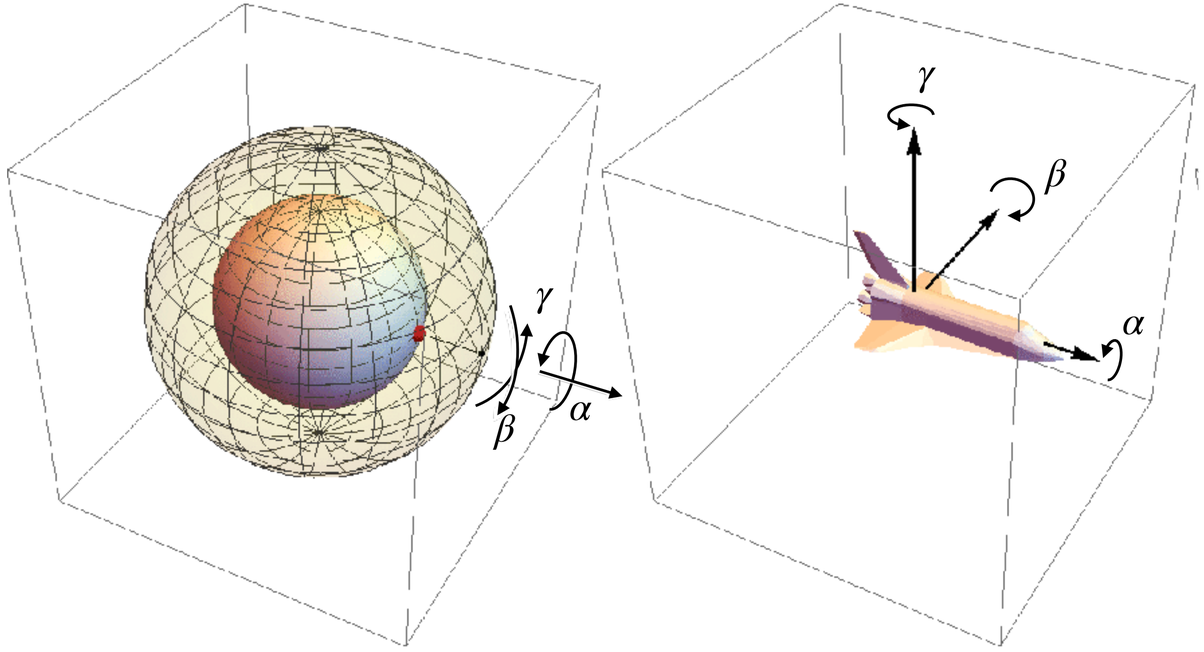
The sphere S^2 is a homogeneous space of 3D rotations $SO(3)$

The 3D rotation group $SO(3)$

Representation in parameter space (XYZ-Euler angles)

Rotation by $R \in SO(3)$

$$R = R_{e_z,\gamma} R_{e_y,\beta} R_{e_x,\alpha}$$



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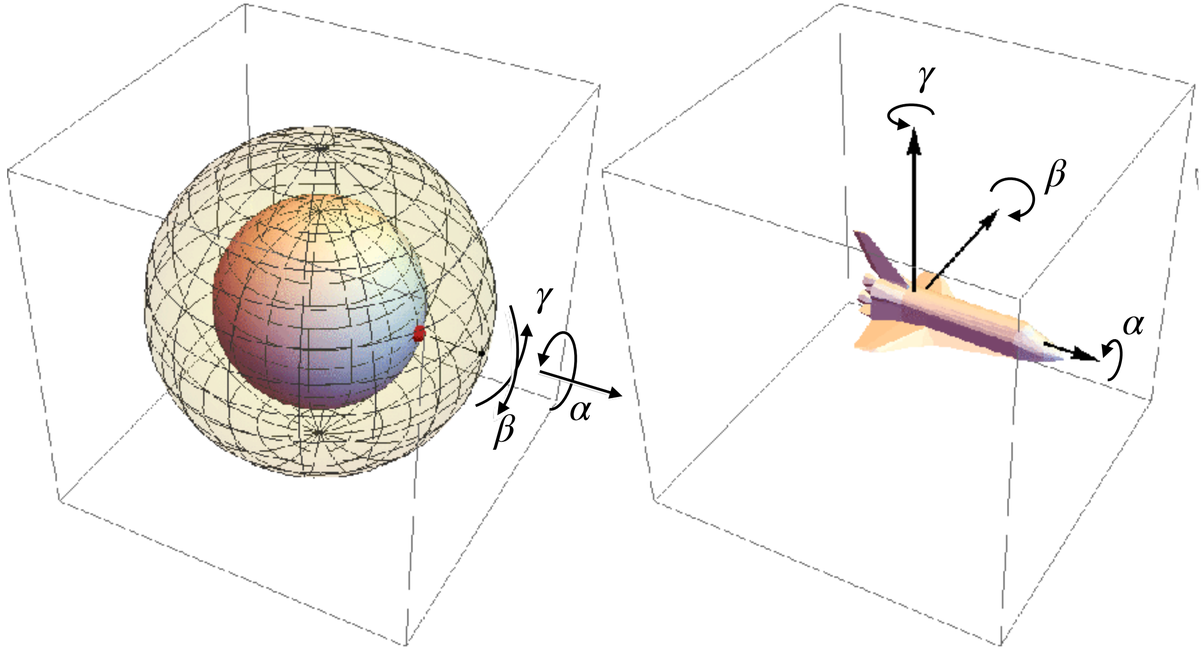

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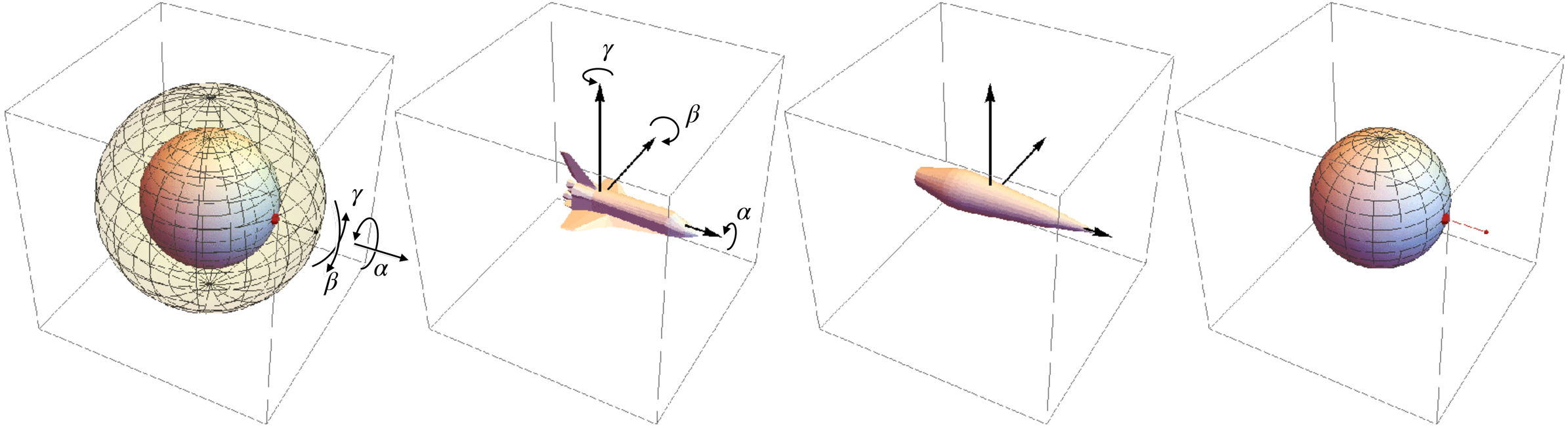
The 2-sphere as a quotient space

Representation in parameter space (XYZ-Euler angles)

Rotation by $R \in SO(3)$

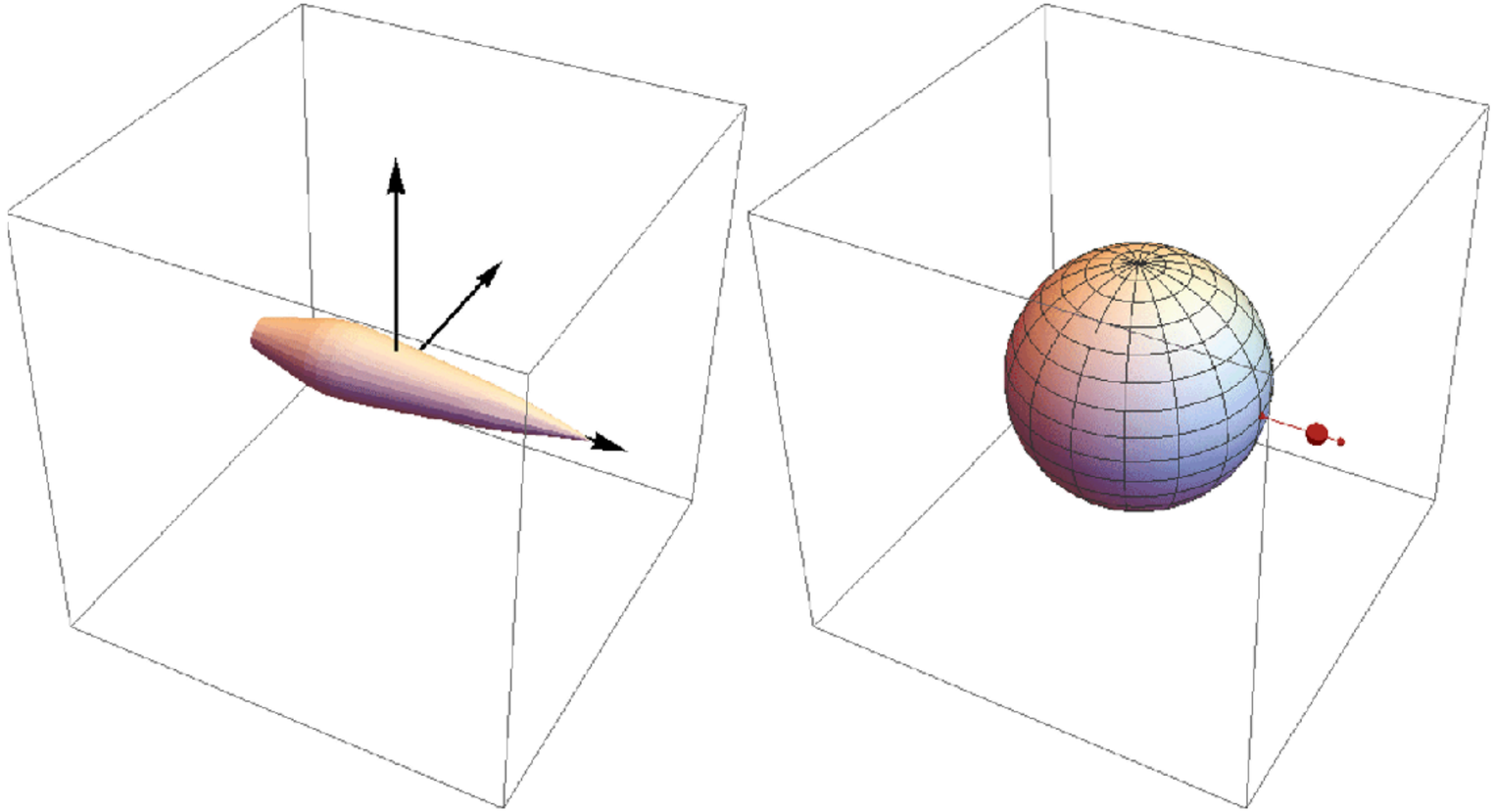
$R = R_{e_z,\gamma} R_{e_y,\beta} R_{e_x,\alpha}$

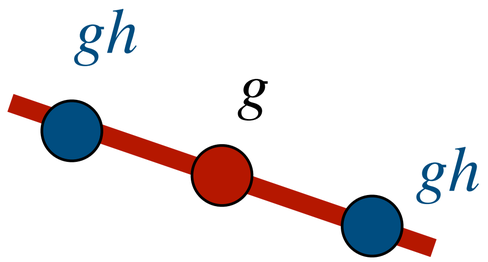
$S^2 \equiv SO(3)/SO(2)$



Quotient space

Quotient space G/H: The space of unique cosets $gH = \{gh \,|\, h \in H\}$. Elements of the space G/H are cosets.





