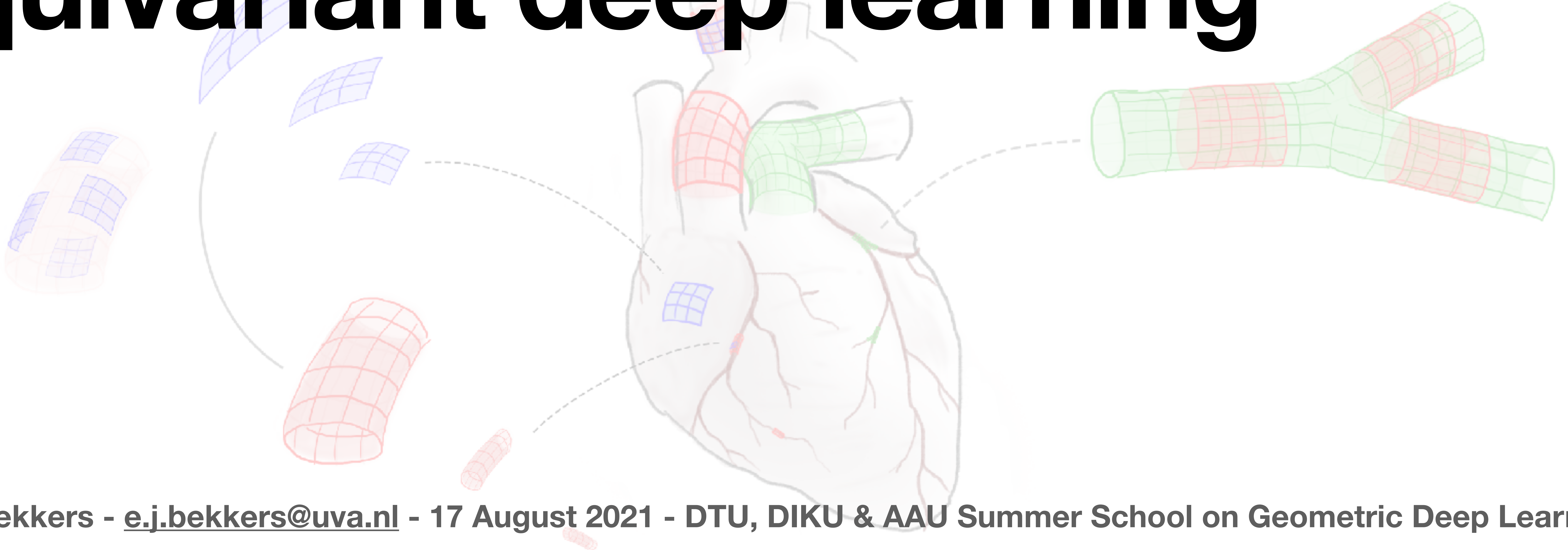
UNIVERSITY OF AMSTERDAM

Introduction to group equivariant deep learning



Erik J Bekkers - e.j.bekkers@uva.nl - 17 August 2021 - DTU, DIKU & AAU Summer School on Geometric Deep Learning

Content

Part I: Introduction to group convolutions

* Motivation
* Introduction to group theory
* Regular group convolutional neural networks
* Applications

Part II: General theory for group equivariant deep learning

* Group convolutions are all you need!
* Deeper into group theory: representation theory, homogeneous spaces
* Characterization of types of group equivariant layers

Part III: Steerable group convolutions

* Deep dive into group theory: irreducible representations, steerable operators and vector spaces
* Examples of steerable group convolutions: Spherical data and Volumetric data/3D point clouds

Lecture notes, slides and exercises available at

https://uvagedl.github.io

An Introduction to Equivariant Convolutional Neural Networks for Continuous Groups
Lecture Notes

dr.ir. Erik J. Bekkers

August 2021

Contents

1

Exercise 2.4. Show transitivity (Definition 2.8) of the action of G given in Eq. (29).

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 translating 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.

Lemma 2.1 shows that a quotient space G/H of a group G with H is a homogeneous space. We can also approach this in the other direction and state that any homogeneous space of G is equivalent to a quotient space G/H for some H. This is stated in the following Lemma, for which we first need to introduce the notion of a stabilizer.

Definition 2.13 (Stabilizer). Let G act on X via the action $\odot$. For every $x \in X$, the stabilizer subgroup of G with respect to the point x is denoted with $\mathrm{Stab}_G(x)$ is the set of all elements in G that fix x:

$$\mathrm{Stab}_G(x) = \{g \in G \mid g \odot x = x\}. \tag{30}$$

Lemma 2.2. Let X be a homogeneous space of G. Then X can be identified with G/H with $H = \mathrm{Stab}_G(x_0)$ for any $x_0 \in X$.

Affine groups Finally when it comes to types of groups and homogeneous spaces we note that often we are interested in groups that act on $\mathbb{R}^d$, as most often one deal with data on $\mathbb{R}^d$. It is therefore useful to introduce the following class of groups.

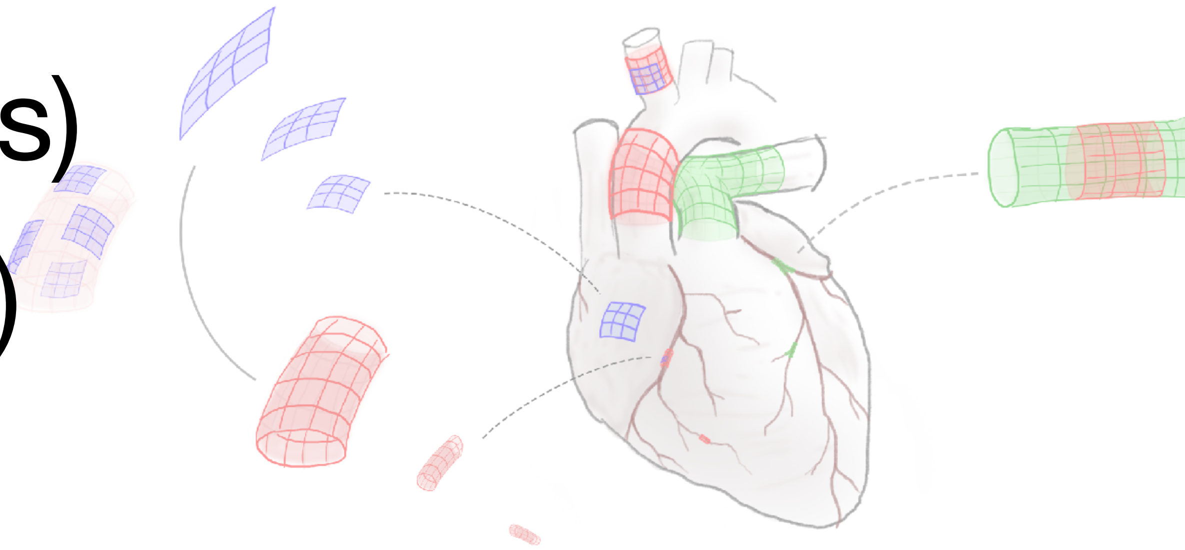
Definition 2.14 (Affine groups). Affine groups $G = \mathbb{R}^d \rtimes H$ are a class of groups that are the semidirect product of a group $H \subseteq GL(\mathbb{R}^d)$ acting on $\mathbb{R}^d$, with $GL(\mathbb{R}^d$ the group of general linear transformations acting on $\mathbb{R}^d$.

The transformations in $H \subseteq GL(\mathbb{R}^d)$ are commonly represented as invertible matrices $\mathbf{A}$ which act on $\mathbb{R}^d$ via matrix-vector multiplication, by which the group

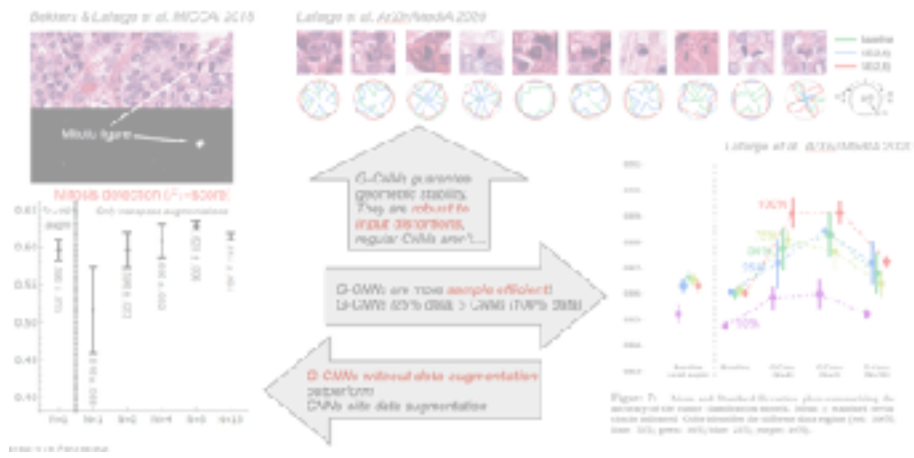
Part I

1. Why do we want equivariant learning models?
   - Geometric guarantees + weight sharing/sample efficiency

2. A group theoretical view on **recognition by components** (capsule nets)
   - Group theoretical prerequisites (**group product** and **representations**)
   - **Group convolutions** perform pattern recognition by components



3. Experimental examples



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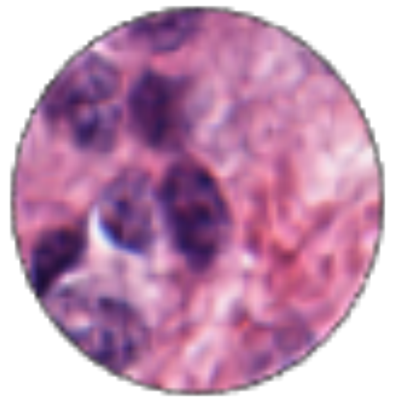
4. Theorem: Linear maps between feature maps are equivariant iff they are group convolutions

Motivation: Geometric Guarantees (invariance)

Example: Detection of pathological cells



Motivation: Geometric Guarantees (invariance)

Example: Detection of pathological cells

Healthy

?

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Pathological

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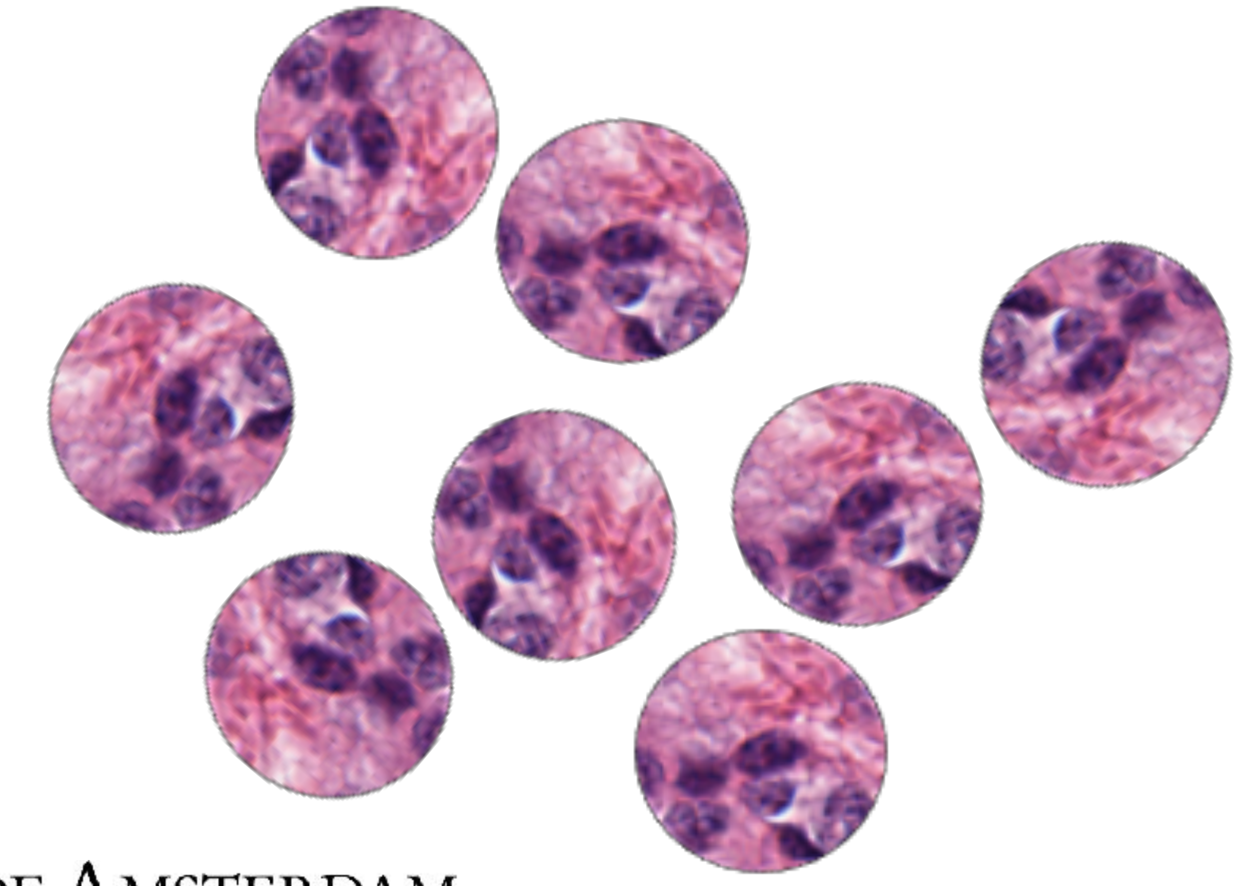
Common approach: data-augmentation



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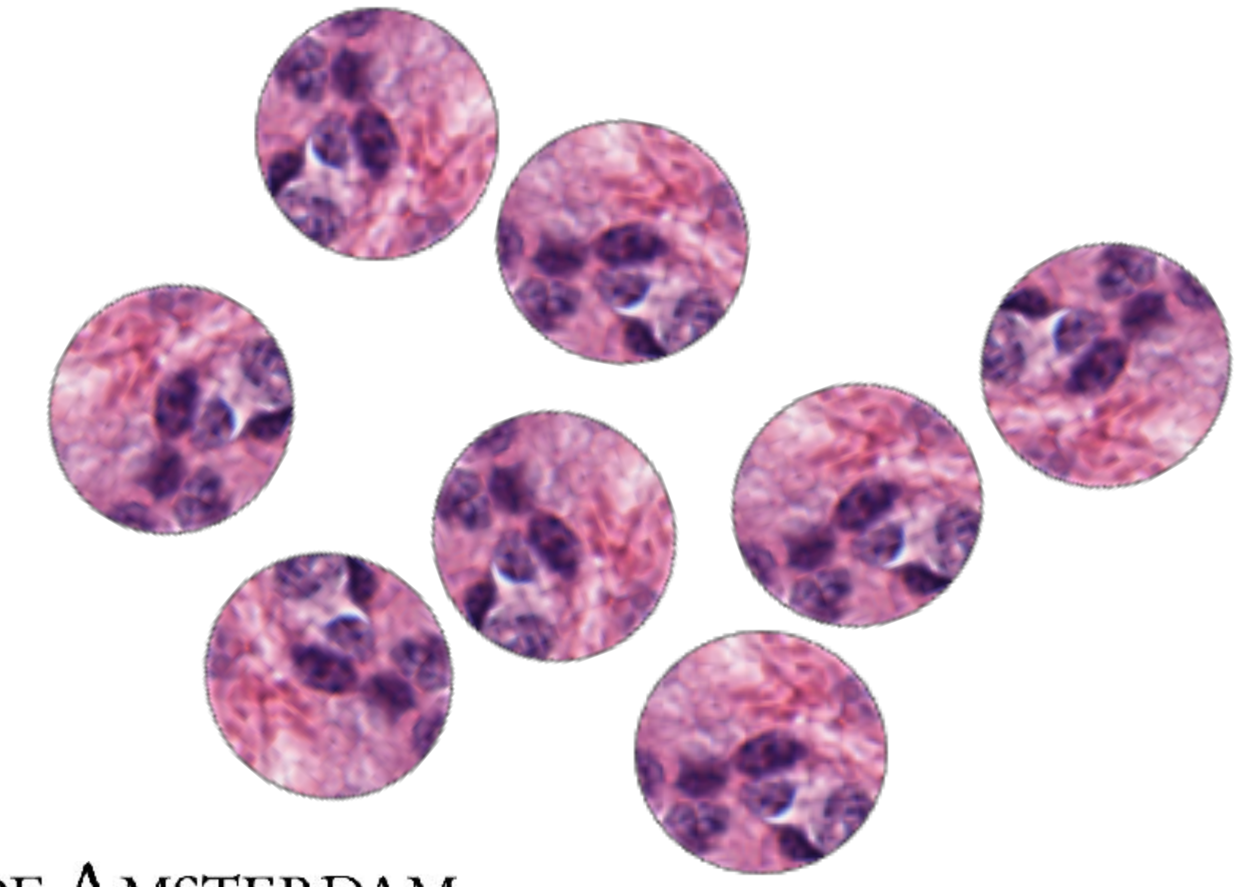

Issues:
- Still no guarantee of invariance
- Valuable net capacity is spend on learning invariance
- Redundancy in feature repr.