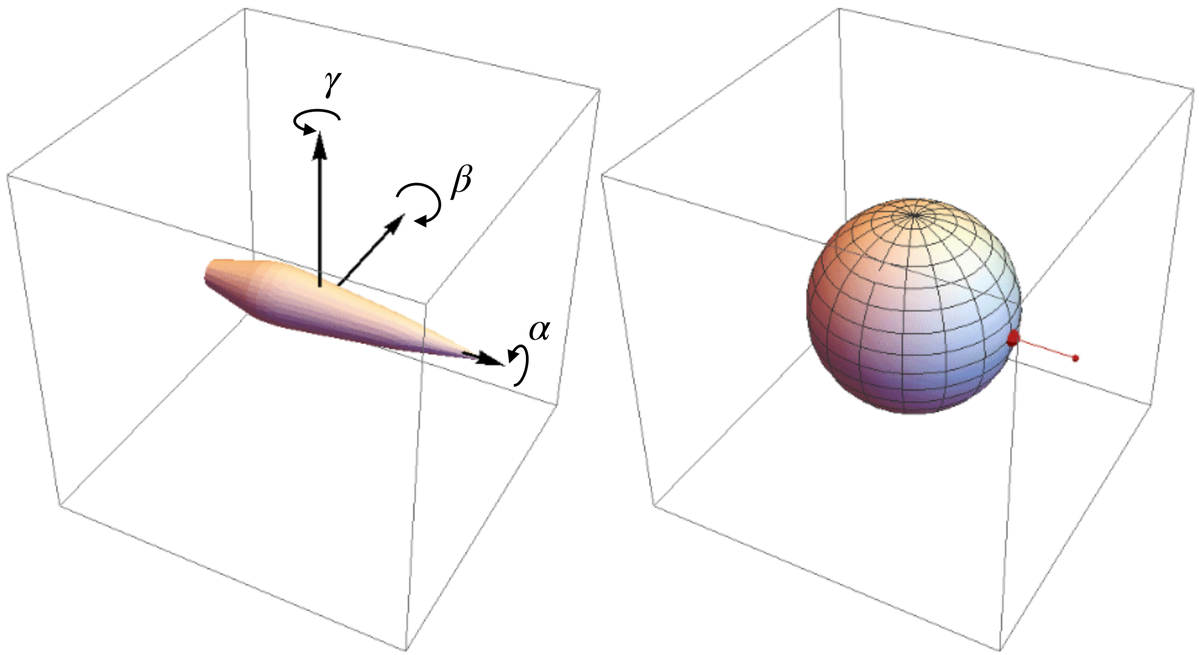
$$gH = \{gh \,|\, h \in H\}$$

Stabilizer

Stabilizer: $\mathrm{Stab}_G(x_0)$ is a subset of G that leaves x_0 unchanged. I.e.,
$\mathrm{Stab}_G(x_0) = \{g \,|\, gx_0 = x_0\}$

Rotation by $R \in SO(3)$

$$R = R_{e_z,\gamma} R_{e_y,\beta} \boxed{R_{e_x,\alpha}}$$



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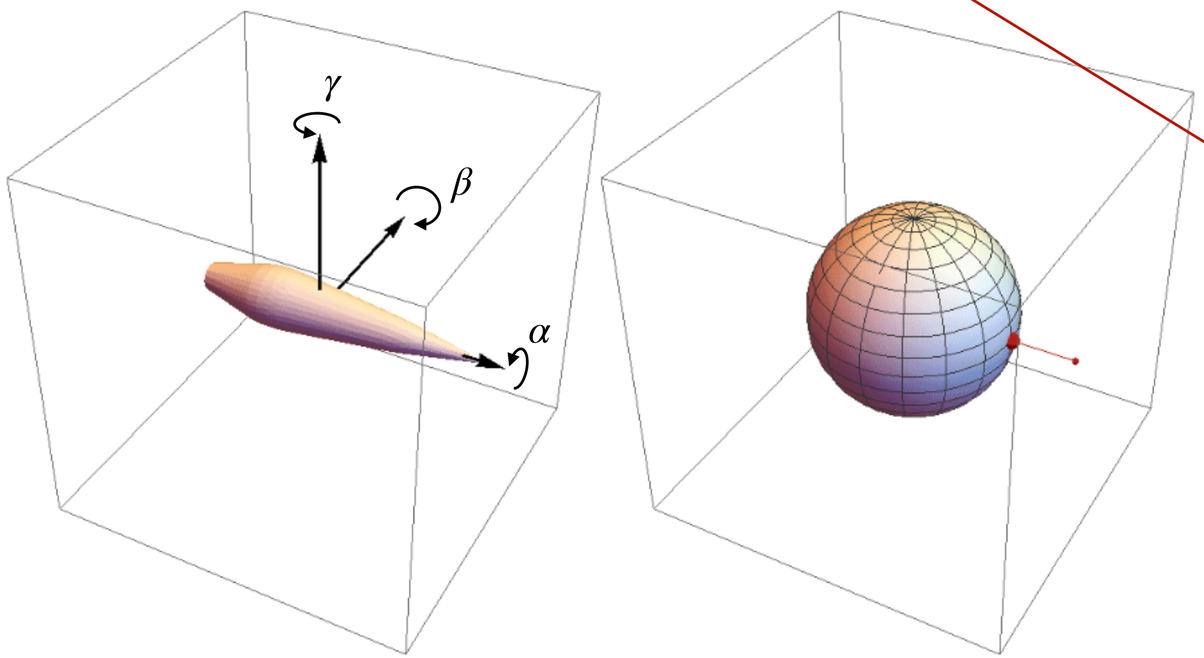


So the sphere is a quotient space

$$S^2 \equiv SO(3)/H$$

with

$$H = \mathrm{Stab}_{SO(3)}(\mathbf{e}_x)$$

Homogeneous space $\equiv$ Quotient space

Any quotient space is a homogeneous space

Any homogeneous space is a quotient space

Quotient space: the Euclidean plane $\mathbb{R}^d$

Lecture notes

Example 2.7 (Quotient space $\mathbb{R}^d = SE(d)/SO(d)$). Let $H = (\{\mathbf{0}\} \times SO(d)$ the subgroup of rotations in $SE(d)$, with $\mathbf{0}$ the identity element of the translationg roup $(\mathbb{R}^d, +)$. The the cosets gH are given by

$$\begin{aligned} gH &= \{g \cdot (\mathbf{0}, \tilde{\mathbf{R}}) \mid \tilde{\mathbf{R}} \in SO(d)\} \\ &= \{(\mathbf{R}\mathbf{e} + \mathbf{x}, \mathbf{R}\tilde{\mathbf{R}}) \mid h \in SO(d)\} \\ &= \{(\mathbf{x}, \mathbf{R}\tilde{\mathbf{R}}) \mid \tilde{\mathbf{R}} \in SO(d)\} \\ &= \{(\mathbf{x}, \tilde{\mathbf{R}}) \mid \tilde{\mathbf{R}} \in SO(d)\}, \end{aligned}$$

with $g = (\mathbf{x}, \mathbf{R})$. So, the cosets are given by all possible rotations for a fixed translation vector $\mathbf{x}$, the vector $\mathbf{x}$ thus indexes these sets. We can therefore make the identification

$$\mathbb{R}^d \equiv SE(d)/SO(d).$$

We already saw in Exercise 2.1 that $\mathbb{R}^d$ is a homogeneous space of $SE(d)$, this is a consequence of Lemma 2.1.

Conclusion

- A homogeneous space X is a space on which a group G acts transitively

- This is important as then we can reach any point in X via the action of G (when template matching we want to scan the entire space)

- Any homogeneous X space can be identified with a quotient space $X \equiv G/H$ (there is a point that is left invariant by a sub-group H)

UNIVERSITY OF AMSTERDAM

AMLAB Amsterdam Machine Learning Lab

Group Equivariant Deep Learning

Lecture 1 - Regular group convolutions

Lecture 1.7 - Group convolutions are all you need!

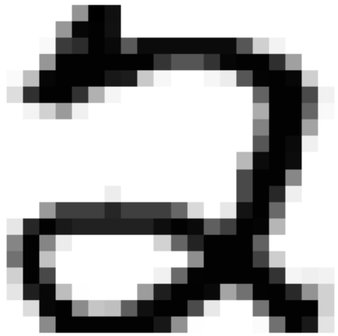
Equivariant linear layers between feature maps are group convolutions

Erik Bekkers, Amsterdam Machine Learning Lab, University of Amsterdam

This mini-course serves as a module with the UvA Master AI course Deep Learning 2 https://uvadl2c.github.io/

Classical artificial neural networks

What's my input? $\underline{x}^0 \in \mathscr{X} = ?$



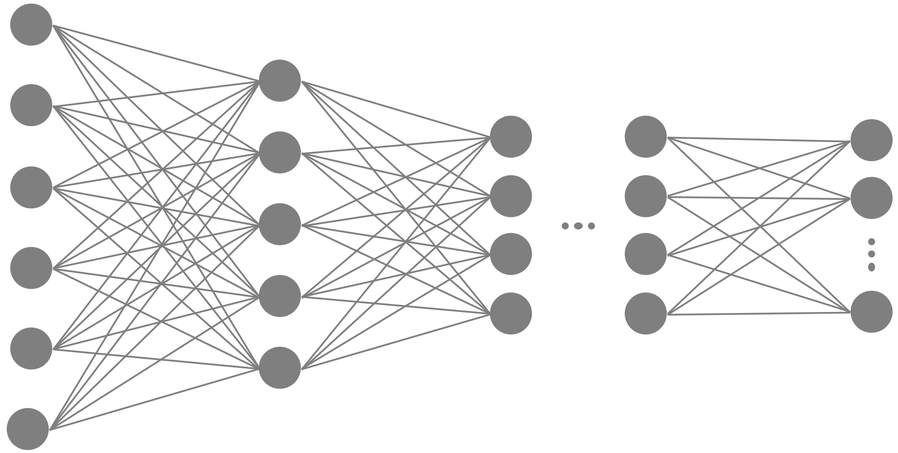


Image analyst: $\underline{x}^0 \in \mathscr{X} = \mathbb{L}_2(\mathbb{R}^2)$

Naive deep learner: $\underline{x}^0 \in \mathscr{X} = \mathbb{R}^{784}$

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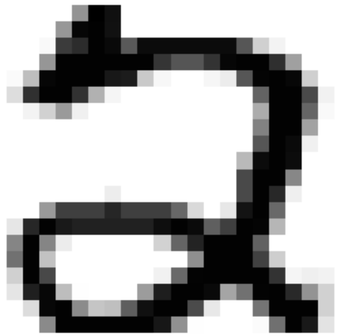
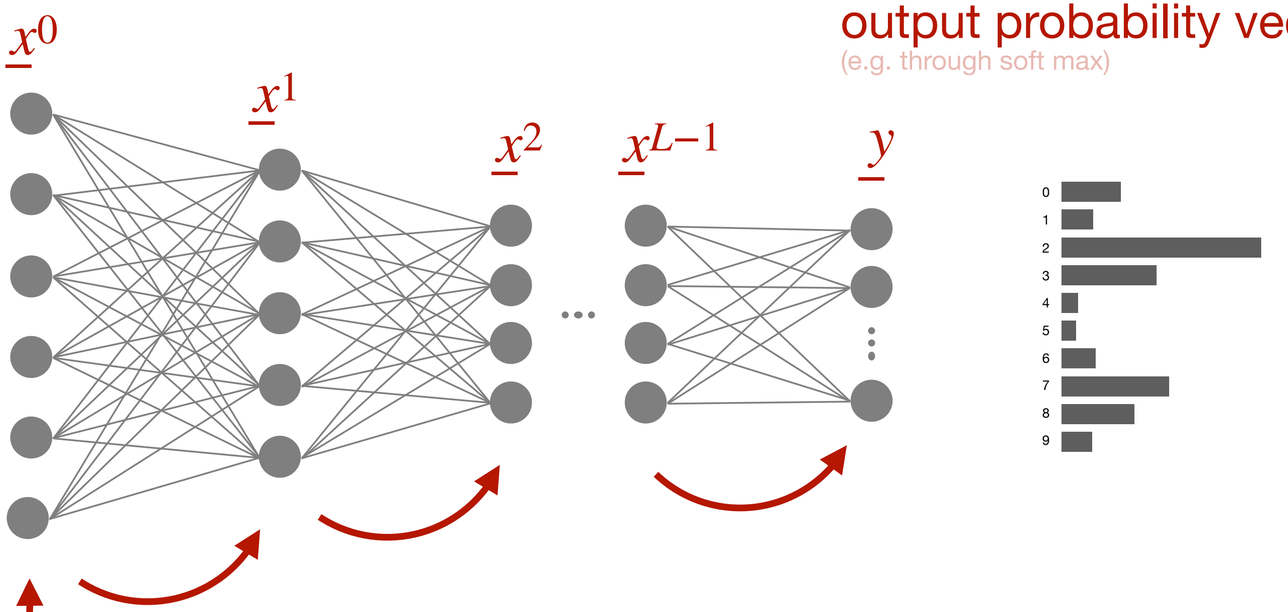


input vector

output probability vector
(e.g. through soft max)



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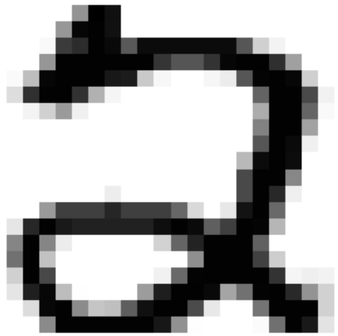

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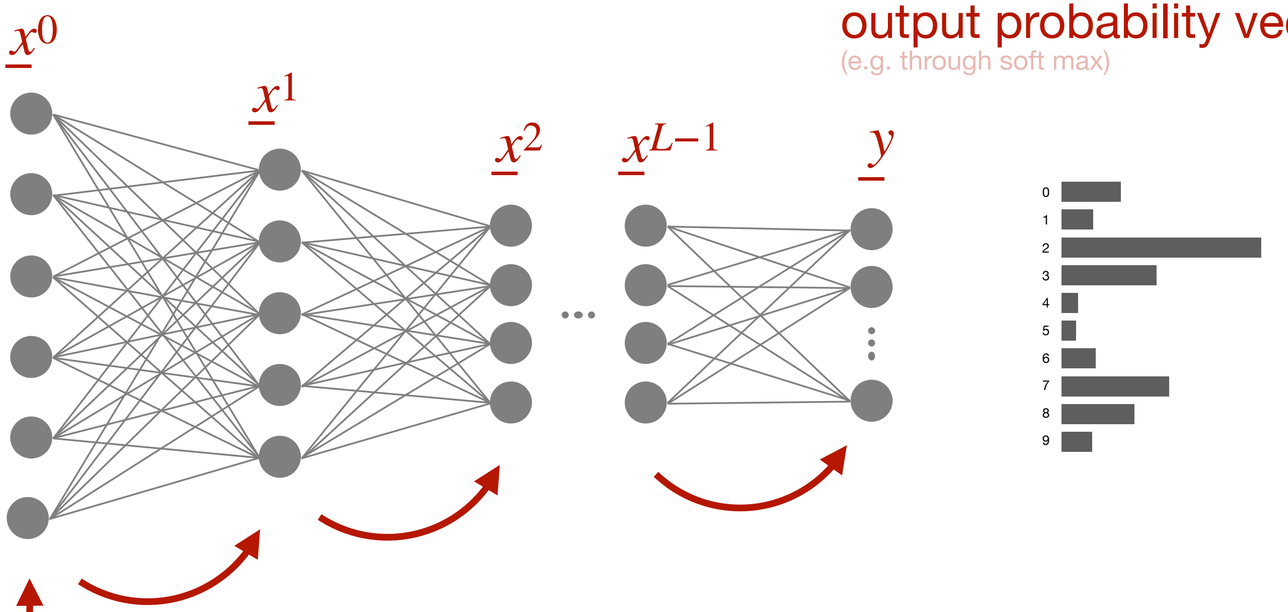