Motivation: Geometric Guarantees (invariance)

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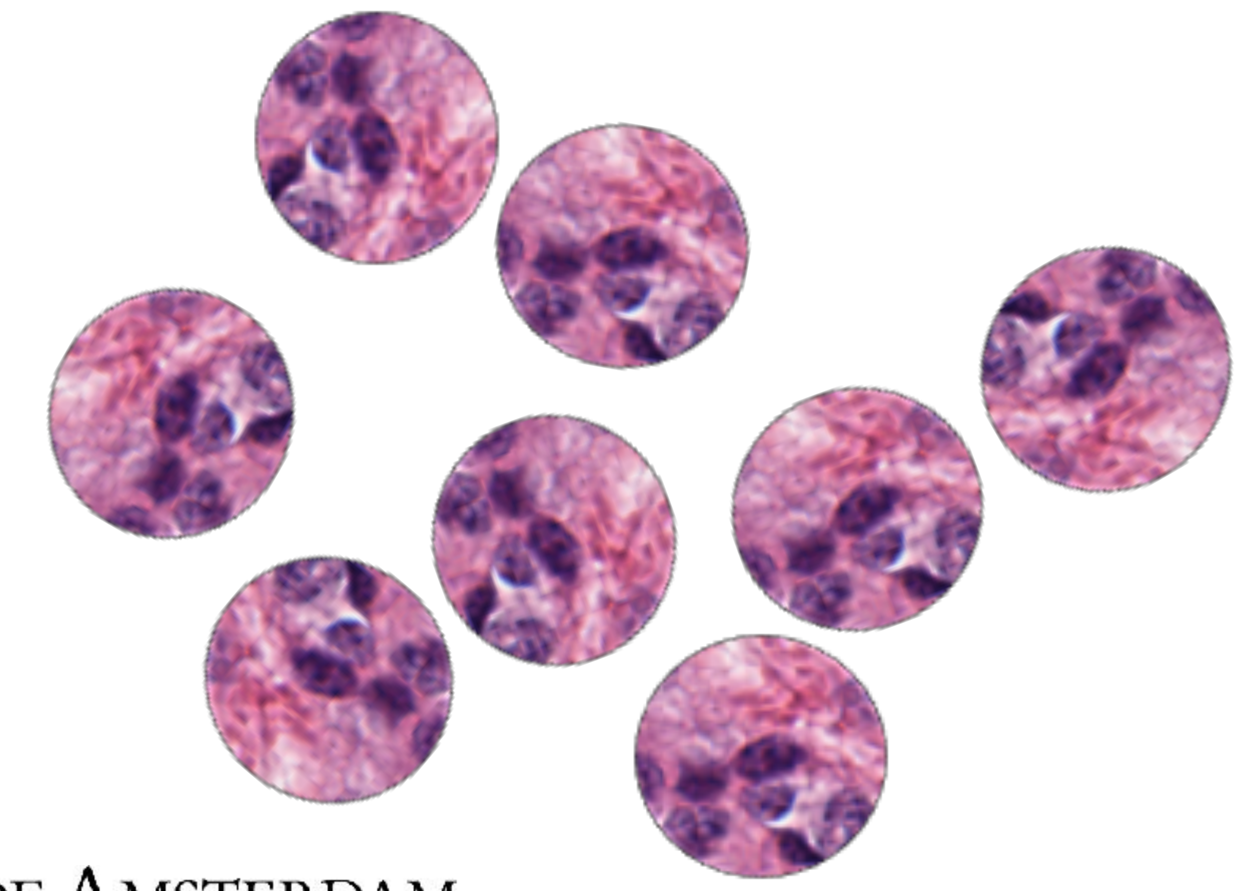
Common approach: data-augmentation



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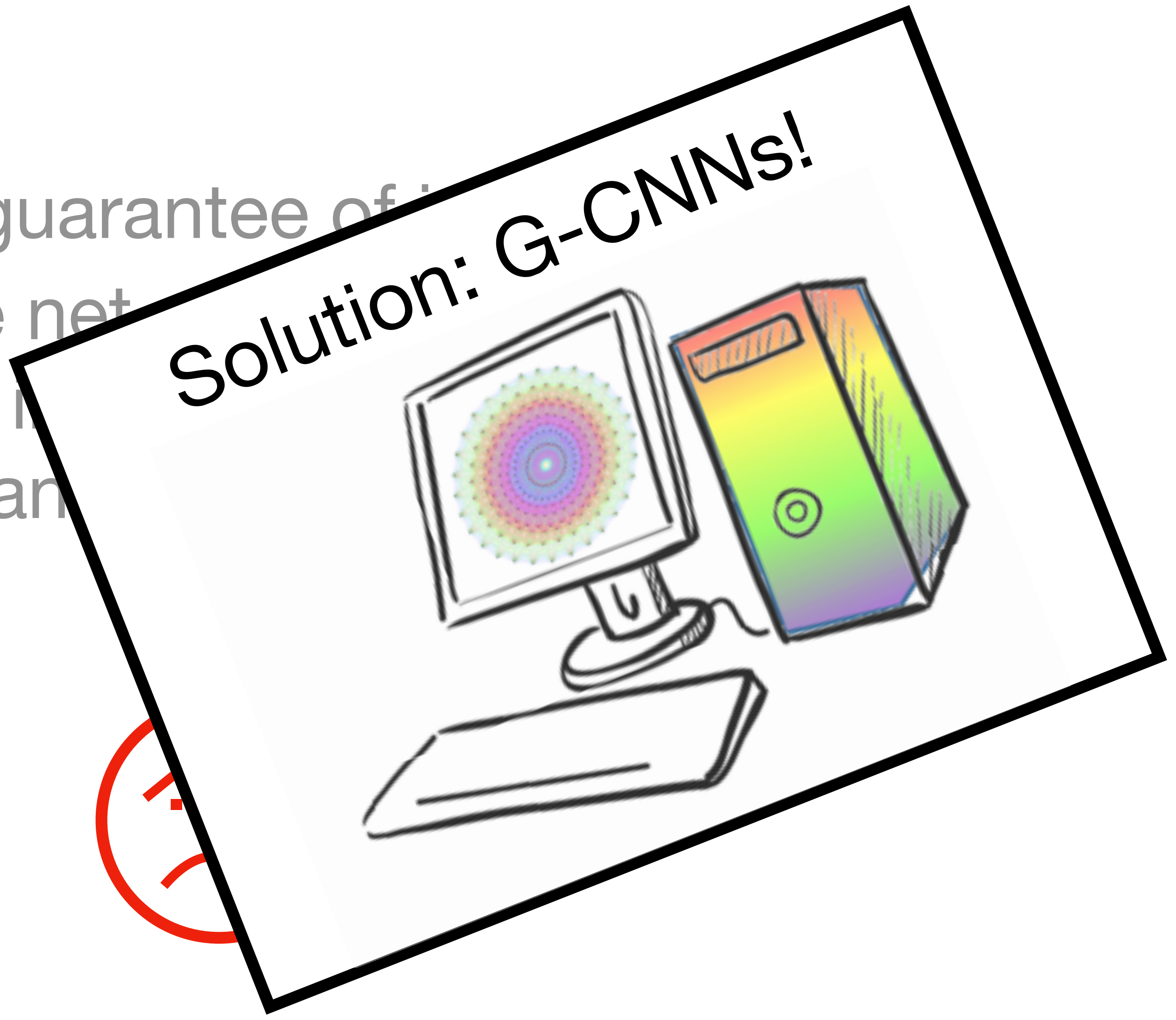

Motivation: Geometric Guarantees (equivariance)

CNNs are translation equivariant

Via convolutions

Motivation: Geometric Guarantees (equivariance)

CNNs are translation equivariant

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Motivation: Geometric Guarantees (equivariance)

CNNs are not rotation equivariant

Via convolutions

Stabilized view

Motivation: Geometric Guarantees (equivariance)

CNNs are not rotation equivariant

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Stabilized view

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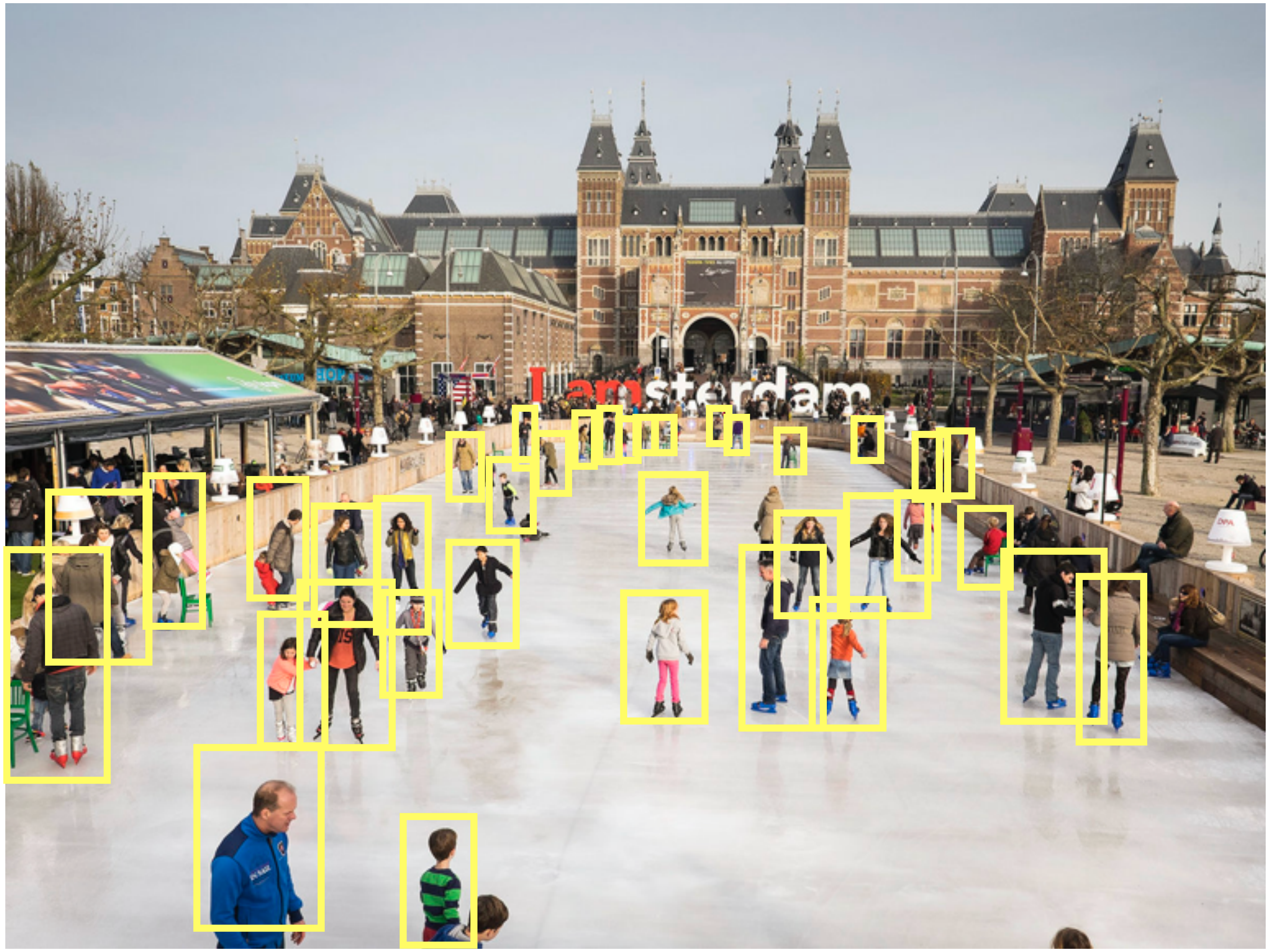


Importance of equivariance:

- No information is lost when the input is transformed
- Guaranteed stability to (local + global) transformations