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Iteratively transform the vector via

$$\underline{x}^l = \varphi(K_{\mathbf{w}_l}\underline{x}^{l-1} + \underline{b}^l)$$

Linear map: matrix-vector multiplication with $K_{\mathbf{w}_l} \in \mathbb{R}^{N^l \times N^{l-1}}$

A fully connect layer as convolution on 1D signal

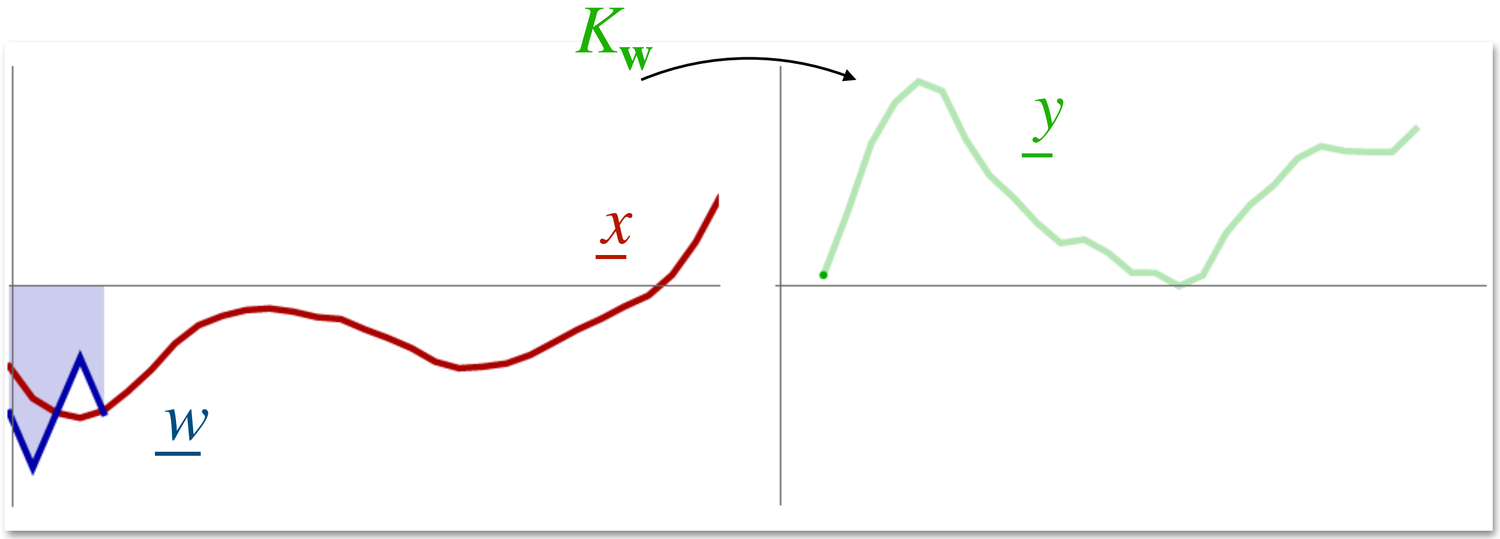
- Way too many degrees of freedom!
- Doest not leverage/preserve structure in data

$$\underline{y} = \varphi(\quad K_{\mathbf{w}} \quad \underline{x} + \underline{b} \quad)$$

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \end{pmatrix} = \varphi \left(\begin{pmatrix} w_{11} & w_{12} & w_{13} & w_{14} & w_{15} & \cdots \\ w_{21} & w_{22} & w_{23} & w_{24} & w_{25} & \cdots \\ w_{31} & w_{32} & w_{33} & w_{34} & w_{35} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ \vdots \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix} \right)$$

A fully connected layer as convolution on 1D signal

Convolution as linear operator
+ Localized transformations
+ Shift equivariance
+ Sparsification of the linear operator
+ Weightsharing



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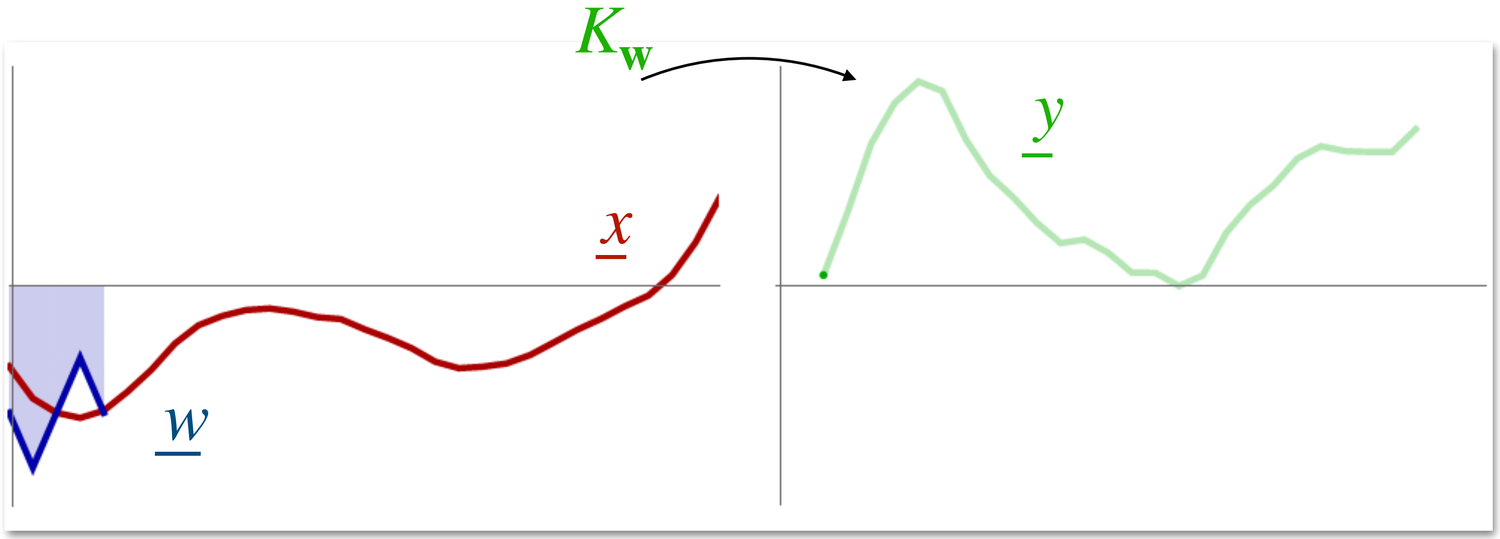

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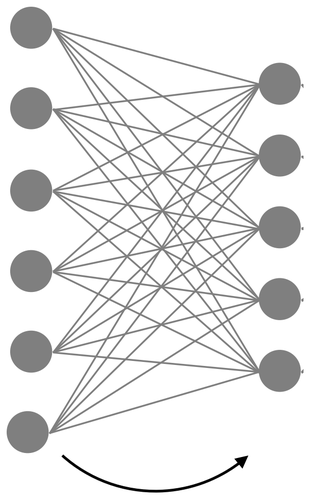
Classical artificial NNs in the continuous world

Working with vectors $\underline{x} \in \mathscr{X} = \mathbb{R}^{N^x}$



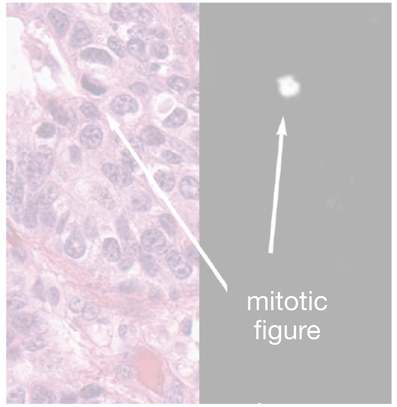
Iteratively transform the **vector** in $\mathbb{R}^{N^x}$ via

$$\underline{y} = \varphi(K\,\underline{x} + \underline{b}^l)$$

Linear map: matrix-vector multiplication with $K \in \mathbb{R}^{N^y \times N^x}$

$$y_j = \sum_i K_{i,j}\, x_i$$

Working with feature maps $f \in \mathscr{X} = \mathbb{L}_2(X)$



Iteratively transform the **feature map** in $\mathbb{L}_2(X)$

$$f^{out} = \varphi(K f^{in} + b^l)$$

Linear map: kernel operator with kernel in $\mathbb{L}_1(Y, X)$

$$(Kf)(y) = \int_X k(y,x) f(x) \mathrm{d}x$$

Classical artificial NNs in the continuous world

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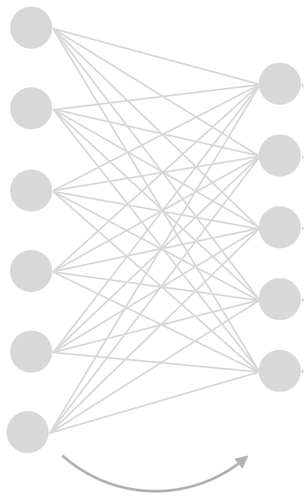

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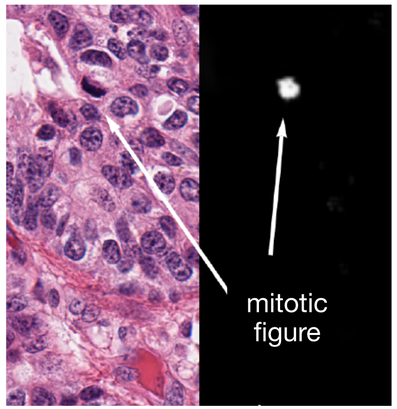

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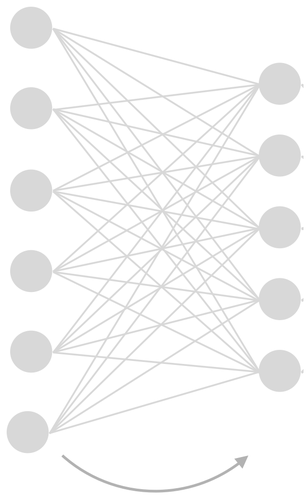

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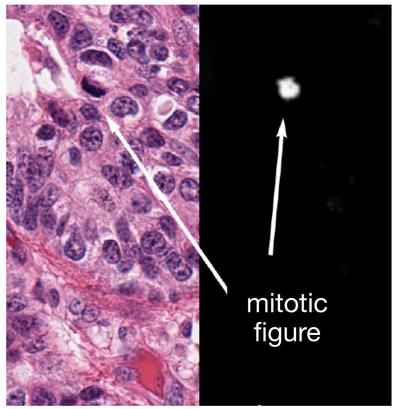
We want K to be equivariant!

Linear map: matrix-vector multiplication with $K \in \mathbb{R}^{N^y \times N^x}$

$$y_j = \sum_i K_{i,j}\, x_i$$

Working with feature maps $f \in \mathscr{X} = \mathbb{L}_2(X)$



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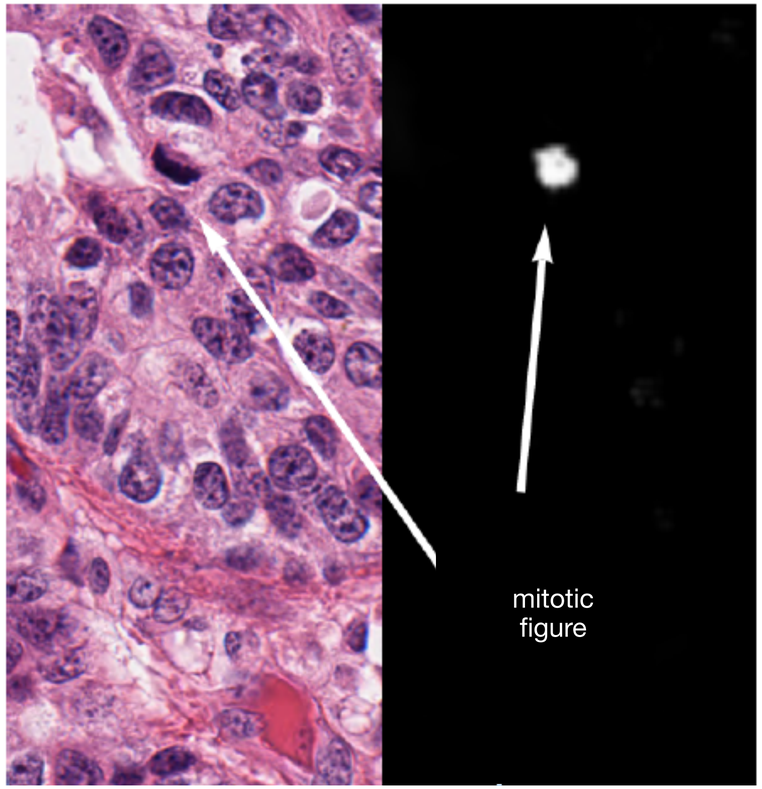
Neural Networks for Signal Data



$$\mathscr{K} : \mathbb{L}_2(X)^{N_l} \to \mathbb{L}_2(Y)^{N_{l+1}}$$

Let's build neural networks for signal data via the layers of the form:

$$\underline{f}^{l+1} = \sigma(\mathscr{K}\,\underline{f}^{l} + \mathbf{b}^{l})$$

The linear map has to be an integral transform with a two-argument kernel
(Dunford-Pettis theorem)

$$(\mathscr{K}f)(y) = \int_X \mathbf{k}(y,x)\underline{f}(x)\mathrm{d}x$$

Theorem (G-convs are all you need)

Bekkers ICLR 2020, Thm. 1*

Let $\mathscr{K} : \mathbb{L}_2(X) \to \mathbb{L}_2(Y)$ map between signals on homogeneous spaces of G.