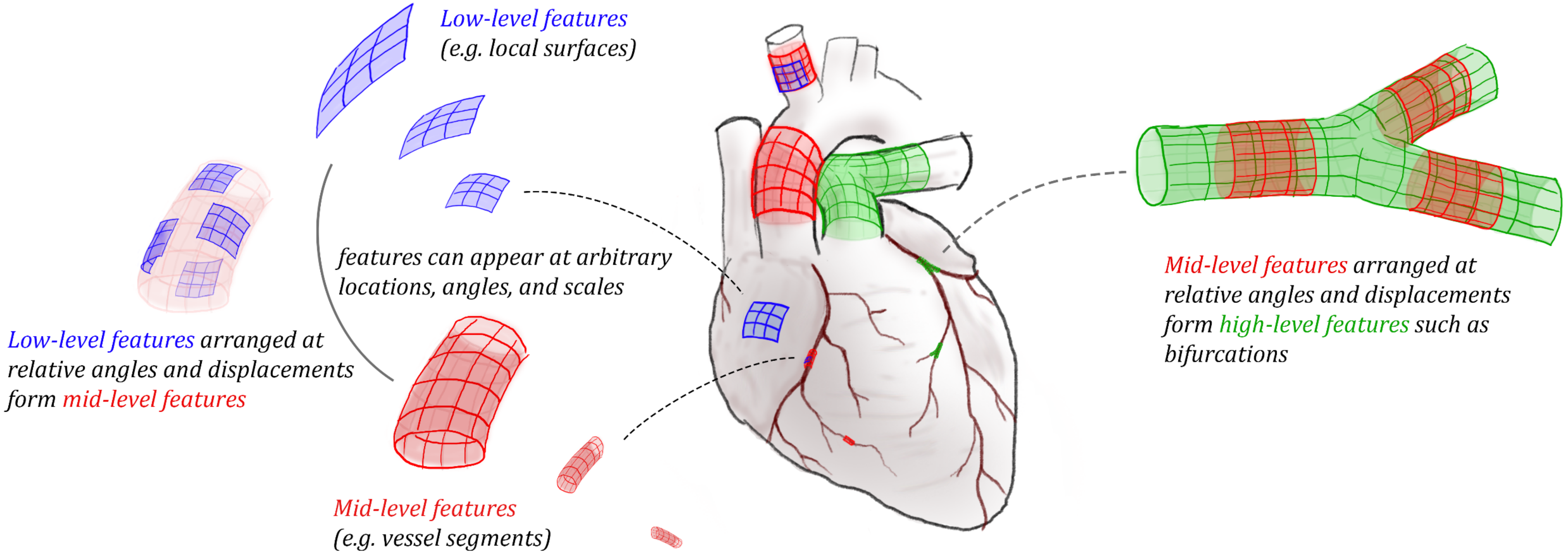
Group convolutions:

- Equivariance beyond translations
- Geometric guarantees
- Increased weight sharing

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

Motivation: Recognition by components

In a group theoretical setting



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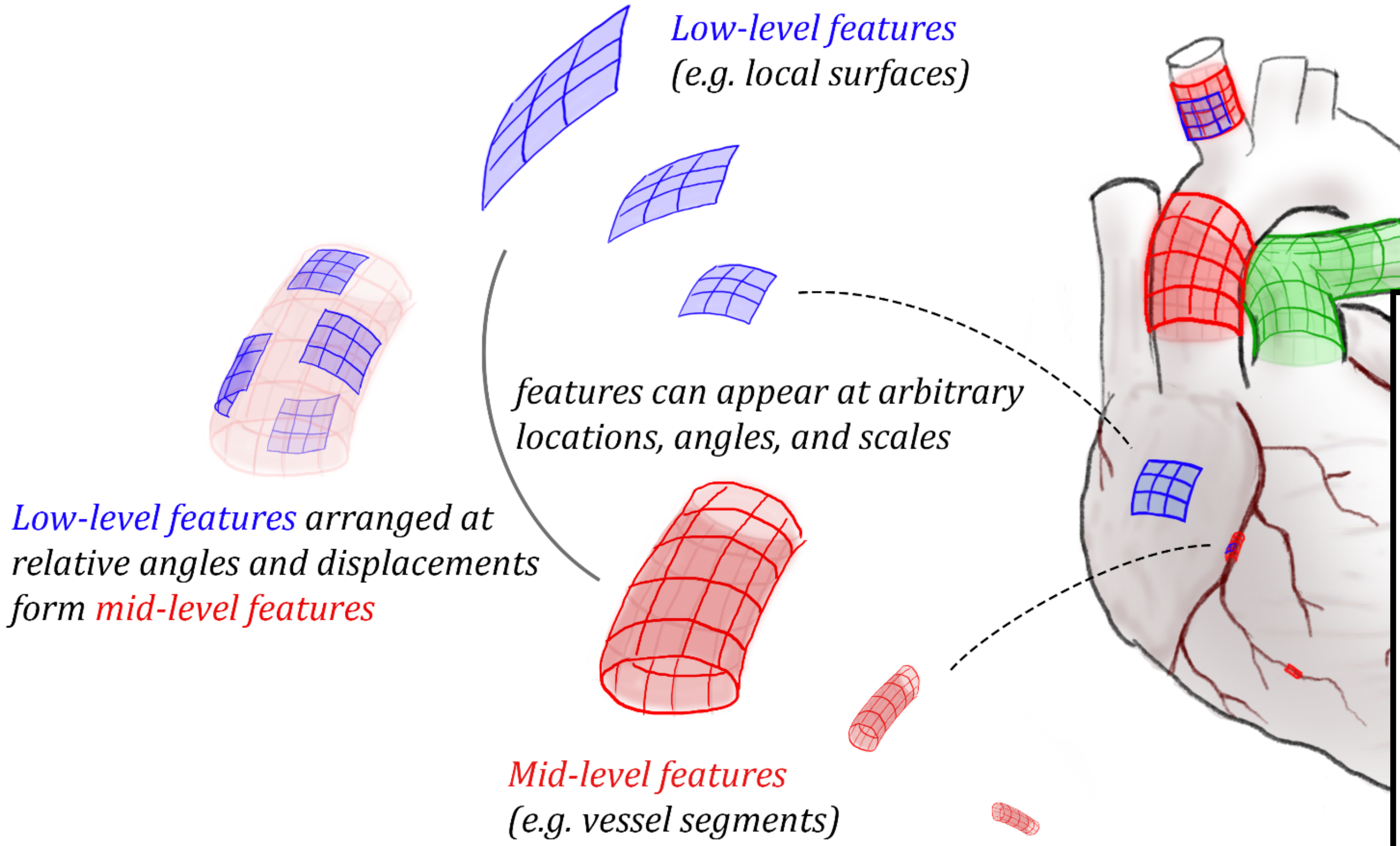

Rationale behind capsule networks

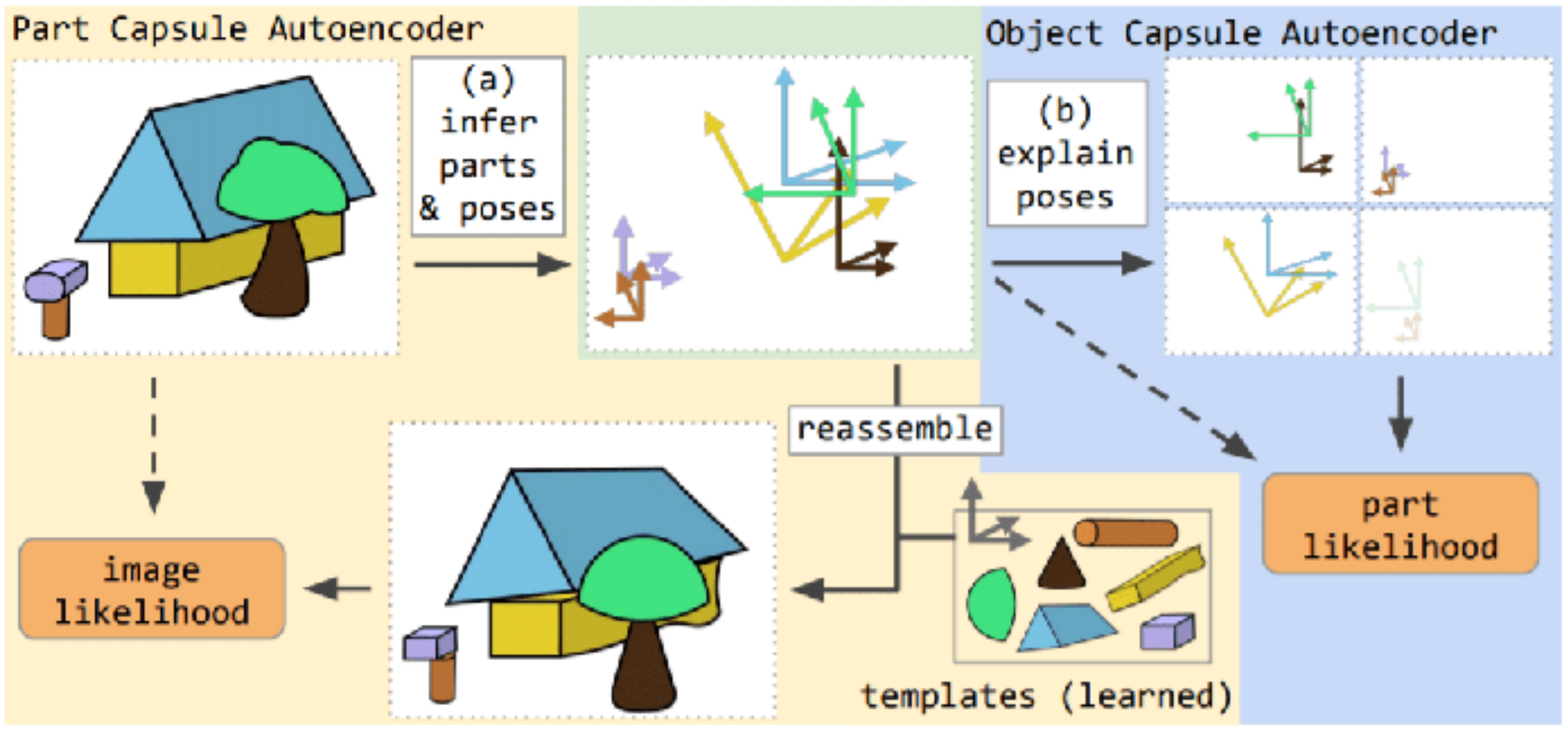

Fig from Kosiorek et al. 2019

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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:

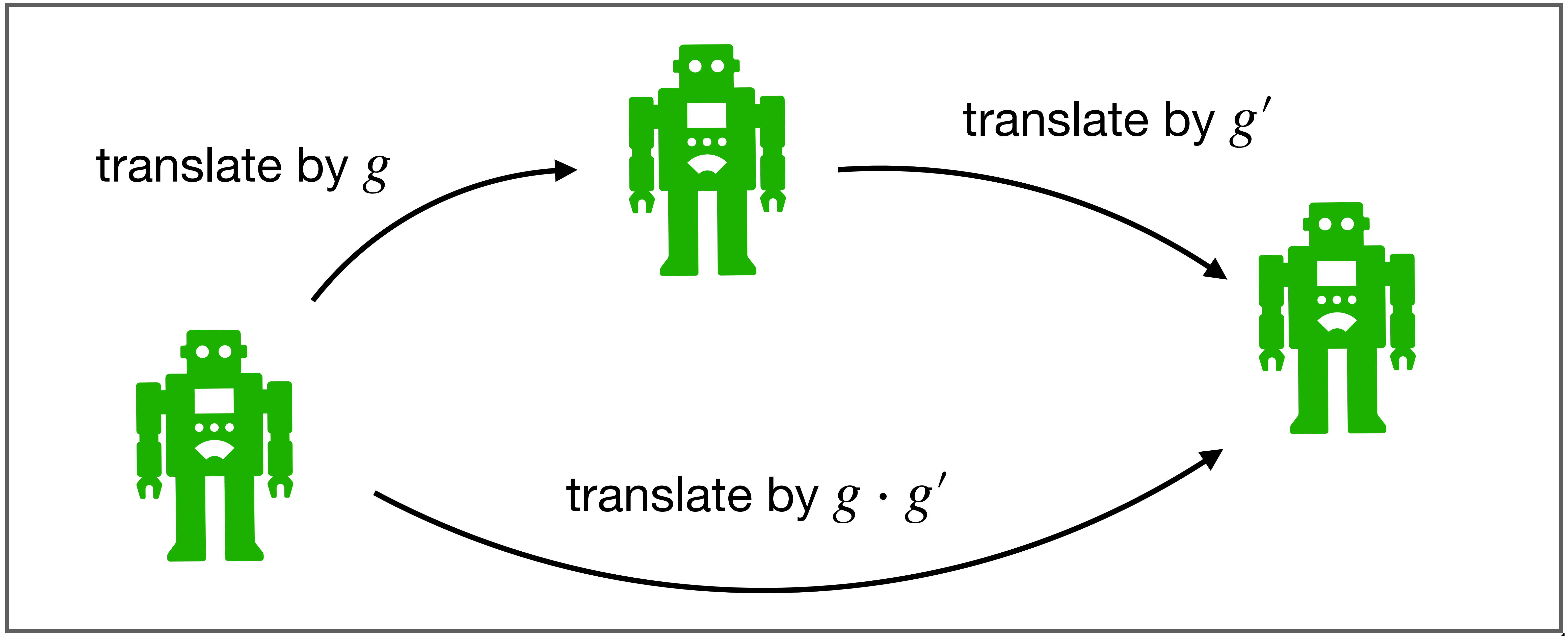
- **Closure**: Given two elements g and h of G, the product $g \cdot h$ is also in G.
- **Associativity**: For $g, h, i \in G$ the product $\cdot$ is associative, i.e., $g \cdot (h \cdot i) = (g \cdot h) \cdot i$.
- **Identity element**: There exists an identity element $e \in G$ such that $e \cdot g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

The 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 $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2$.



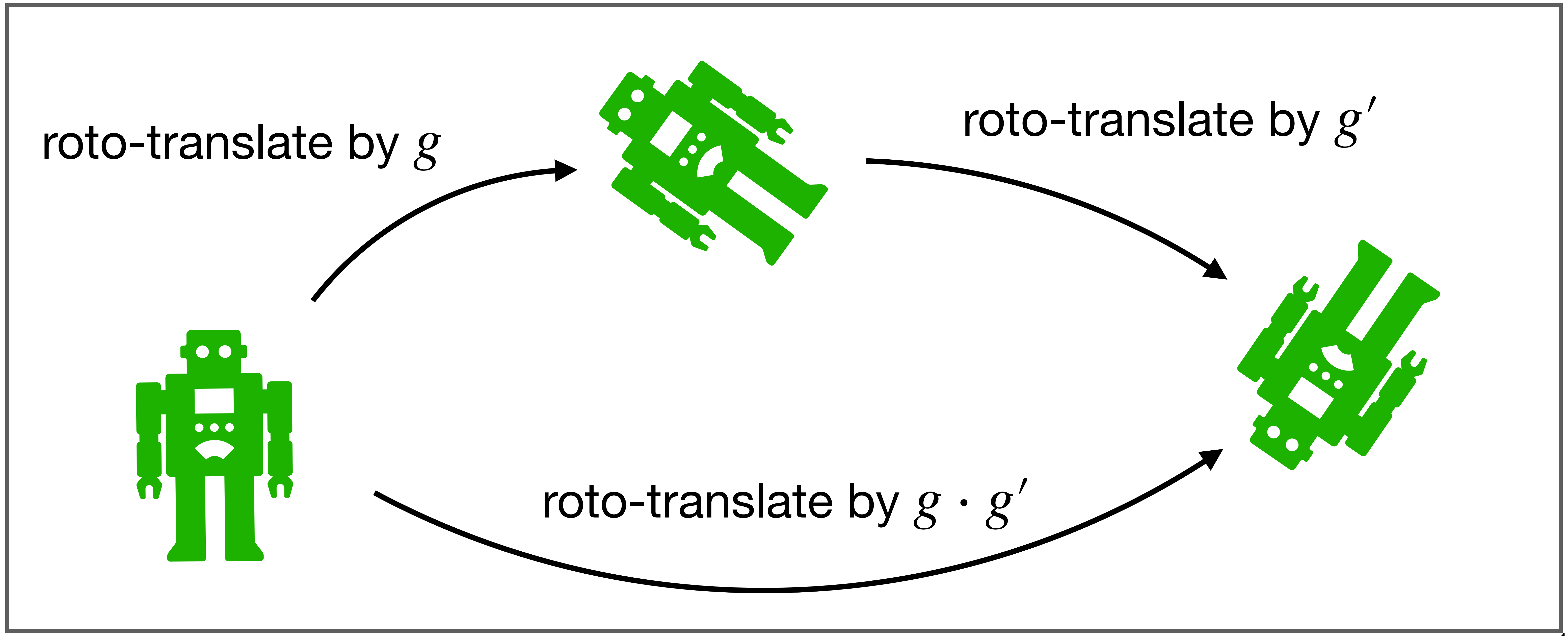
The roto-translation group $SE(2)$

*2D **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 $g = (\mathbf{x}, \mathbf{R}_\theta)$, $g' = (\mathbf{x}', \mathbf{R}_{\theta'})$.



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

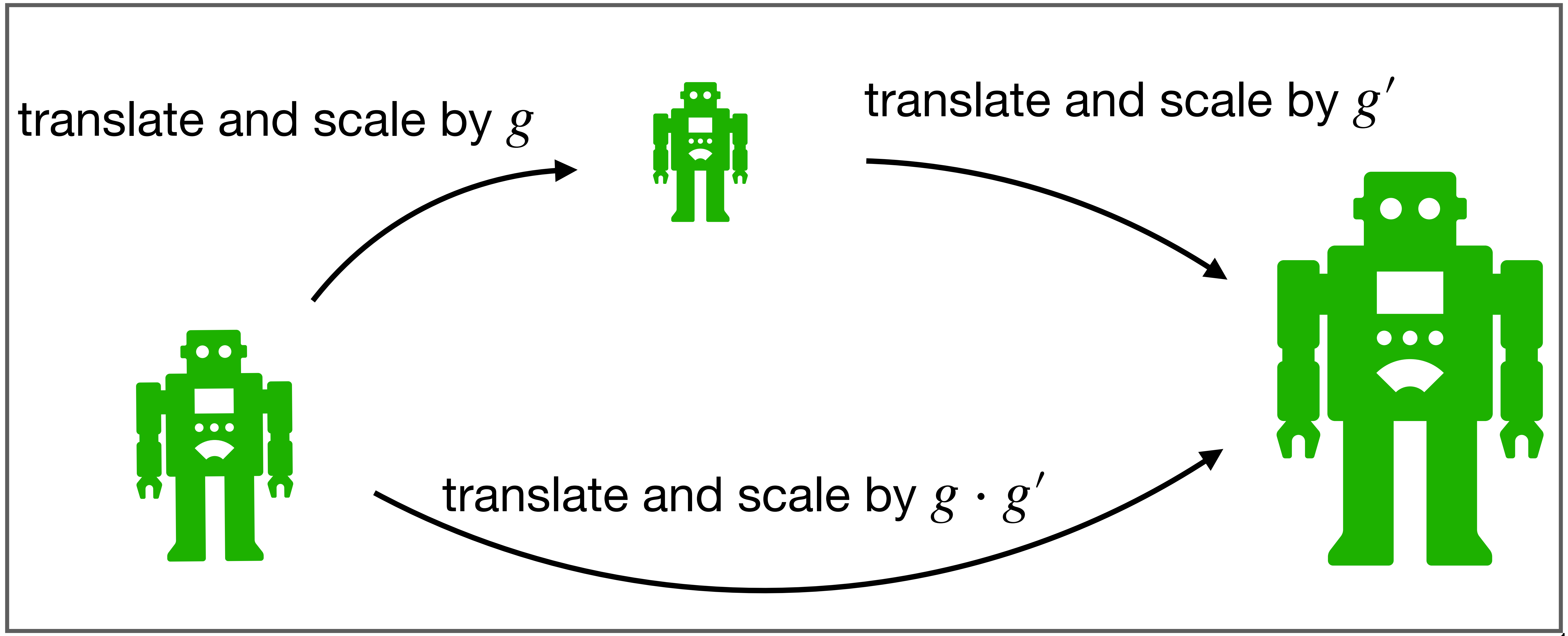
The scale-translation group of space $\mathbb{R}^2 \times \mathbb{R}^+$ of translations vectors in $\mathbb{R}^2$ and scale/dilation factors in $\mathbb{R}^+$, and is equipped with the group product and group inverse:

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

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

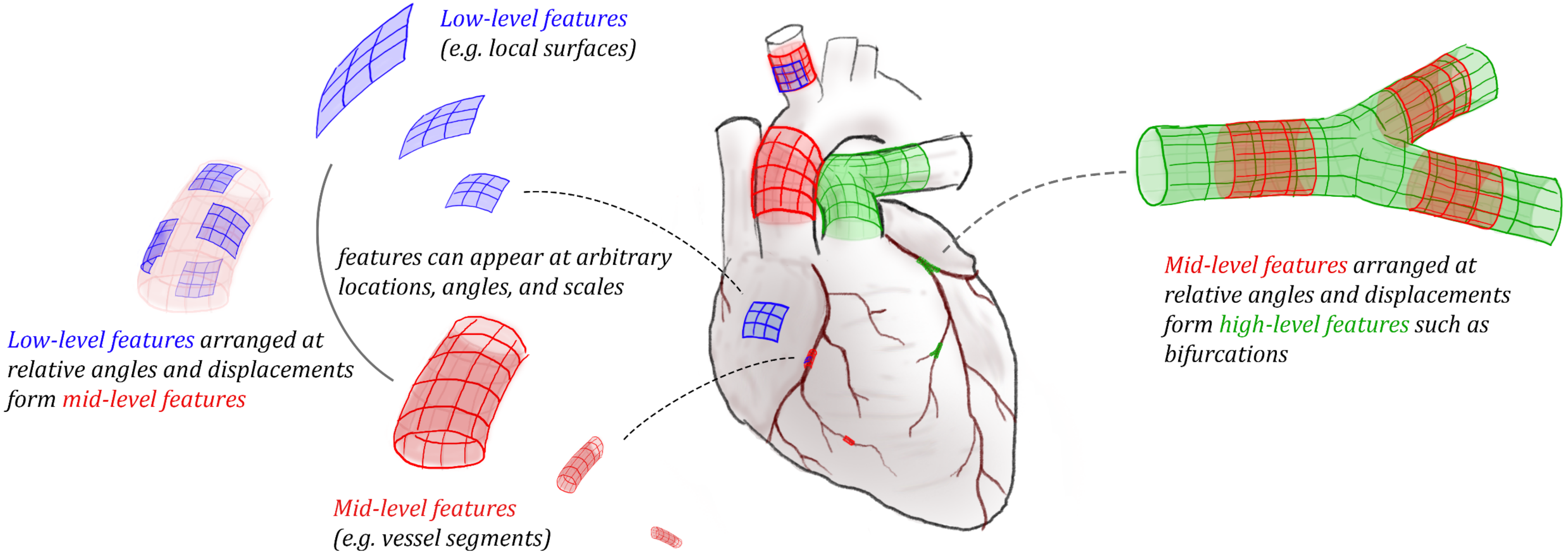
with $g \cdot g^{-1} = e = (\mathbf{0},1)$

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



Motivation: Recognition by components

In a group theoretical setting



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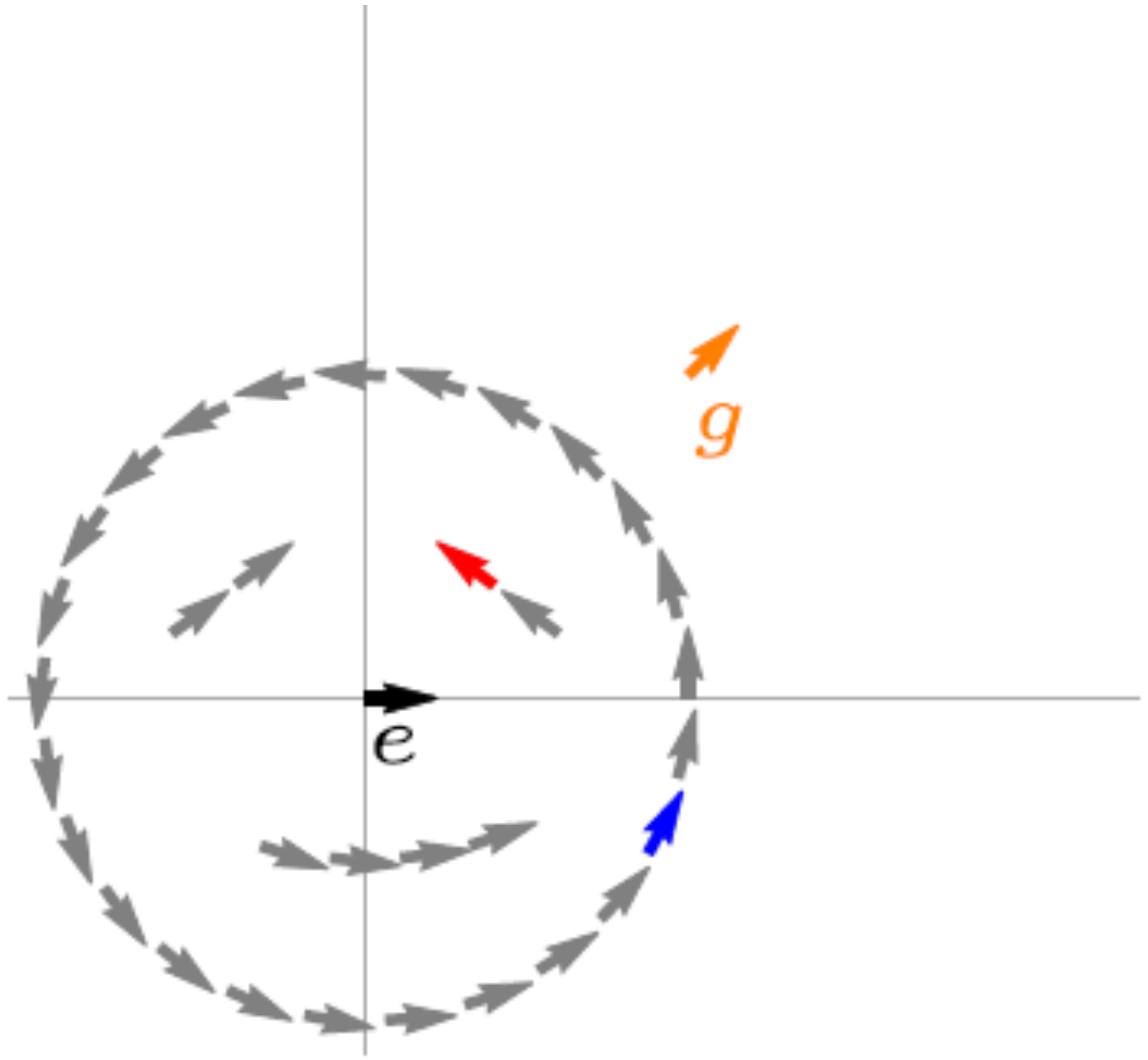

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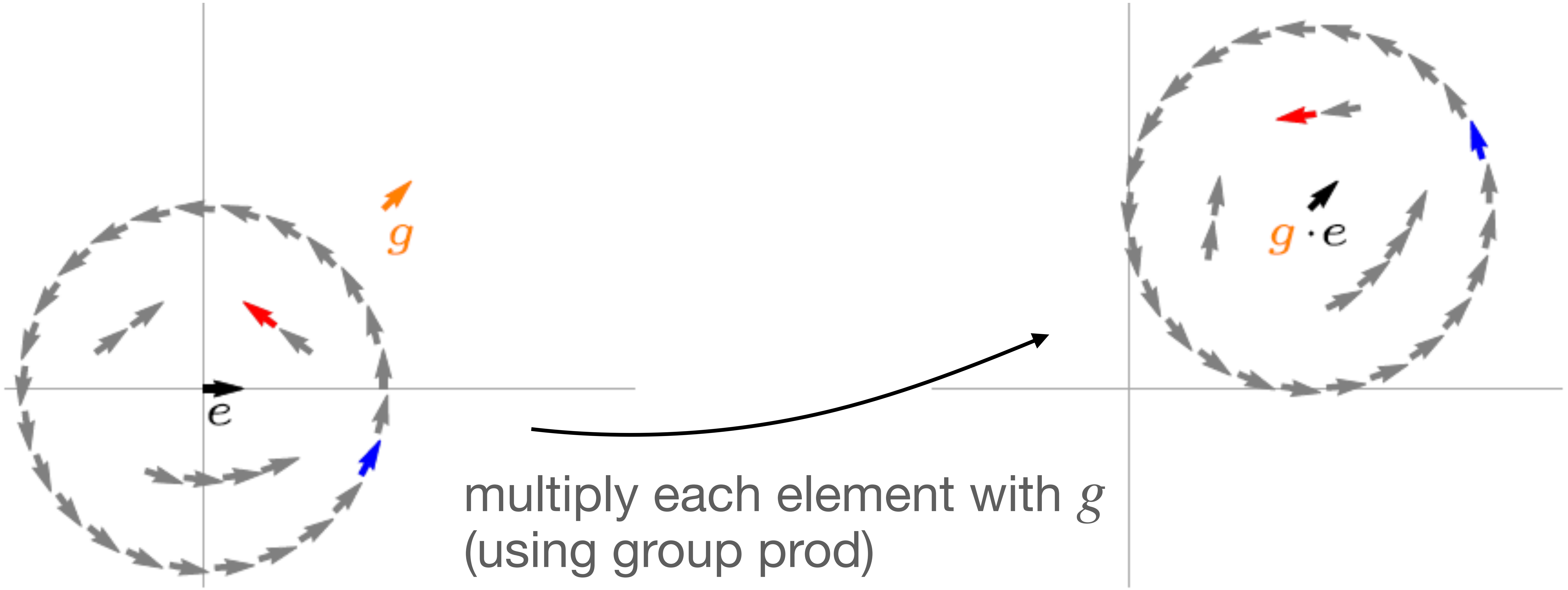
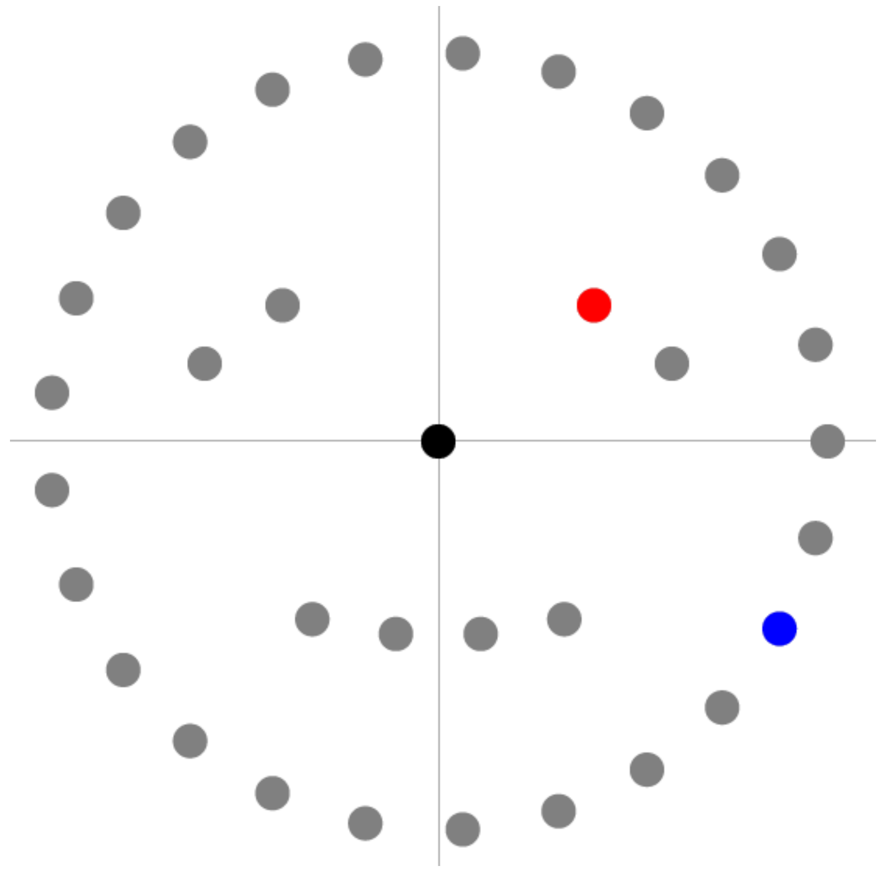
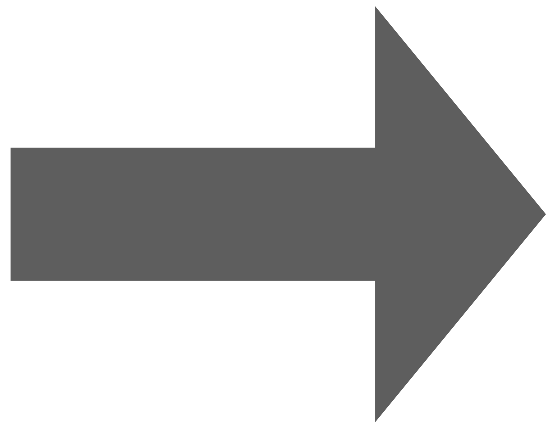