Let homogeneous space $Y \equiv G/H$ such that $H = \mathrm{Stab}_G(y_0)$ for some chosen origin $y_0 \in Y$ and let $g_y \in G$ such that $\forall_{y \in Y} : y = g_y y_0$.

Then $\mathscr{K}$ is equivariant to group G if and only if:

1. It is a group convolution: $[\mathscr{K}f](y) = \int_X \frac{1}{|g_y|} k(g_y^{-1}x) f(x) \mathrm{d}x$

2. The kernel satisfies a symmetry constraint: $\forall_{h \in H} : \frac{1}{|g_y|} k(hx) = k(x)$

*Work with Remco Duits at TU/e.

See also: Duits 2005 – Thm 25, Cohen, Geiger, Weiler 2018 - Thm 6.1, Kondor, Trivedi 2018 - Thm 1

Proof (G-convs are all you need)

First of all, $\mathscr{K}$ is an integral transform:

$$\mathscr{K}[f](y) = \int_X \tilde{k}(y, x) f(x) \mathrm{d}x$$

Proof (G-convs are all you need)

First of all, $\mathscr{K}$ is an integral transform:

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$\forall_{g \in G}$ and $\forall_{f \in \mathbb{L}_2(X)}$:

$$(\mathscr{K} \circ \mathscr{L}_g^{G \to \mathbb{L}_2(X)})(f) = (\mathscr{L}_g^{G \to \mathbb{L}_2(Y)} \circ \mathscr{K})(f)$$

Proof (G-convs are all you need)

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$$\int_X \tilde{k}(y,x) f(g^{-1}x) \mathrm{d}x = \int_X \tilde{k}(g^{-1}y, x) f(x) \mathrm{d}x$$

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(in r.h.s. $x \leftarrow g^{-1}x$)

Proof (G-convs are all you need)

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Proof (G-convs are all you need)

First of all, $\mathscr{K}$ is an integral transform:

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Since this should hold or all $f \in \mathbb{L}_2(X)$ we have $\forall_{g\in G}$: $\tilde{k}(y,x) = \frac{1}{|\det g|}\tilde{k}(g^{-1}y,g^{-1}x)$

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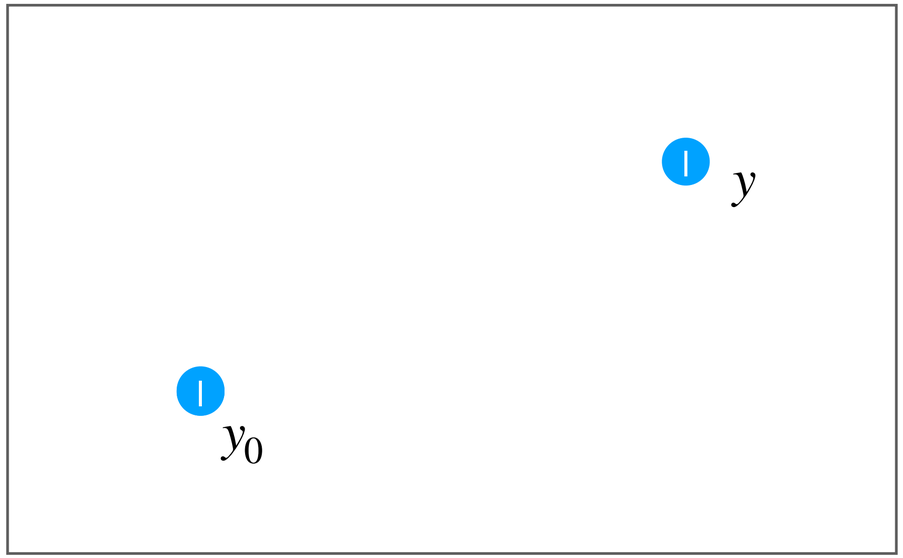

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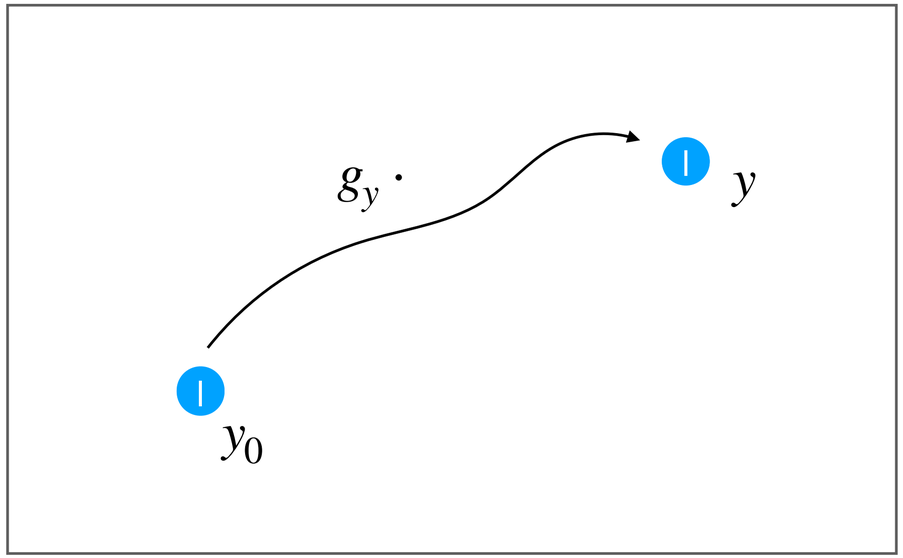

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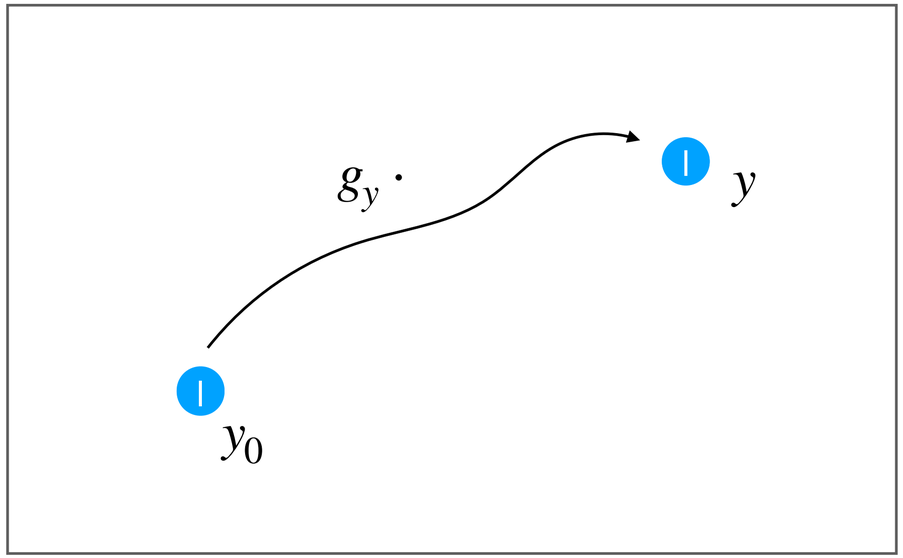

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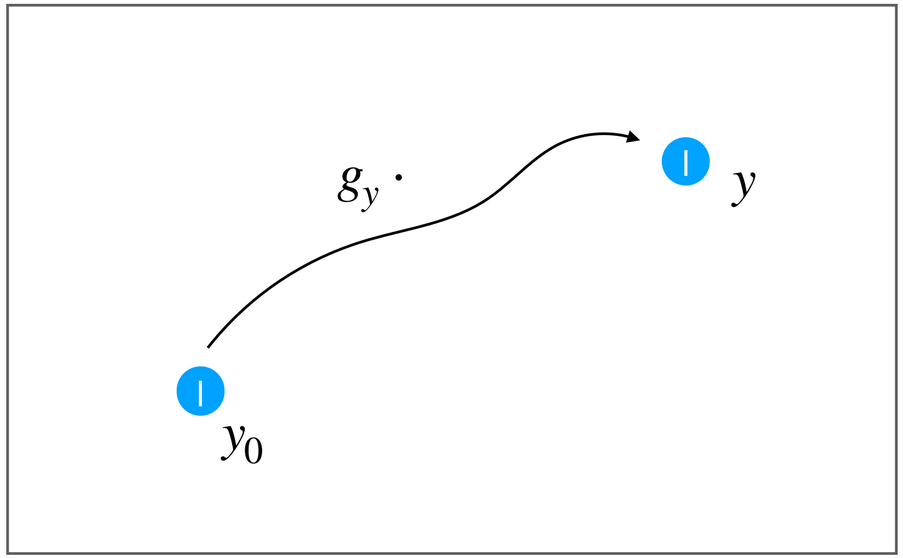

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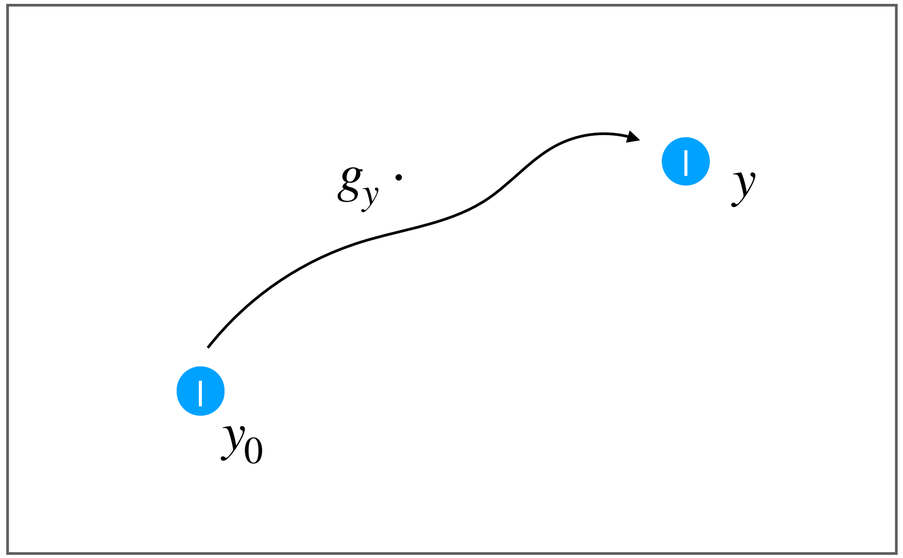

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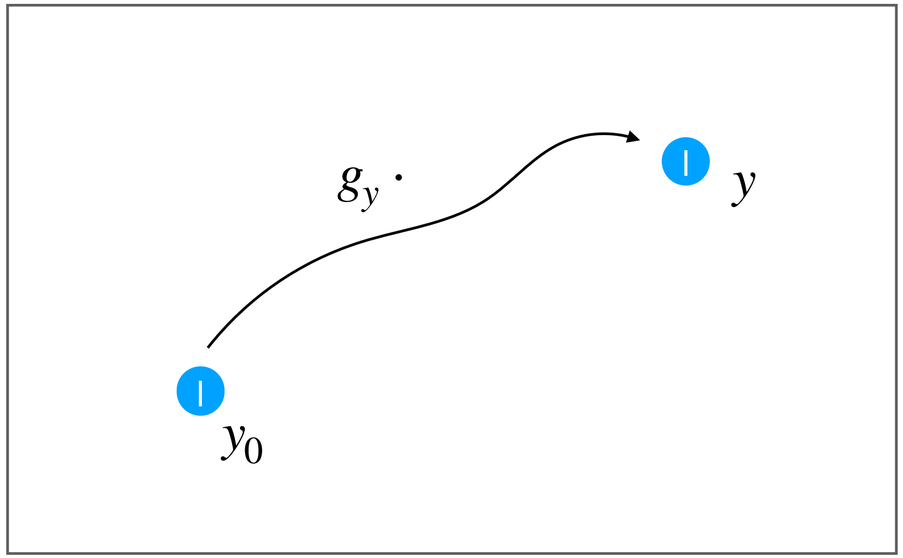

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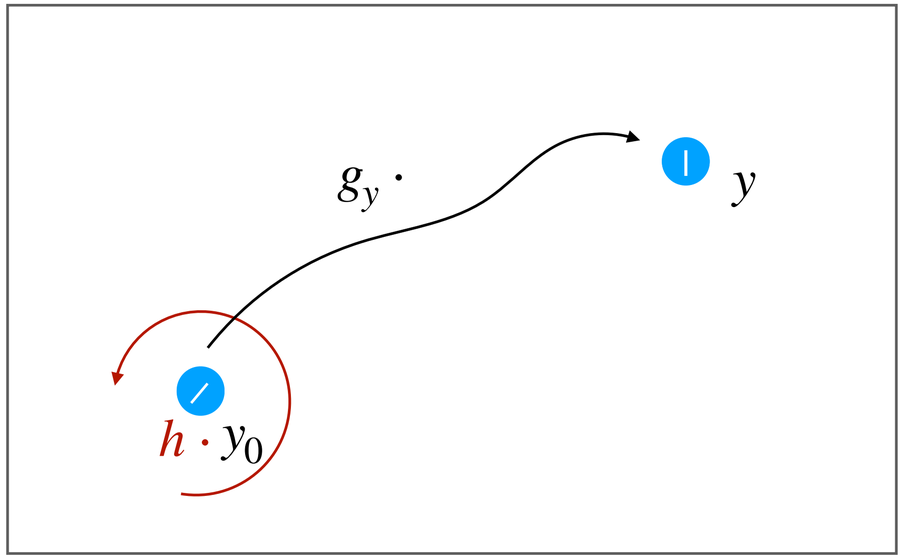

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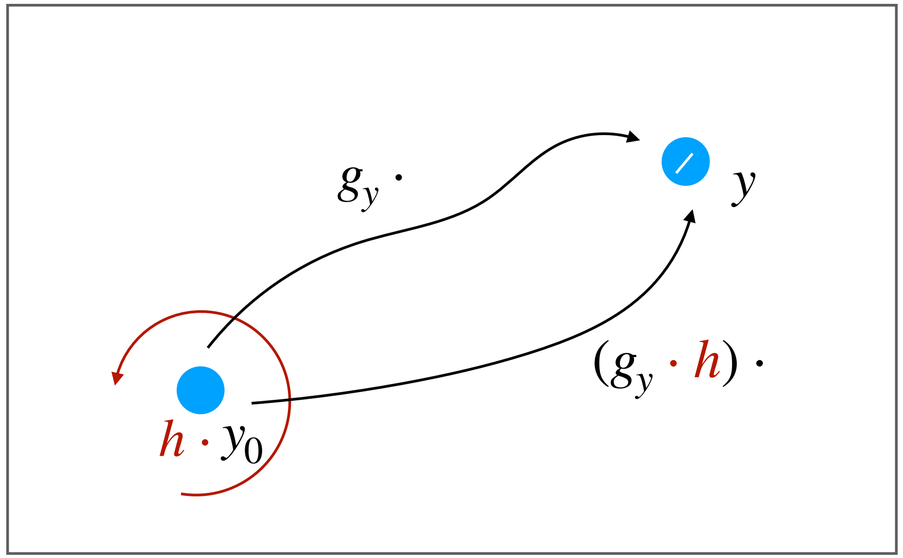

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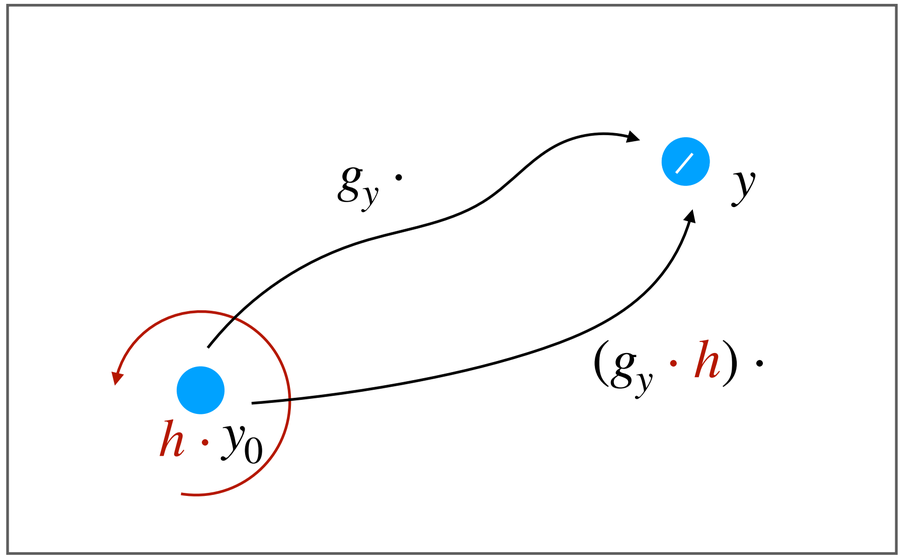

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$$\forall_{h \in H}: \qquad \tilde{k}(h\, y_0, x) = \tilde{k}(y_0, x) \qquad \Leftrightarrow \qquad k(x) = \frac{1}{|\det h|}k(h^{-1}x)$$

Theorem (G-convs are all you need)

Bekkers ICLR 2020, Thm. 1*

Let $\mathscr{K} : \mathbb{L}_2(X) \to \mathbb{L}_2(Y)$ map between signals on homogeneous spaces of G.

Let homogeneous space $Y \equiv G/H$ such that $H = \mathrm{Stab}_G(y_0)$ for some chosen origin $y_0 \in Y$ and let $g_y \in G$ such that $\forall_{y \in Y} : y = g_y y_0$.

Then $\mathscr{K}$ is equivariant to group G if and only if:

1. It is a group convolution: $[\mathscr{K}f](y) = \int_X \frac{1}{|g_y|} k(g_y^{-1}x) f(x) \mathrm{d}x$

2. The kernel satisfies a symmetry constraint: $\forall_{h \in H} : \frac{1}{|g_y|} k(hx) = k(x)$

*Work with Remco Duits at TU/e.

See also: Duits 2005 – Thm 25, Cohen, Geiger, Weiler 2018 - Thm 6.1, Kondor, Trivedi 2018 - Thm 1

Types of layers

$$K : \mathbb{L}_2(\mathbb{R}^2) \to \mathbb{L}_2(\mathbb{R}^2)$$

$(X = Y = G/H)$

Isotropic/Constraint convolutions on spaces of lower dimension than G, $\forall_{h \in H} : k(hx) = k(x)$

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$X = \mathbb{R}^2 \equiv SE(2)/SO(2)$

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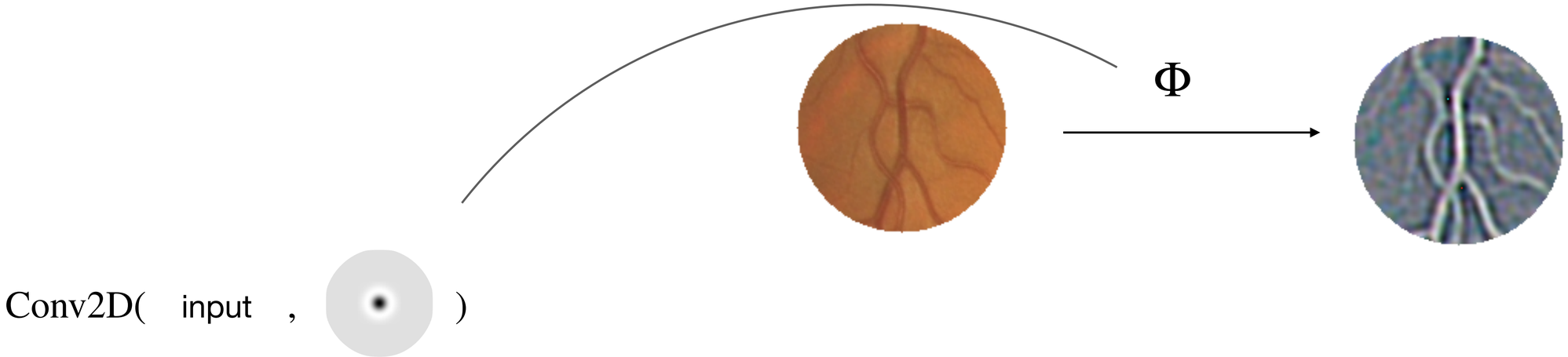

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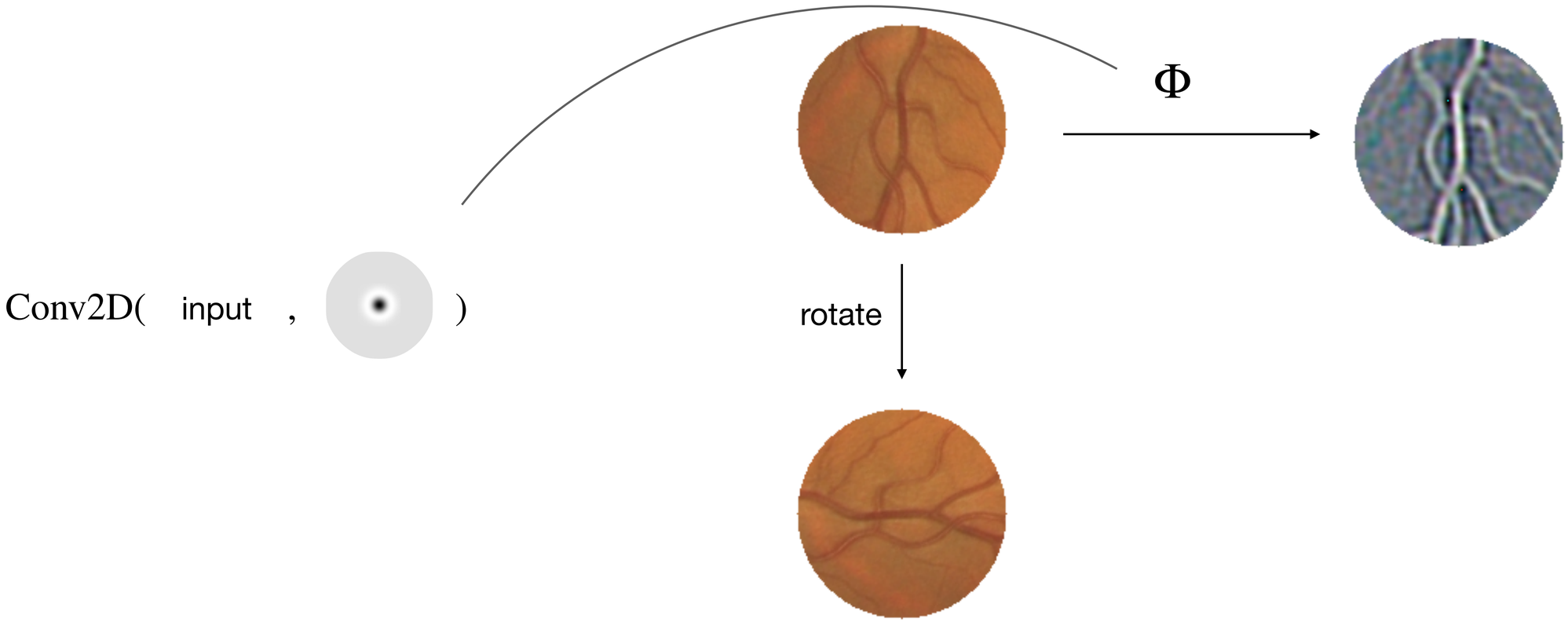

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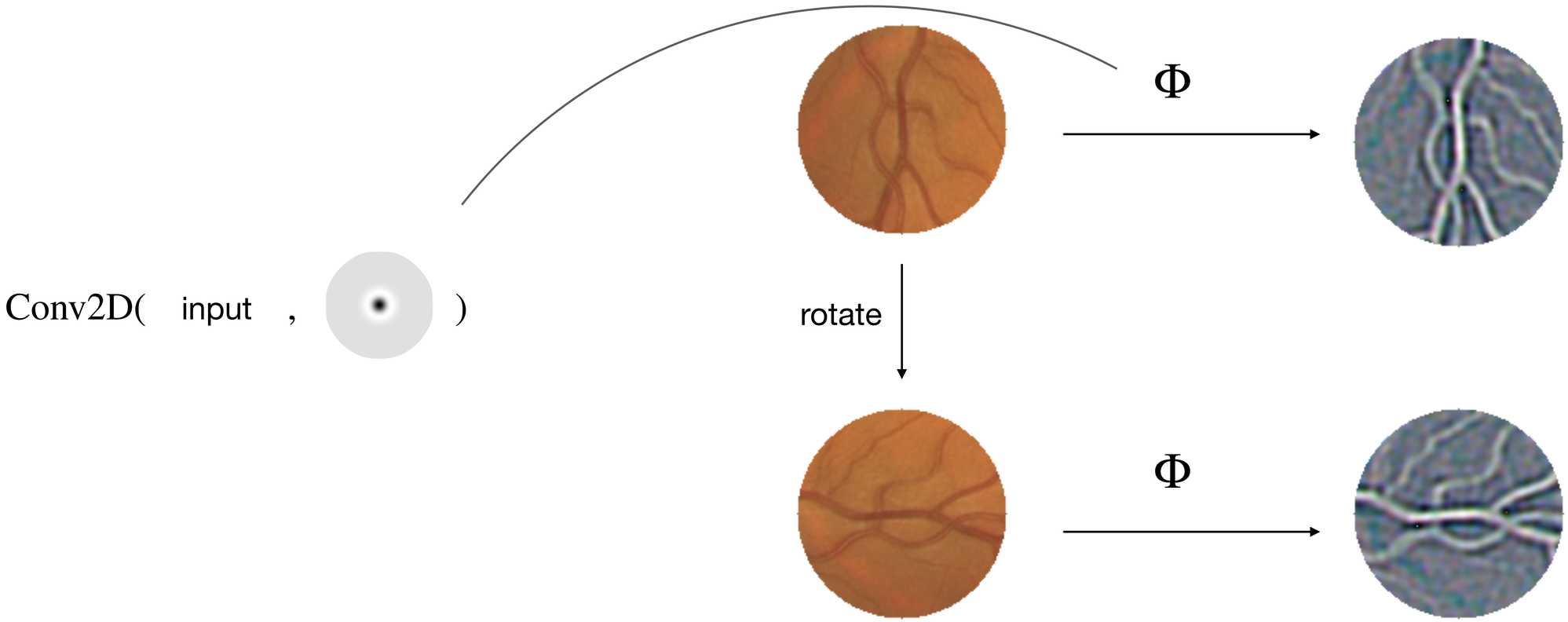