So… How to translate this to (G-)CNNs?

Set of points (group elements)





Convolution kernel

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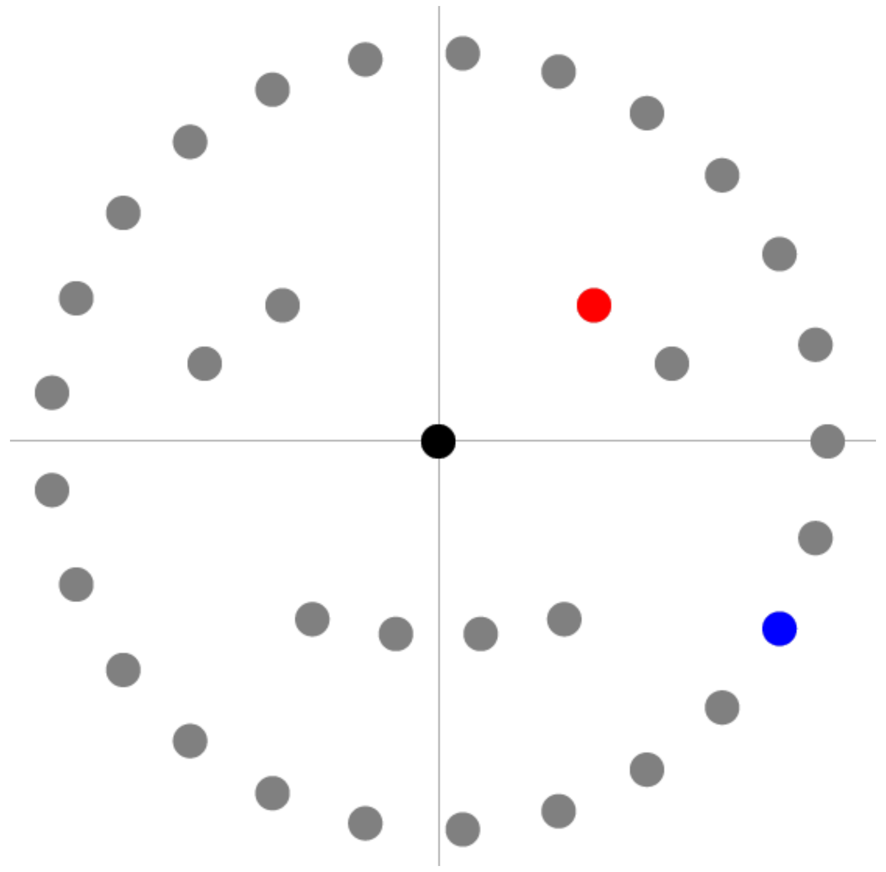
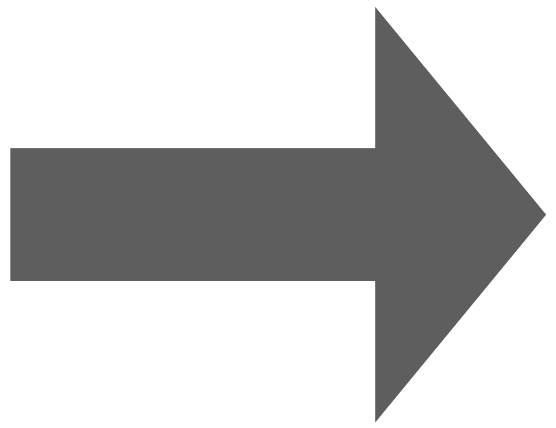


$$\{g_1, g_2, \ldots\} \subset G = (\mathbb{R}^2, +)$$

"A collection of parts in certain poses"



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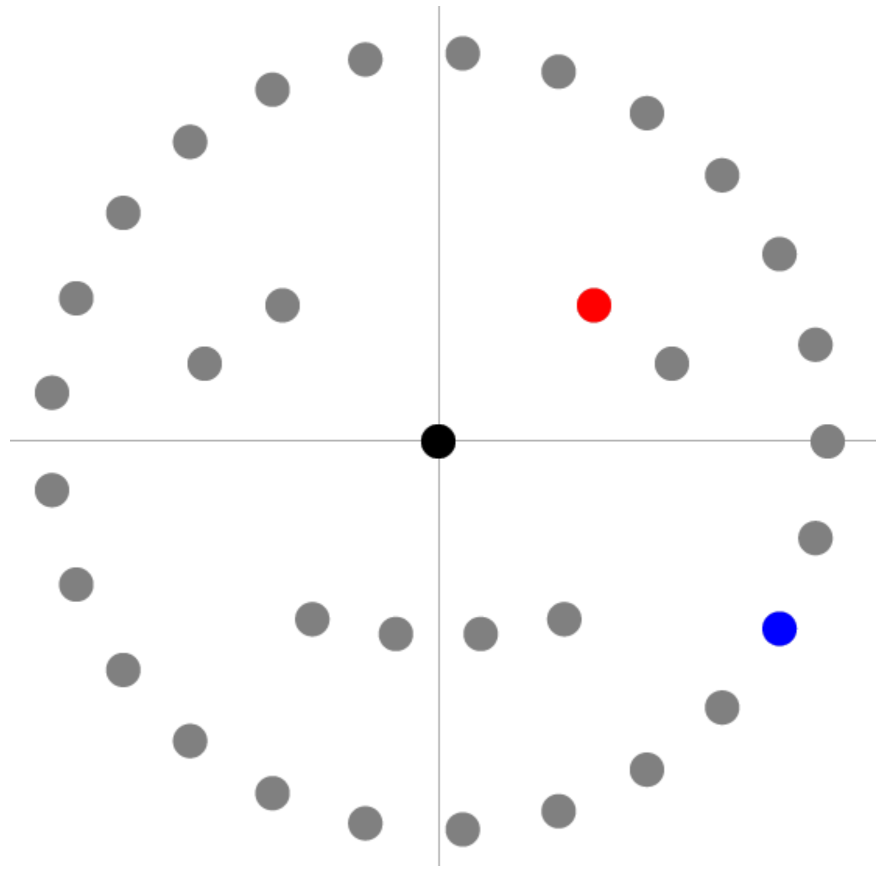


Convolution kernel

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

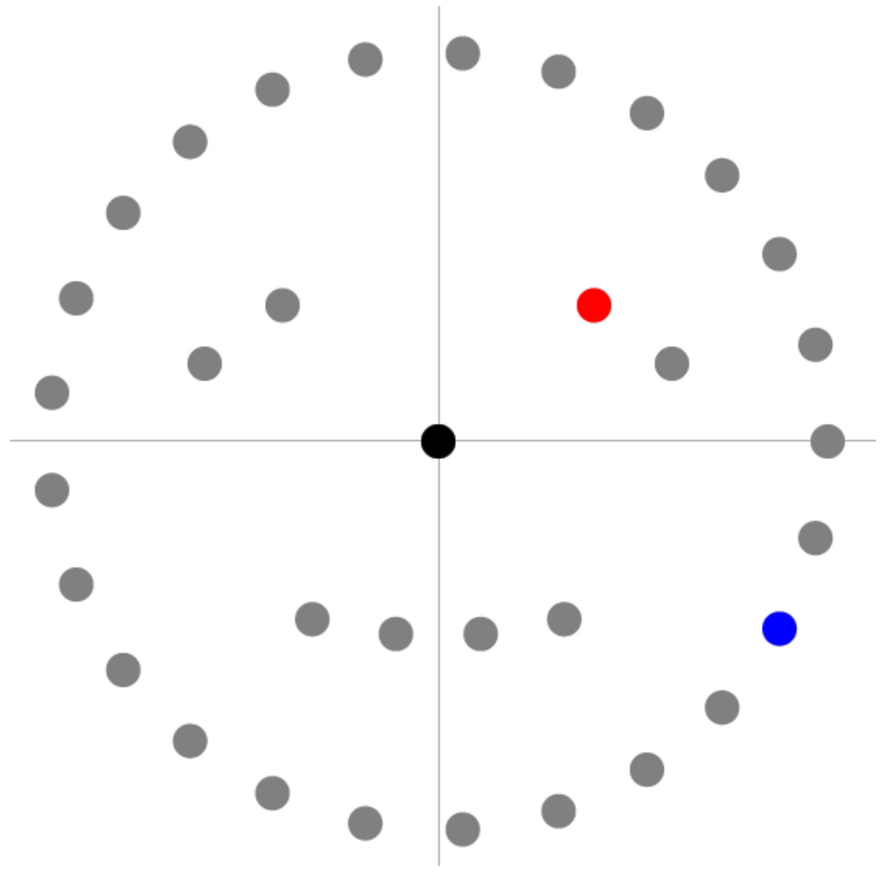
$k \in \mathbb{L}_2(\mathbb{R}^2)$

"A collection of parts in certain poses"

"Assigning weights to relative poses"

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

Set of points (group elements)



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Transforms via group product

Convolution kernel

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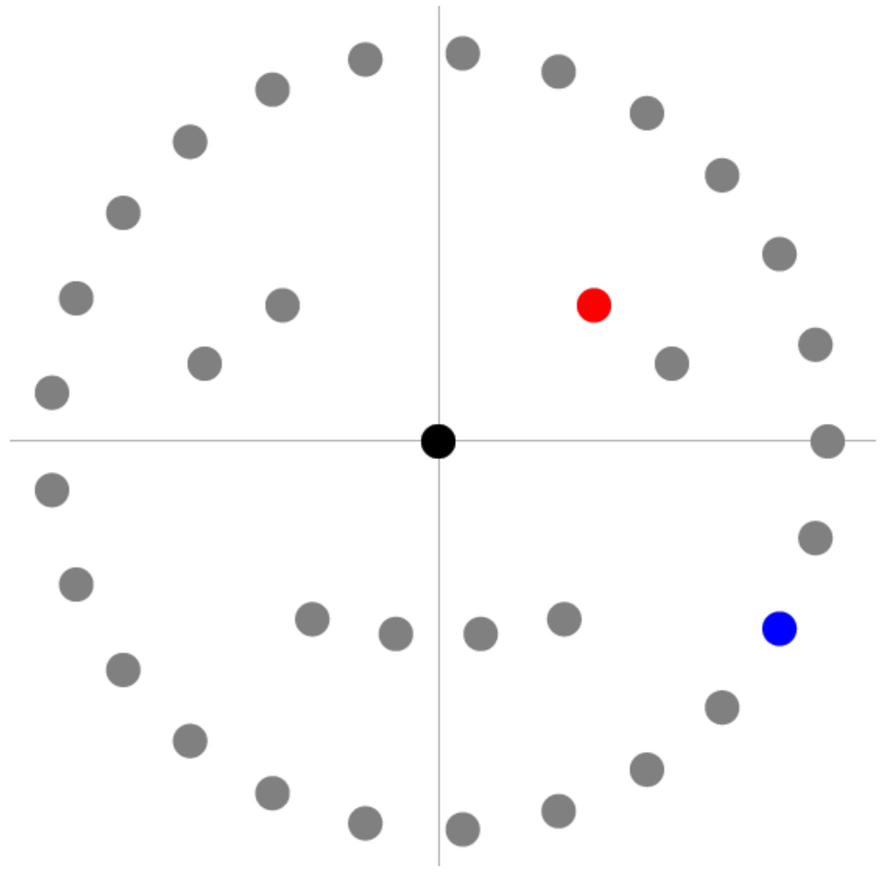
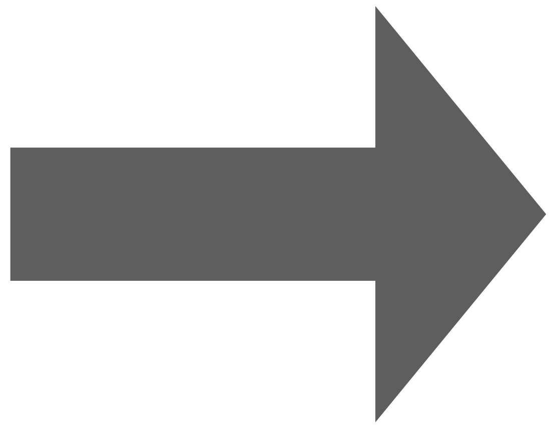