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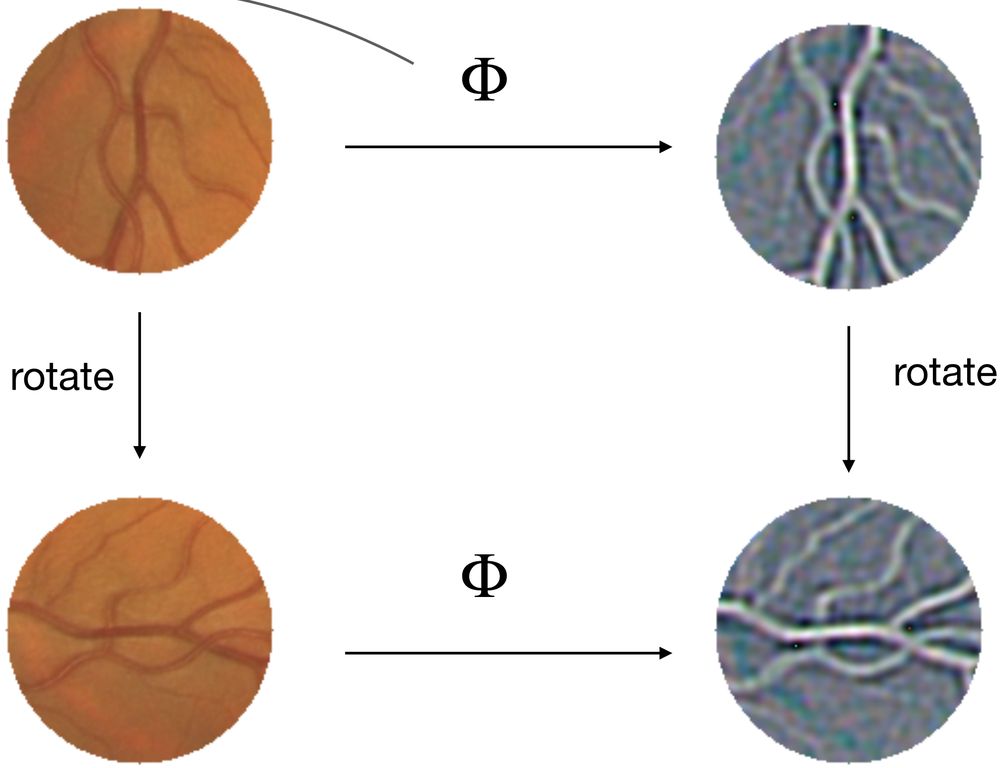

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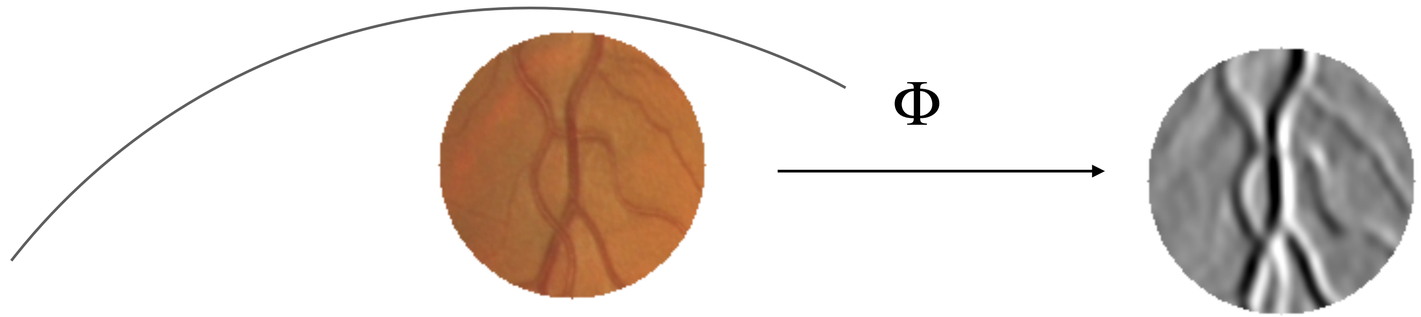
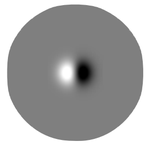


Conv2D(input , )

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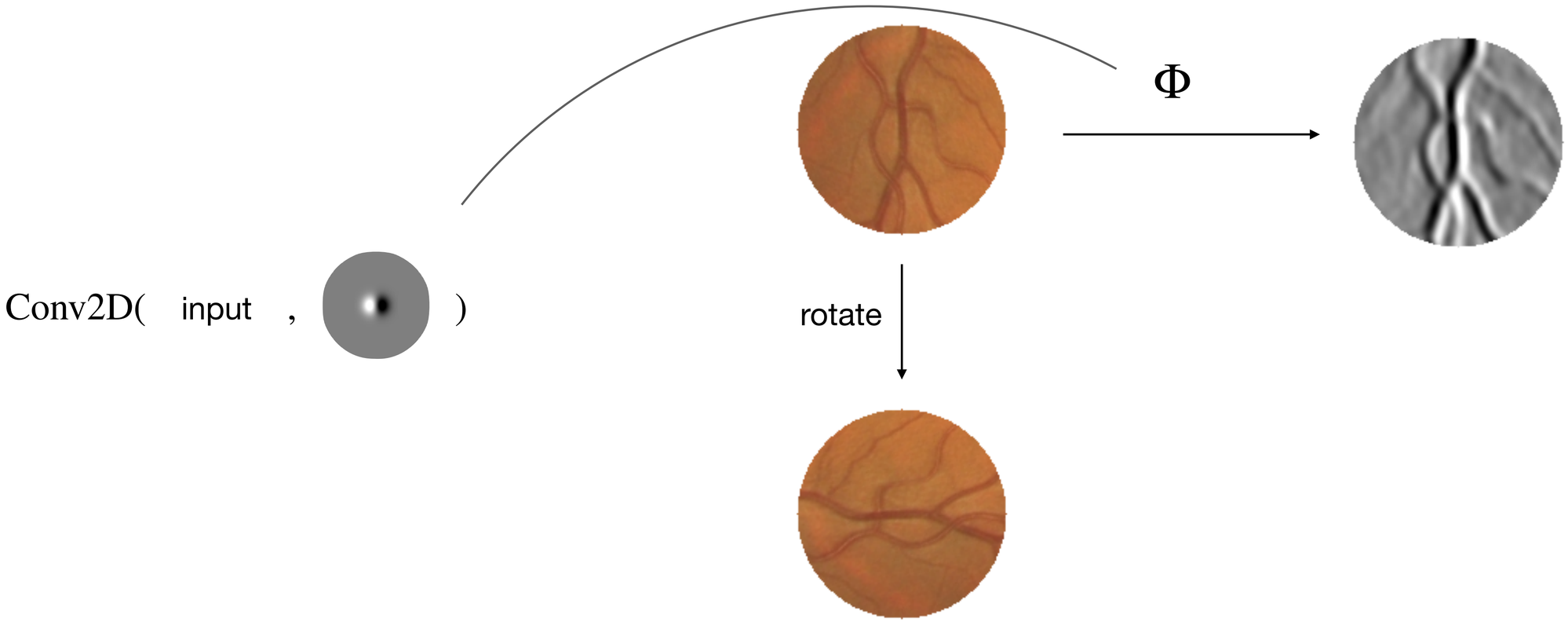

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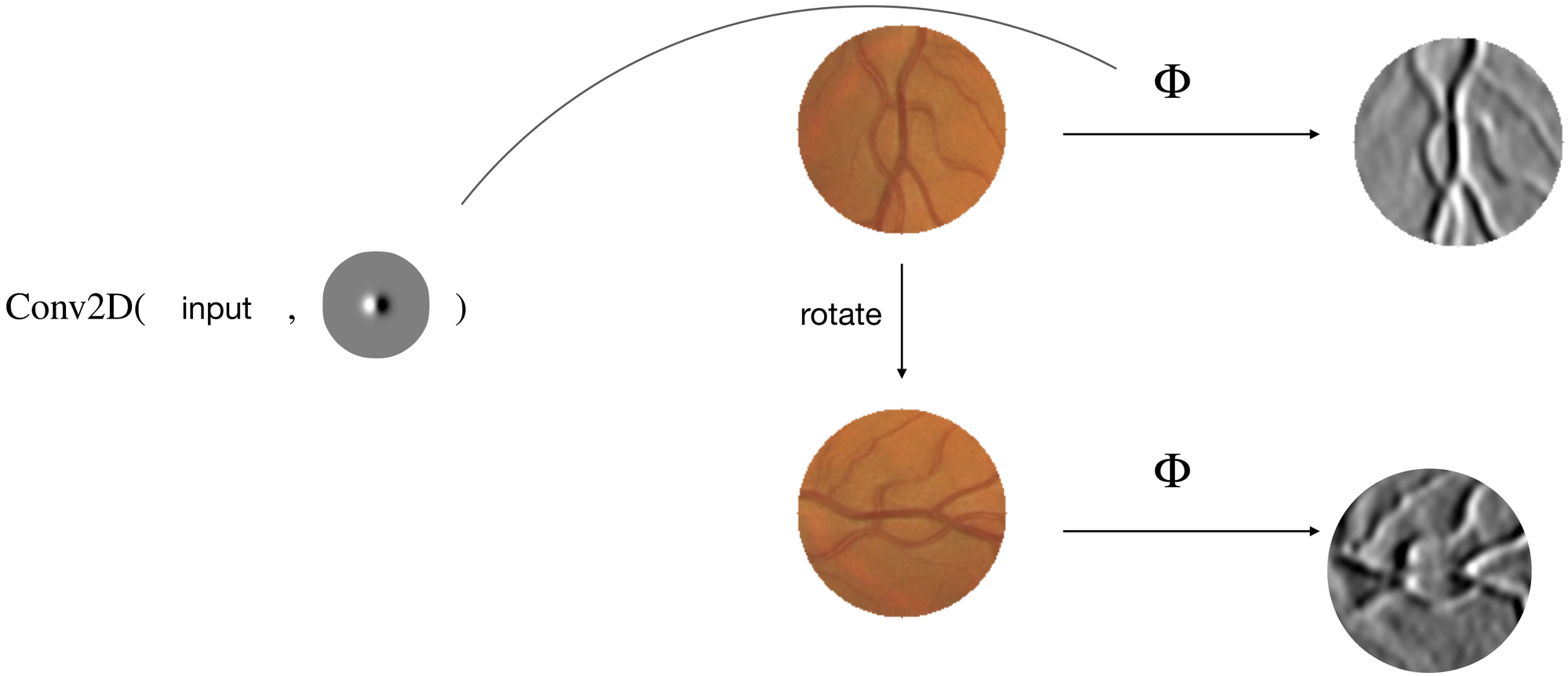

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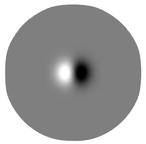
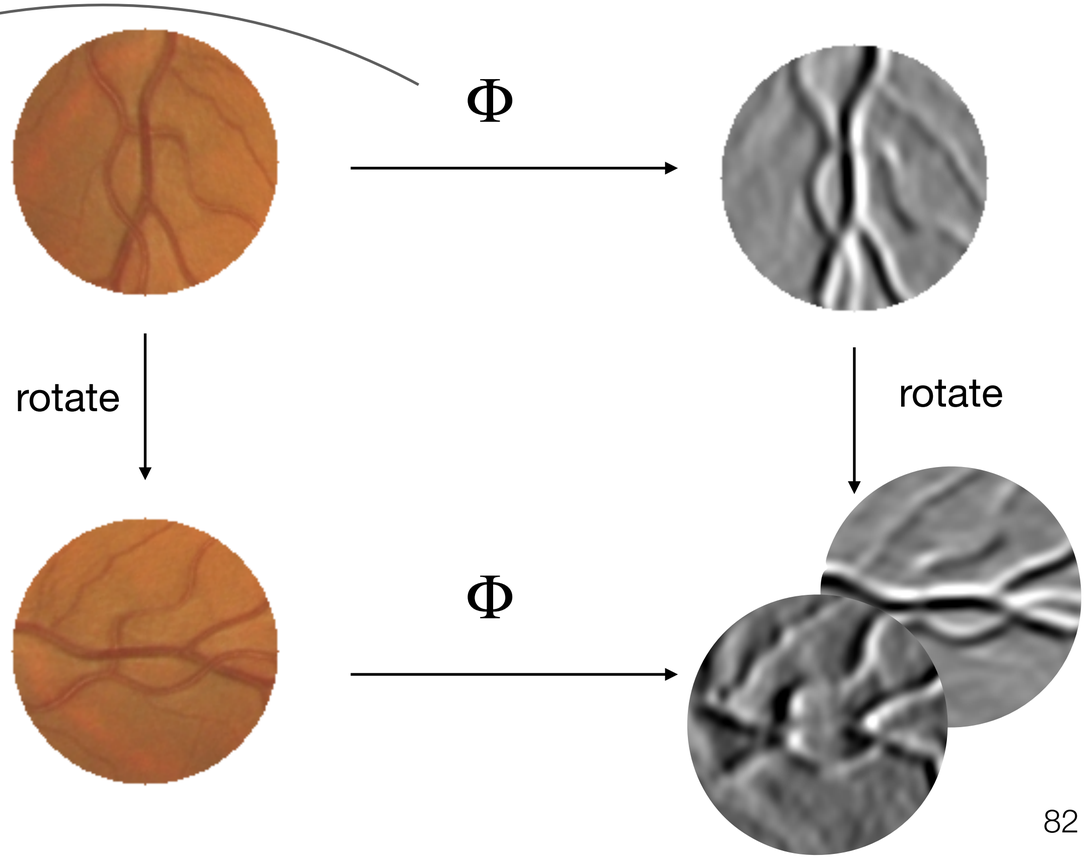
Conv2D(input , )



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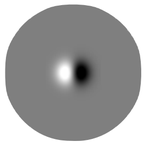
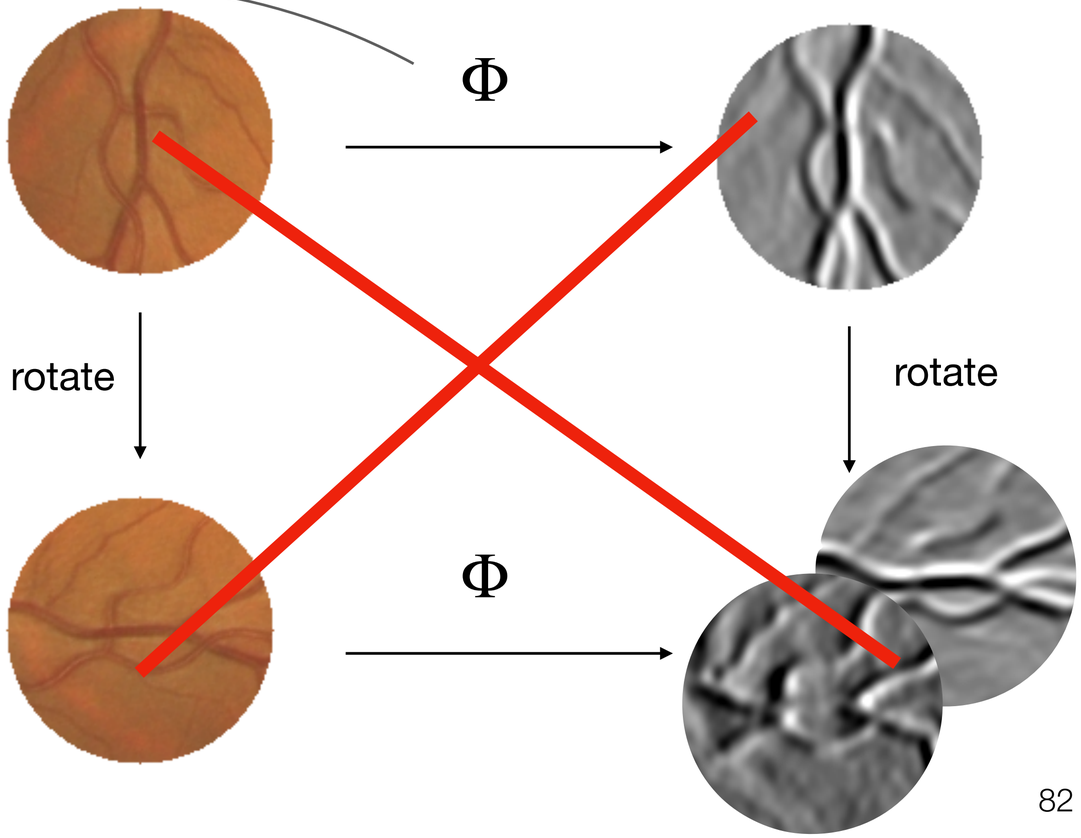
Conv2D(input , )



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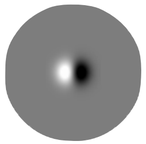
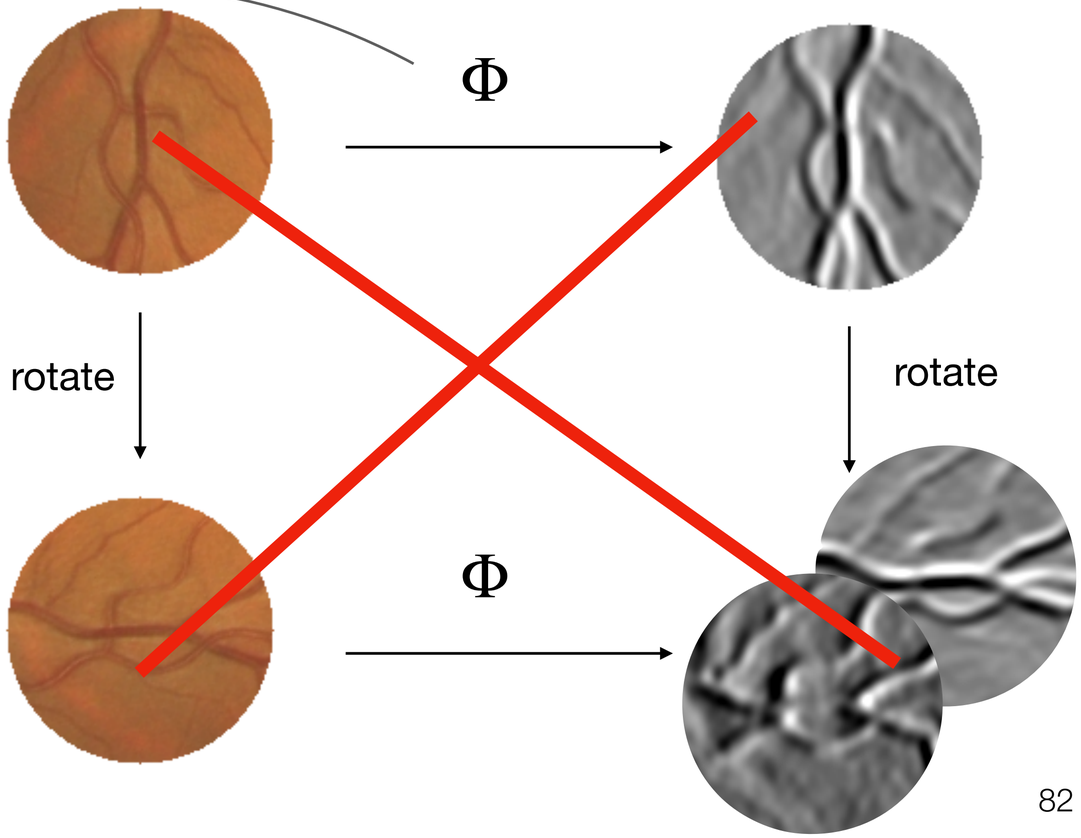
Conv2D(input , )



Types of layers $K : \mathbb{L}_2(\mathbb{R}^2) \to \mathbb{L}_2(SE(2))$

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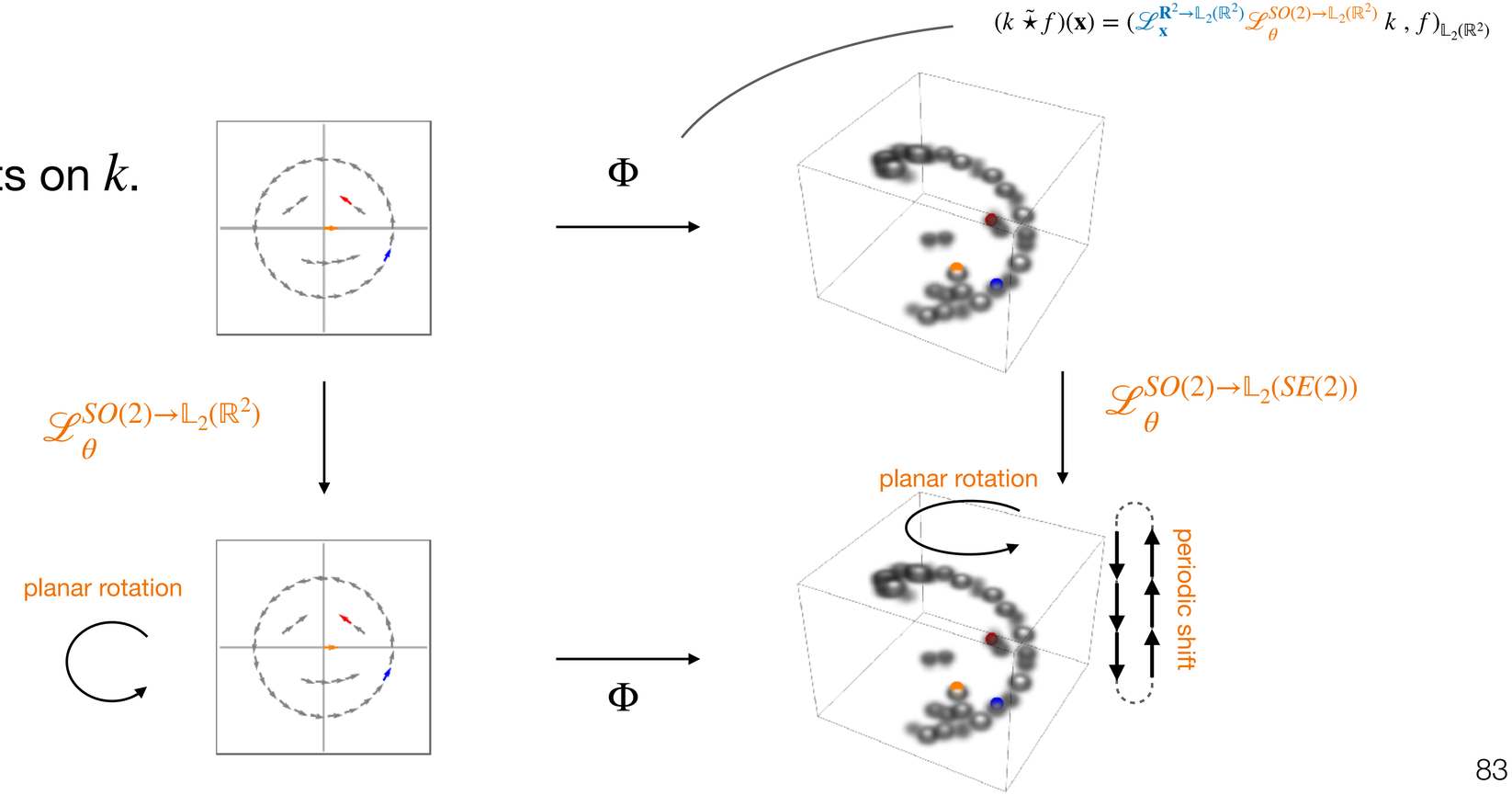
Isotropic/Constraint convolutions on spaces of lower dimension than G, $\forall_{h \in H} : k(hx) = k(x)$

$(X = G/H, Y = G)$

Lifting convolution. No constraints on k.



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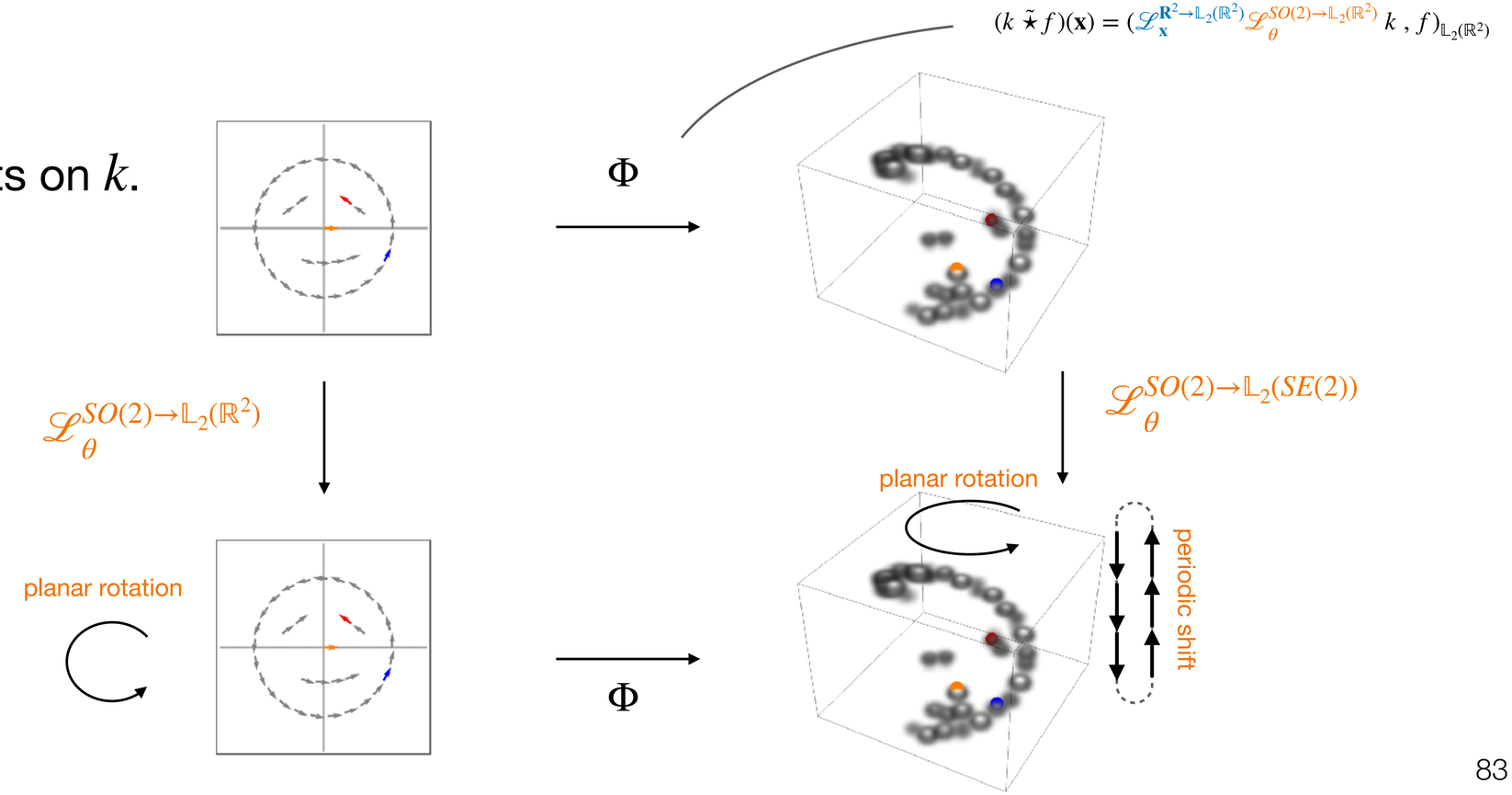