Convolution kernel



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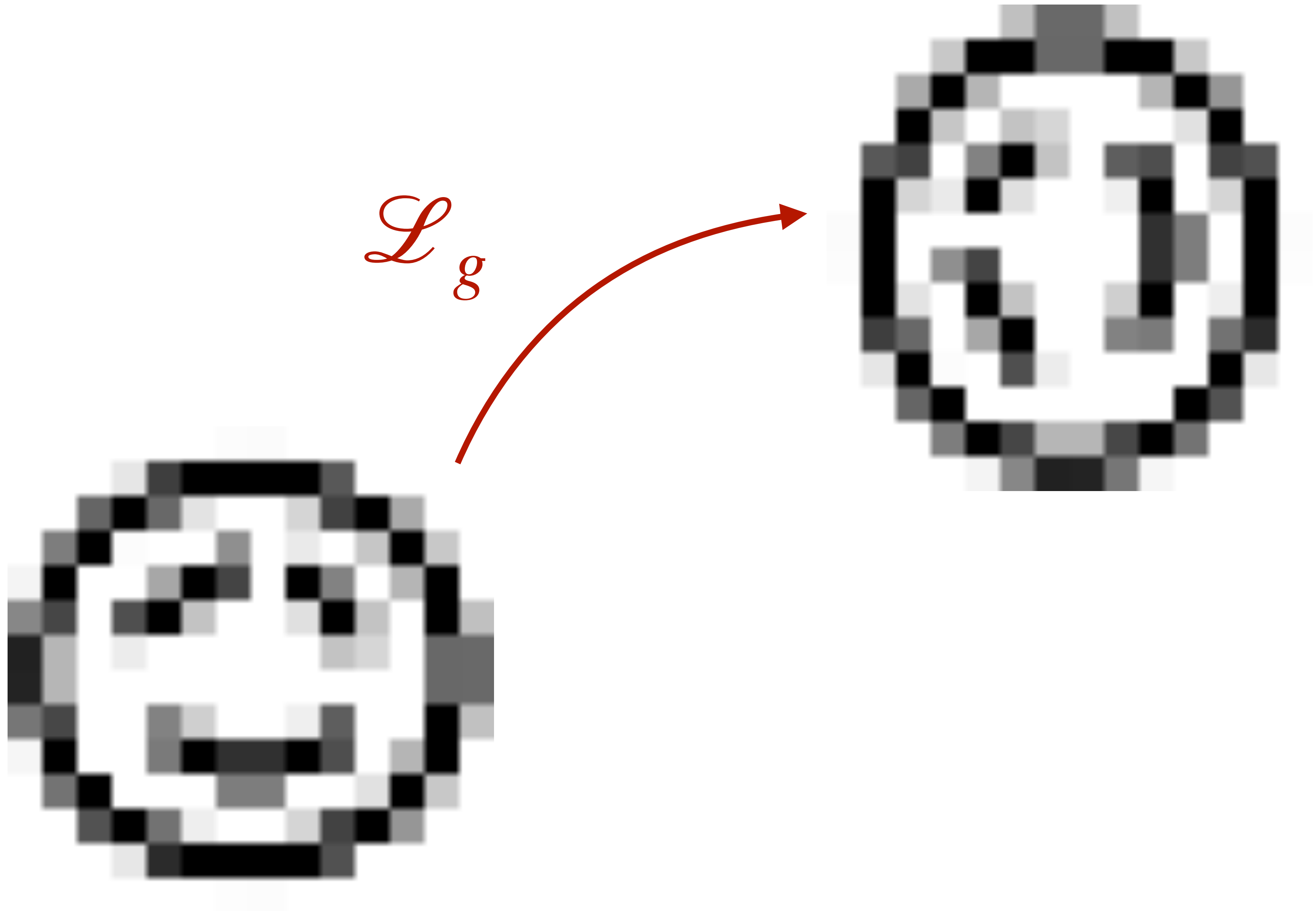
"A collection of parts in certain poses"

"Assigning weights to relative poses"

Transforms via group product

Transforms via group representations

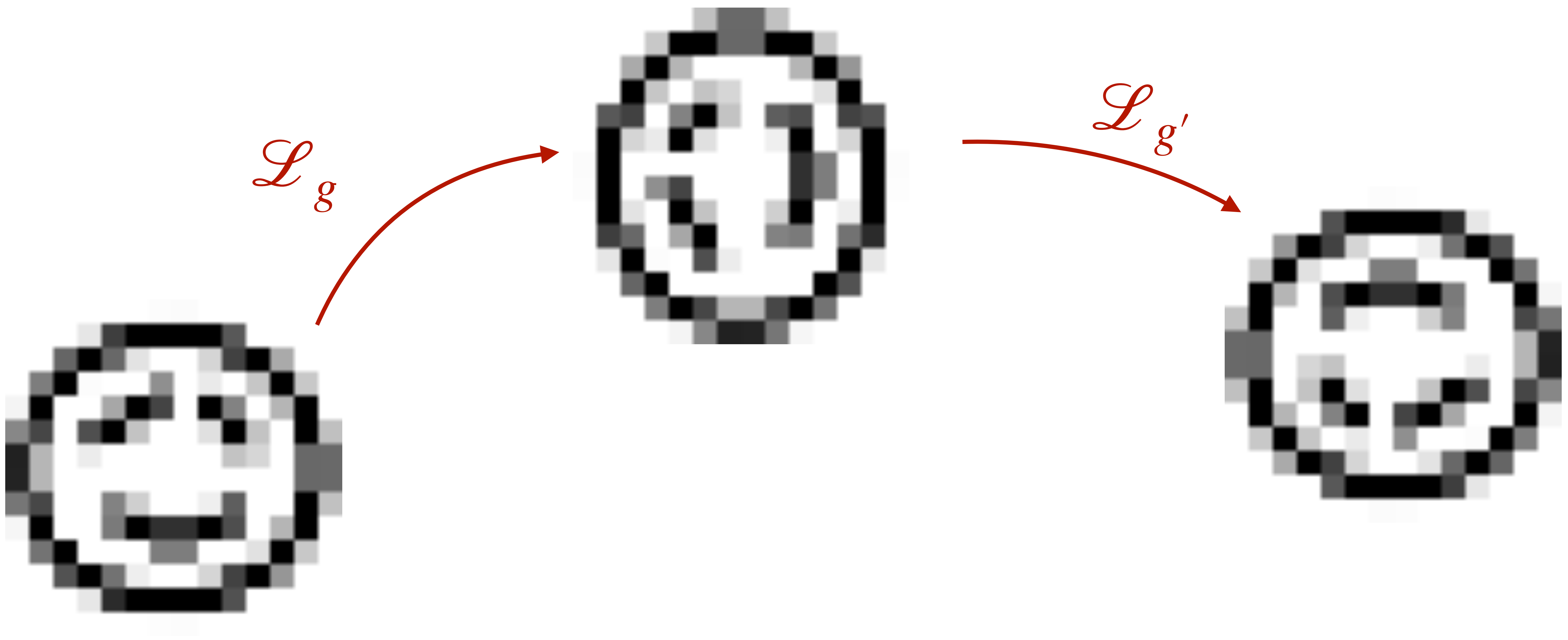
Representations



A linear operator $\mathscr{L}_g$ that is parameterized by group elements $g \in G$ that transforms some object f (e.g. an image) is called a representation of G if it caries the group structure in the following way

$$\mathscr{L}_{g'}(\mathscr{L}_g(f)) = \mathscr{L}_{g' \cdot g}(f)$$

Representations



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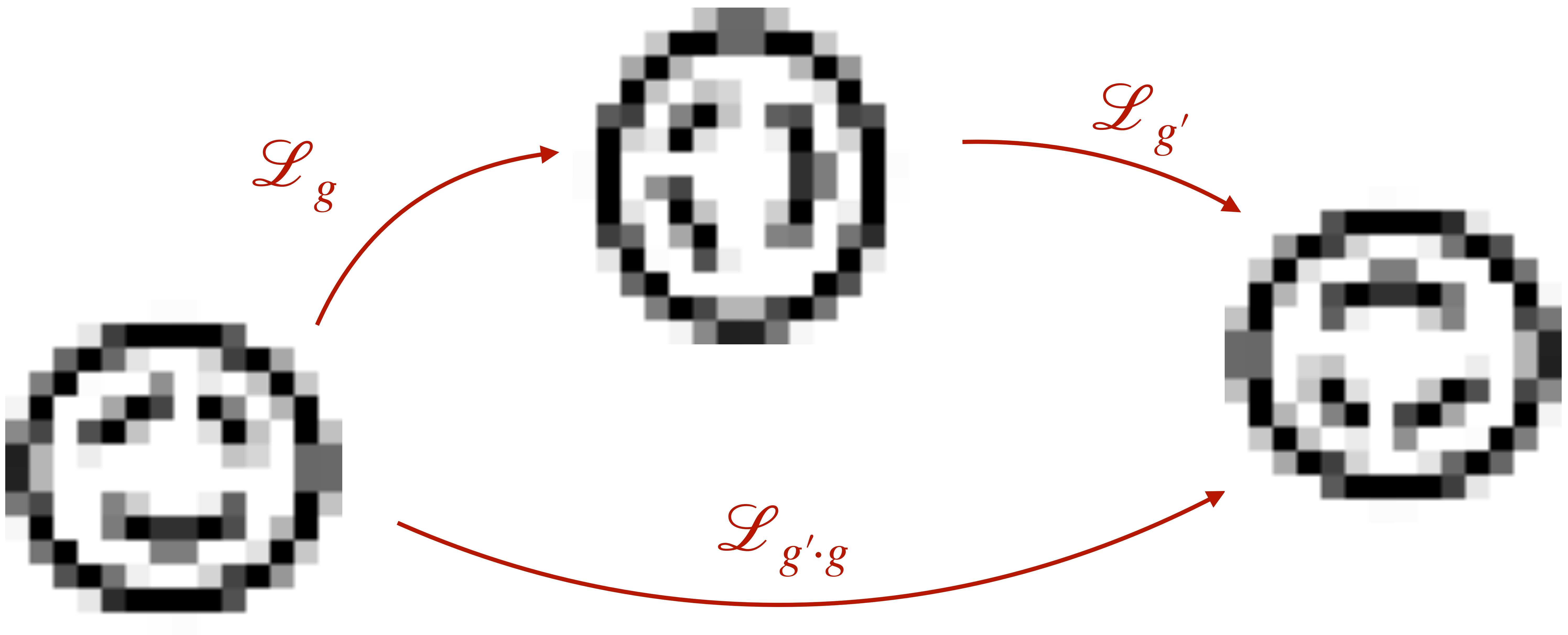

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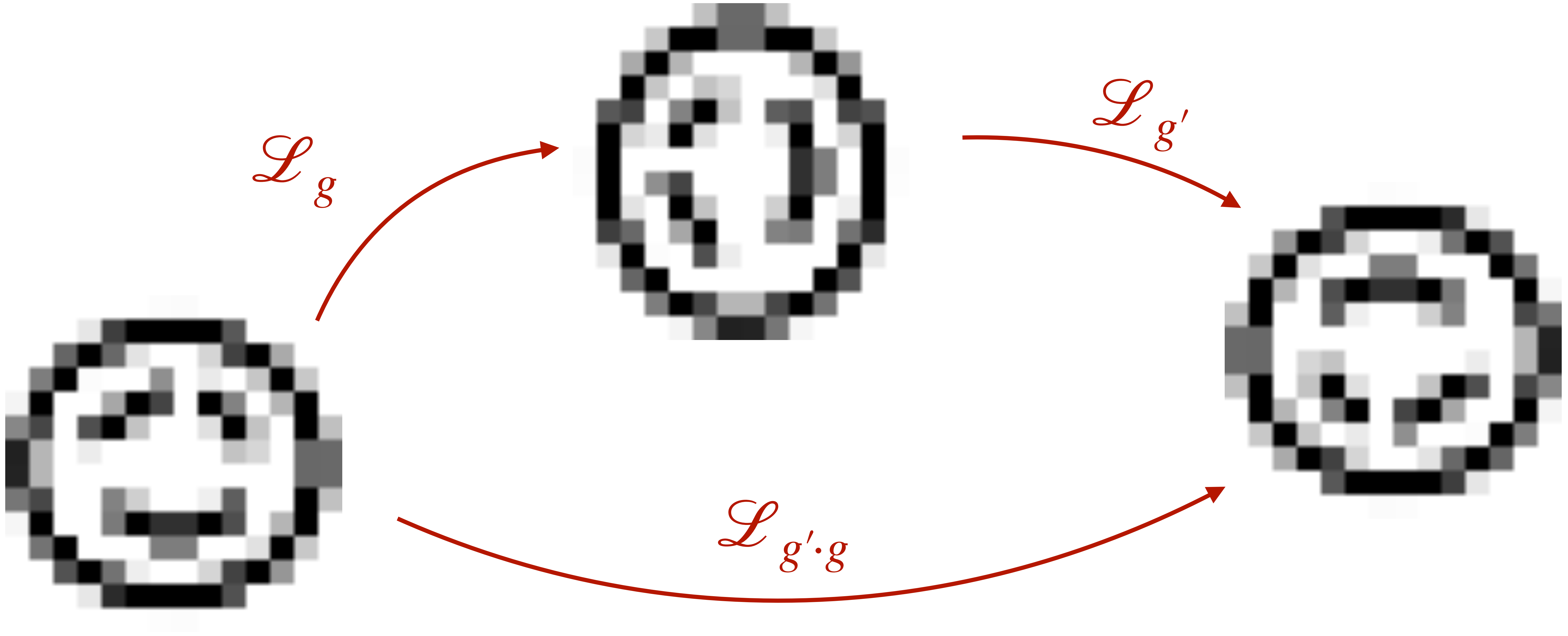
Left-regular representations

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



The left-regular representation of G transforms functions by acting on the domain on which they are defined via

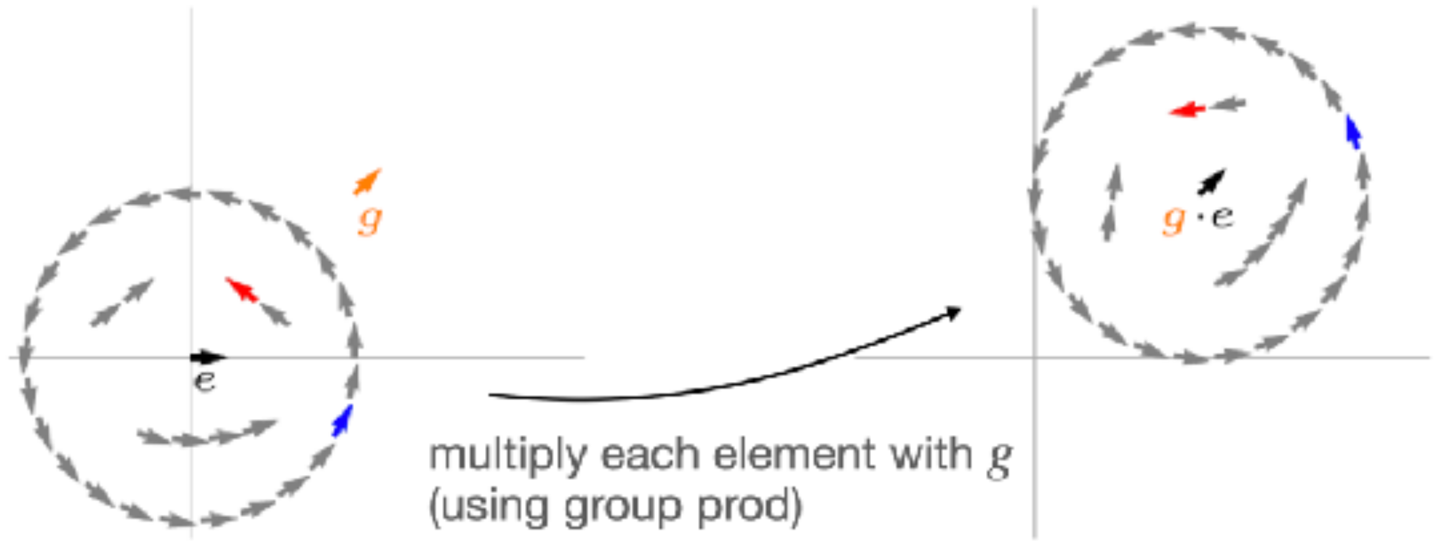
$$\mathscr{L}_g(f)(\mathbf{y}) = f(g^{-1} \odot \mathbf{y})$$

"group action" equals group product when $X = G$

Group actions

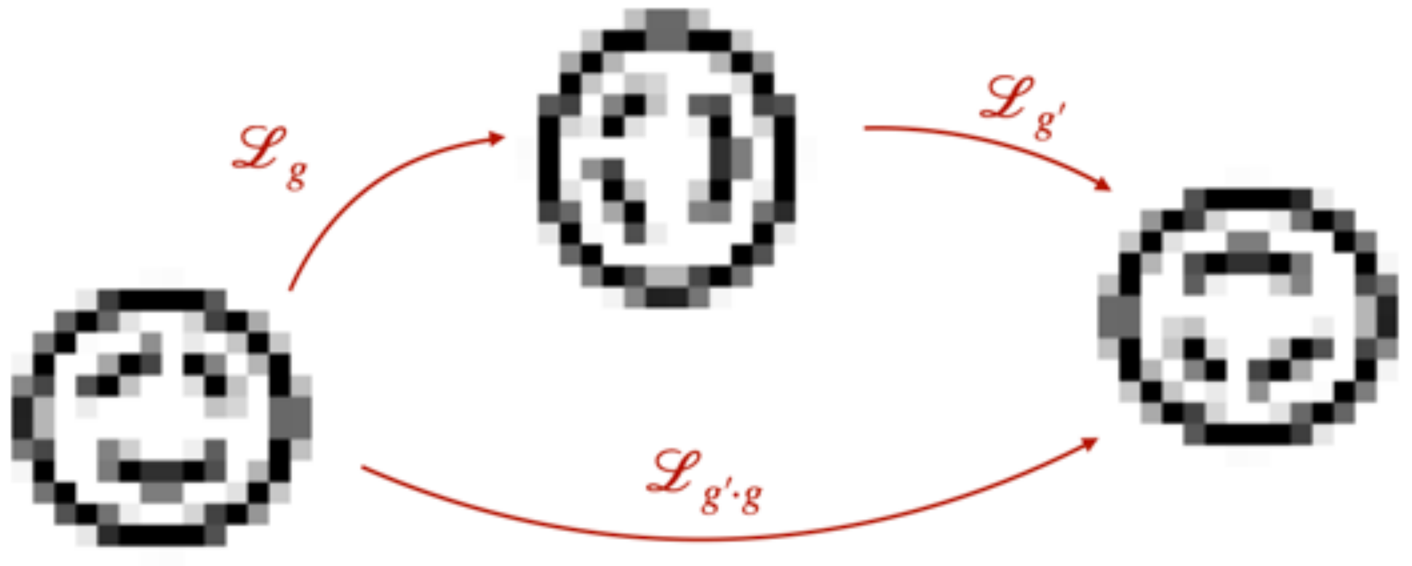
Group product (the action on G)

$$g \cdot g'$$



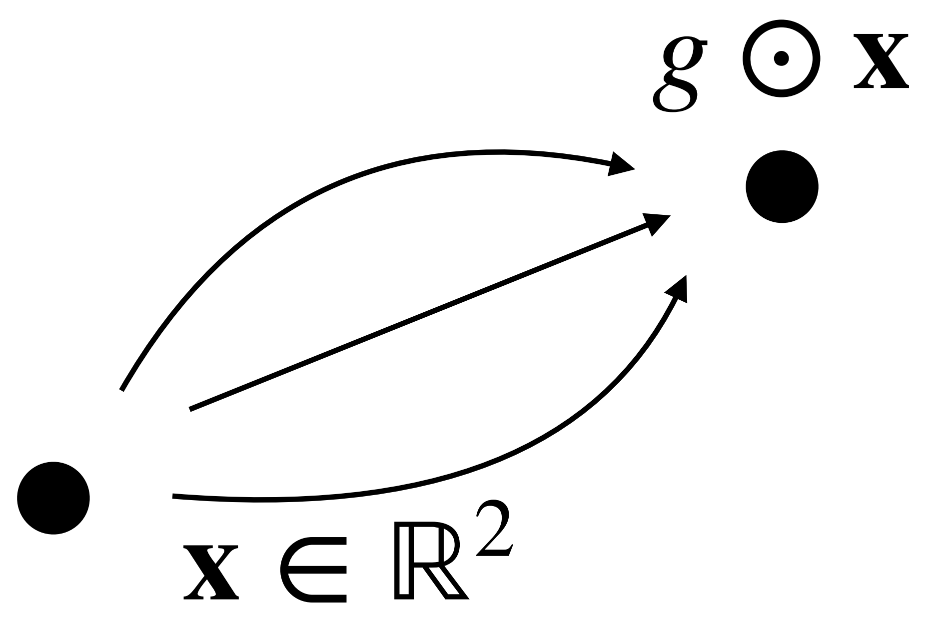
Left regular representation (the action on $\mathbb{L}_2(X)$)

$$\mathscr{L}_g f$$



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

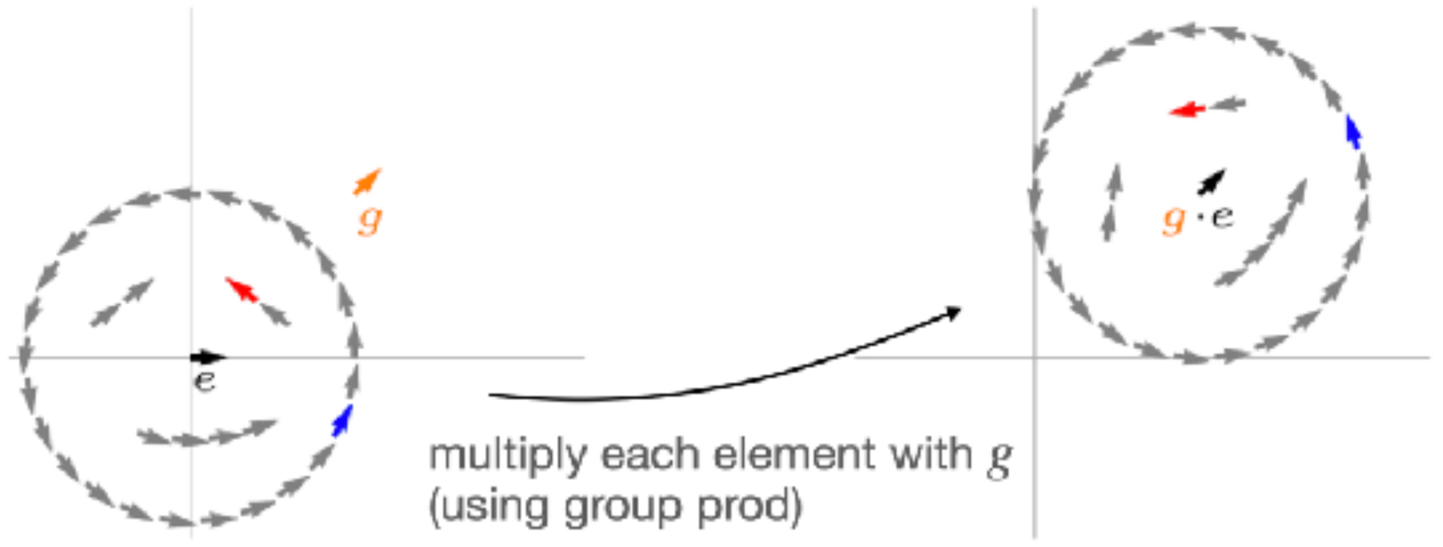
$$g \odot \mathbf{x}$$



Group actions

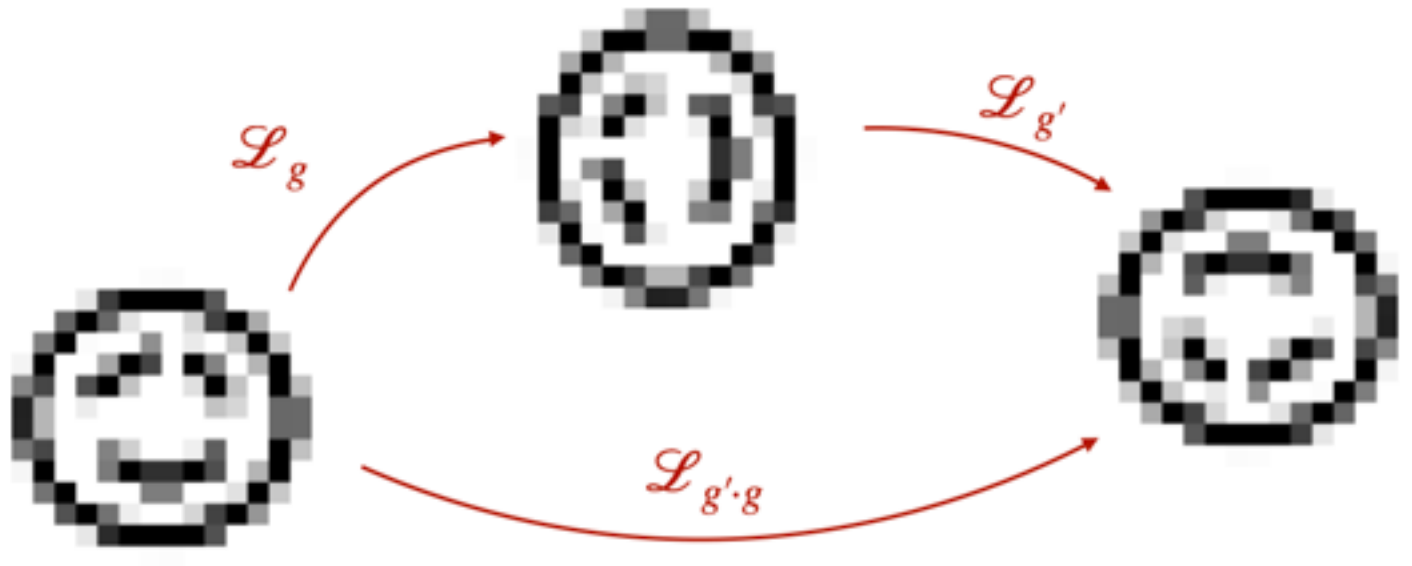
Group product (the action on G)

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



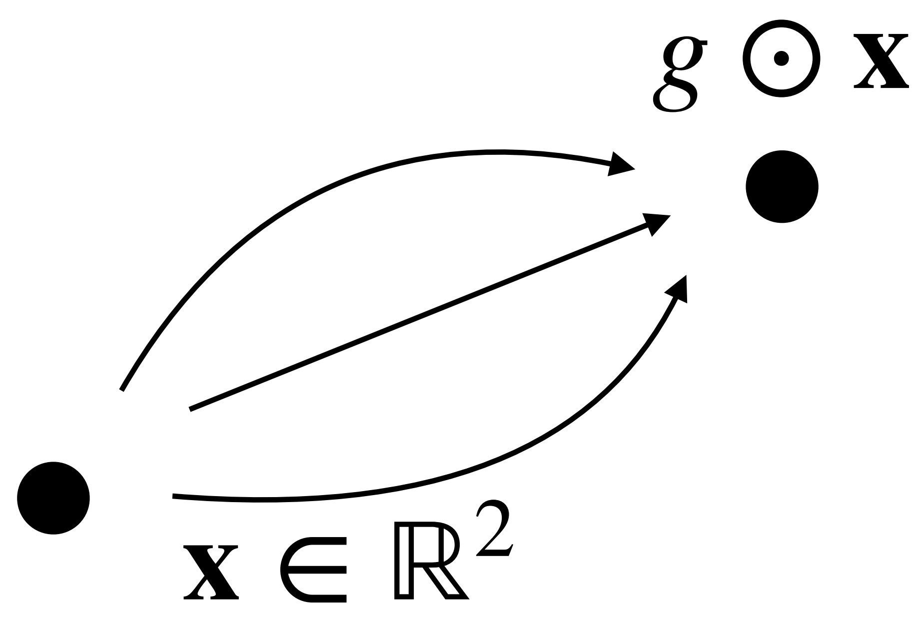
Left regular representation (the action on $\mathbb{L}_2(X)$)

$\mathscr{L}_g f$ $\qquad$ gf



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

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

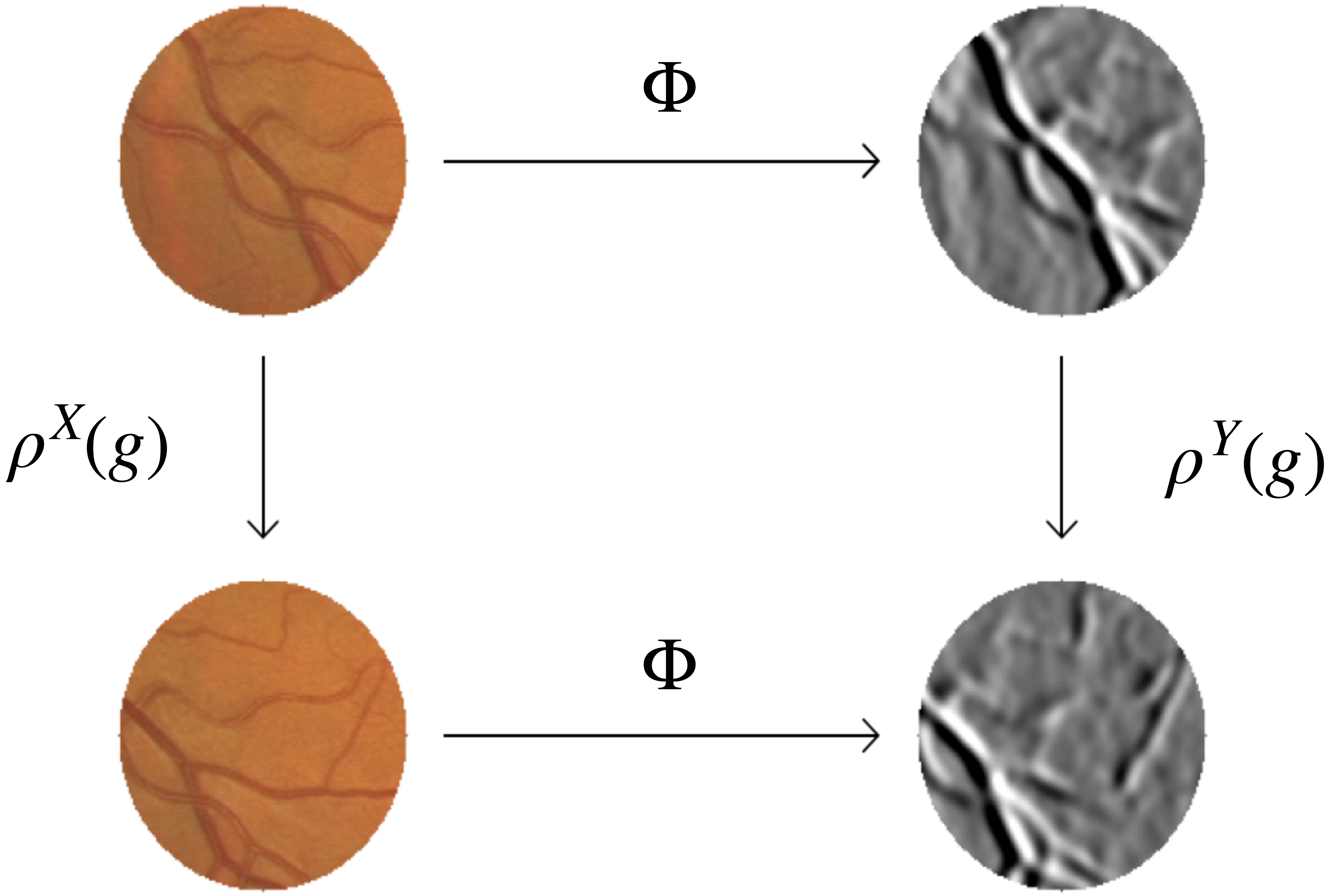


Equivariance

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

$\Phi : X \to Y$

ρ^X and ρ^Y actions of G on X and Y



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   - Geometric guarantees + weight sharing/sample efficiency

2. A group theoretical view on **recognition by components** (capsule nets)
   - Group theoretical prerequisites (**group product** and **representations**)
   - **Group convolutions** perform pattern recognition by components

3. Experimental examples

4. Theorem: Linear maps between feature maps are equivariant iff they are group convolutions

Are convolutions with reflected conv kernels (and vice versa)

Cross-correlations

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

Are convolutions with reflected conv kernels (and vice versa)

Cross-correlations

Representation of the translation group!