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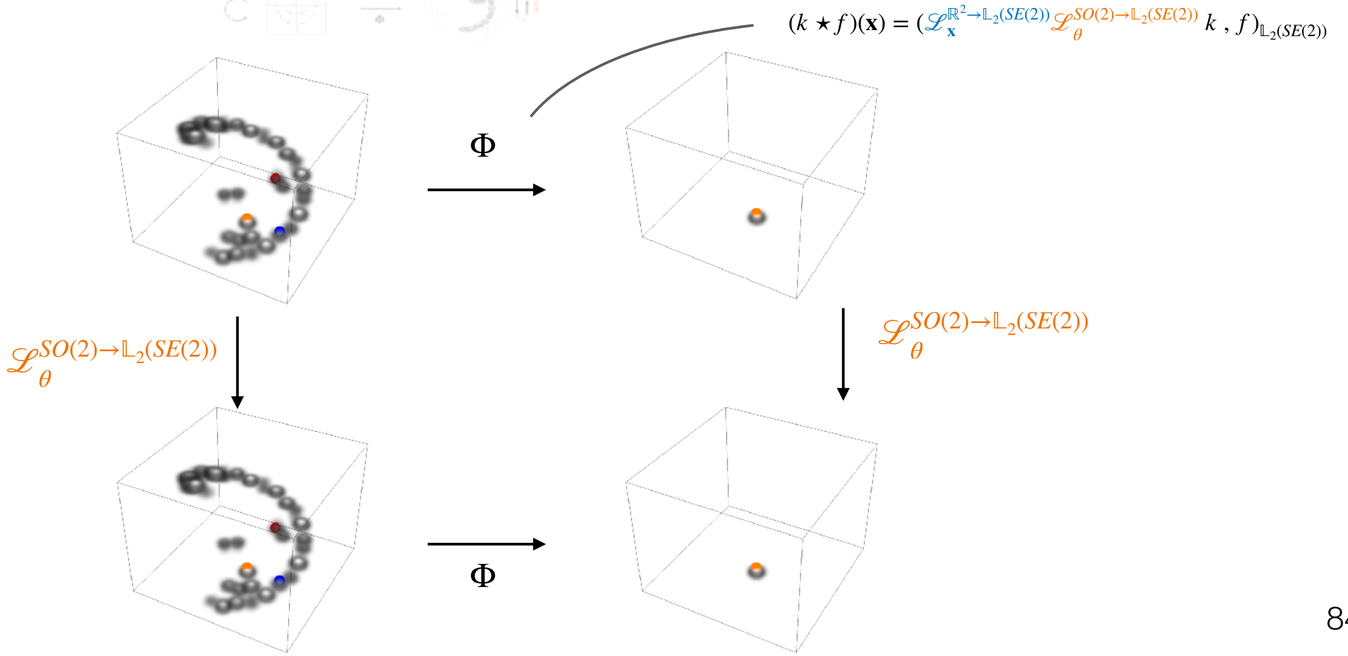
$(X = Y = G)$

Group convolutions. No constraints on k.



Types of layers $K : \mathbb{L}_2(SE(2)) \to \mathbb{L}_2(SE(2))$

$(X = Y = G/H)$

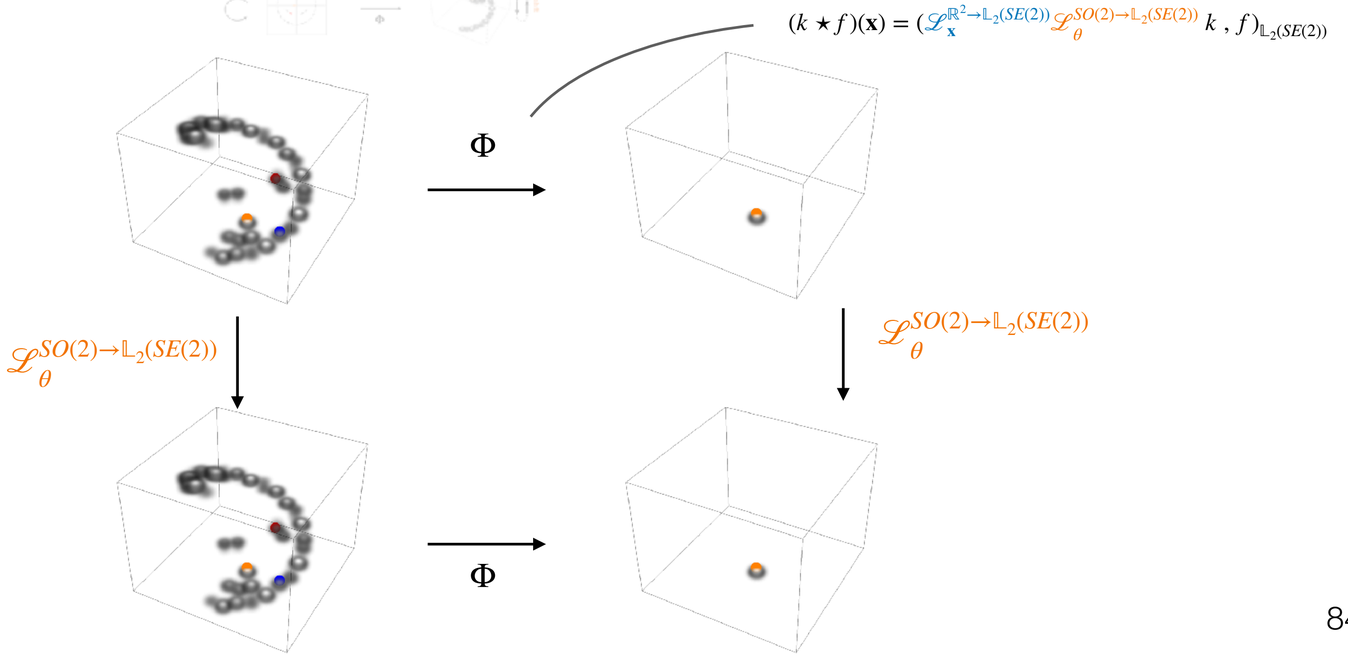
Isotropic/Constraint convolutions on spaces of lower dimension than G, $\forall_{h \in H} : k(hx) = k(x)$

$(X = G/H, Y = G)$

Lifting convolution. No constraints on k.

$(X = Y = G)$

Group convolutions. No constraints on k.



Types of layers

$$K : \mathbb{L}_2(SE(2)) \to \mathbb{L}_2(\mathbb{R}^2)$$

$(X = Y = G/H)$

Isotropic/Constraint convolutions on spaces of lower dimension than G, $\forall_{h \in H} : k(hx) = k(x)$

$(X = G/H, Y = G)$

Lifting convolution. No constraints on k.

$(X = Y = G)$

Group convolutions. No constraints on k.

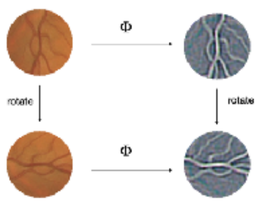
$(X = G, Y = G/H)$

Projection layer. Mean pooling over H.

Types of layers

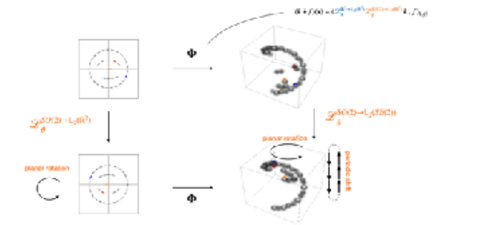
$(X = Y = G/H)$

Isotropic/Constraint convolutions on spaces of lower dimension than G, $\forall_{h \in H} : k(hx) = k(x)$



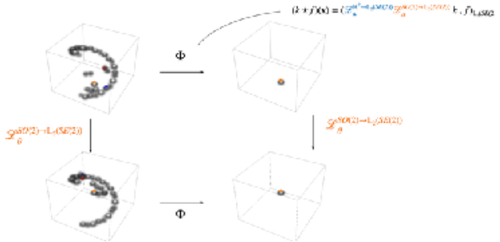
$(X = G/H, Y = G)$

Lifting convolution. No constraints on k.



$(X = Y = G)$

Group convolutions. No constraints on k.

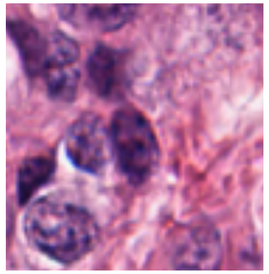


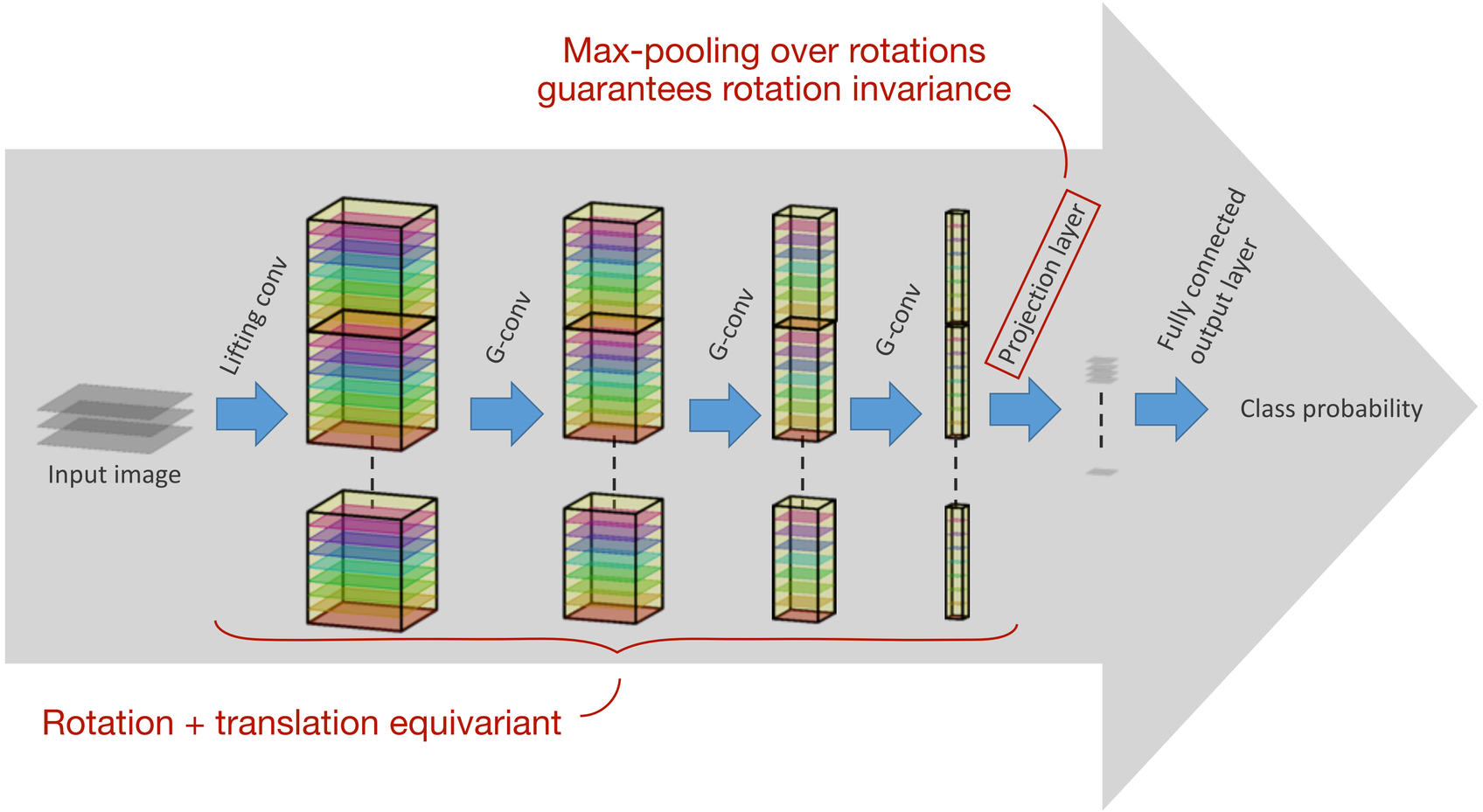
$(X = G, Y = G/H)$

Projection layer. Mean pooling over H.

The most expressive group equivariant architectures are obtained by lifting the feature maps to the group

General group equivariant architecture





“normal” (0)
vs
“mitotic” (1)

Conclusion

If you want to build **equivariant neural networks**

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If you want to build **equivariant neural networks**

Group convolutions are all you need!