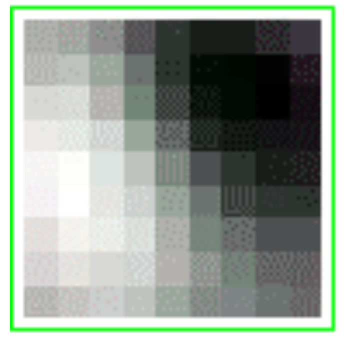
$$(k \star_{\mathbb{R}^2} f)(\mathbf{x}) = \int_{\mathbb{R}^2} k(\mathbf{x}' - \mathbf{x}) f(\mathbf{x}') d\mathbf{x}' = (\mathscr{L}_g\, k\, ,\, f)_{\mathbb{L}_2(\mathbb{R}^2)}$$

Are convolutions with reflected conv kernels (and vice versa)

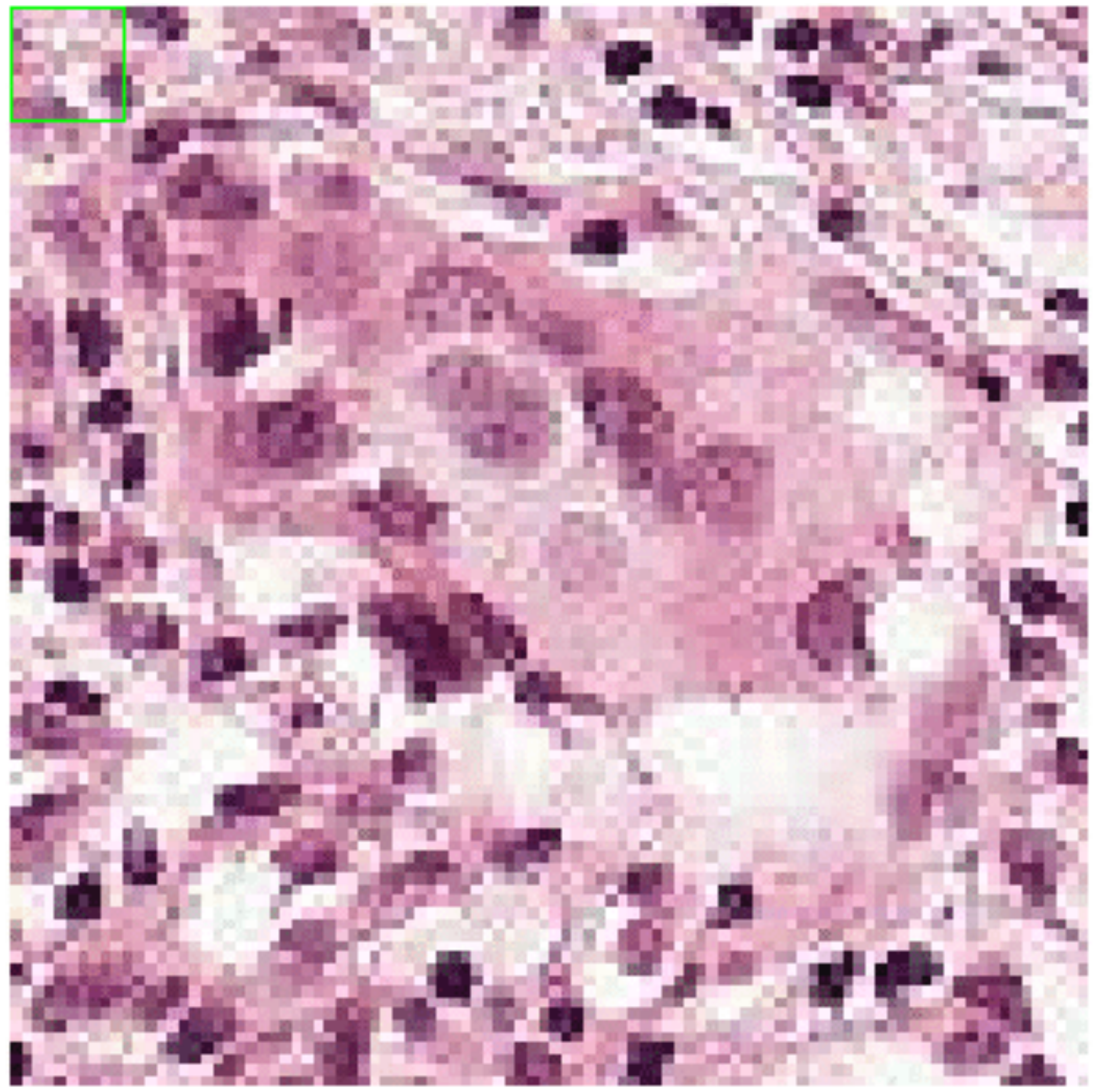
Cross-correlations

Representation of the translation group!

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



$\star_{\mathbb{R}^2}$



$=$

k

2D convolution kernel

f^{in}

2D feature map

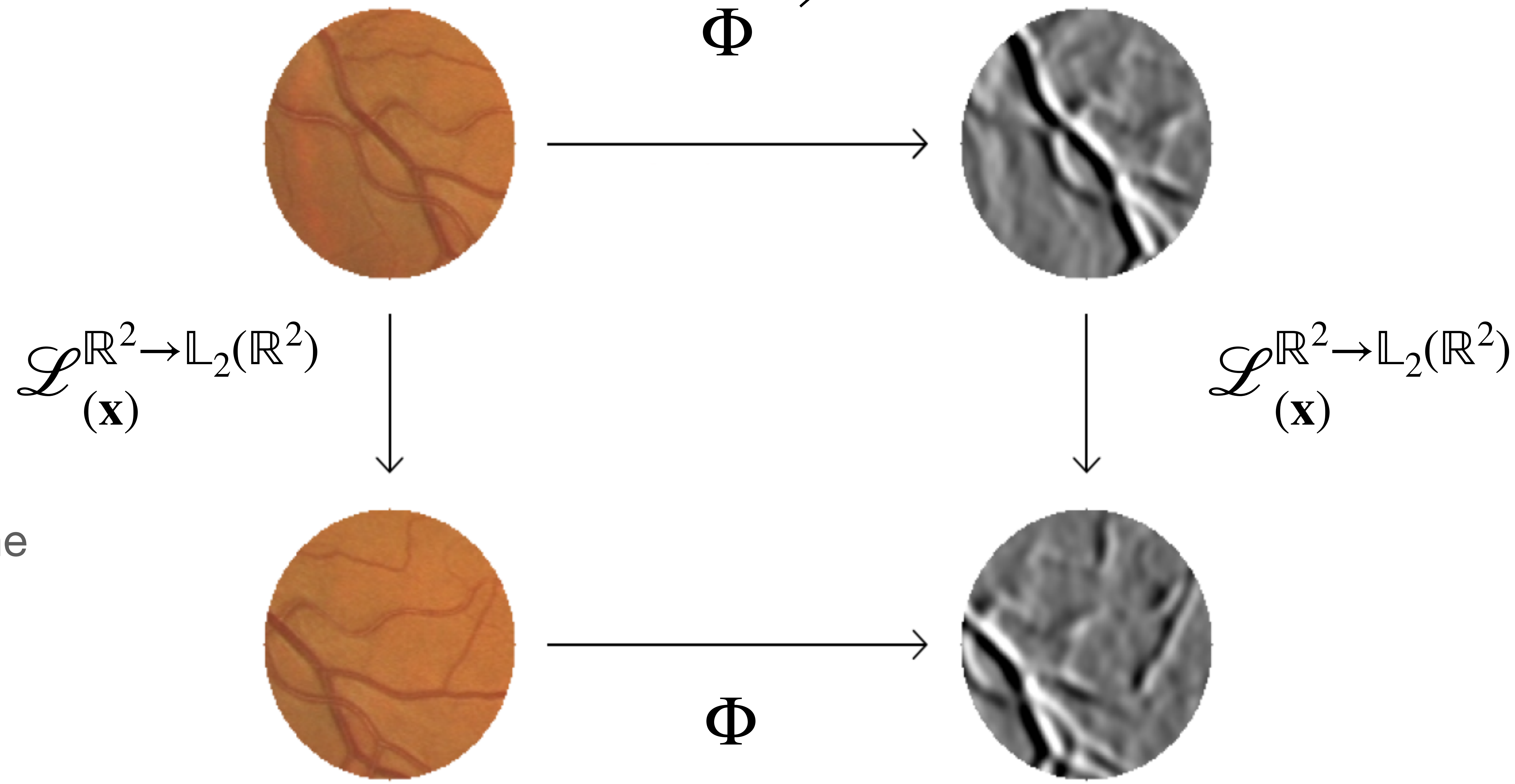
f^{out}

2D feature map (after ReLU)

Group **equivariance**

Convolutions/cross-correlations are translation equivariant

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



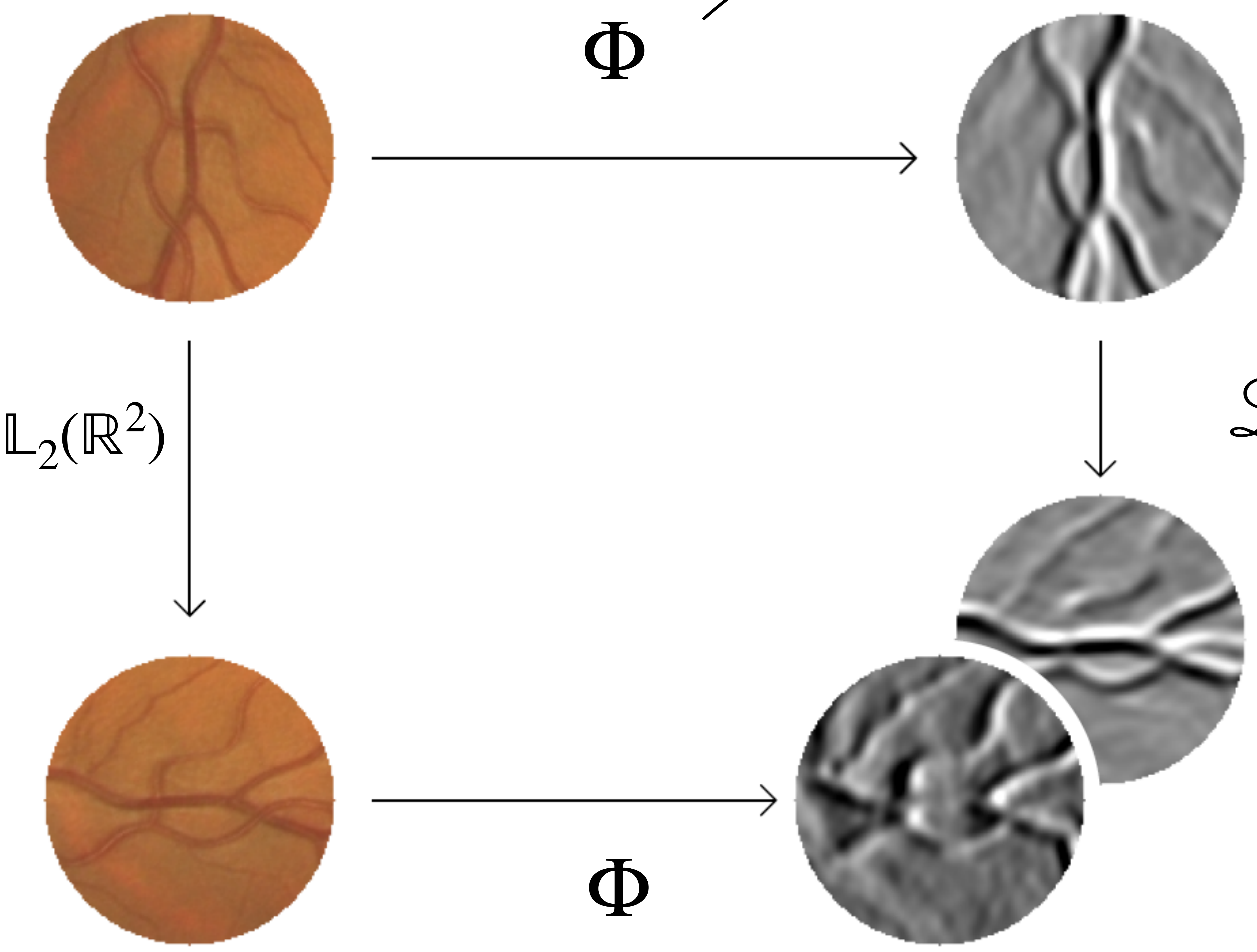
Representation of the translation group

Group **equivariance**

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

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

Representation of the translation group



Representation of the rotation group

SE(2) equivariant cross-correlations

Representation of the roto-translation group!

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

SE(2) equivariant cross-correlations

Representation of the roto-translation group!

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

translation *rotation*

SE(2) equivariant cross-correlations

Representation of the roto-translation group!

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

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

translation *rotation*

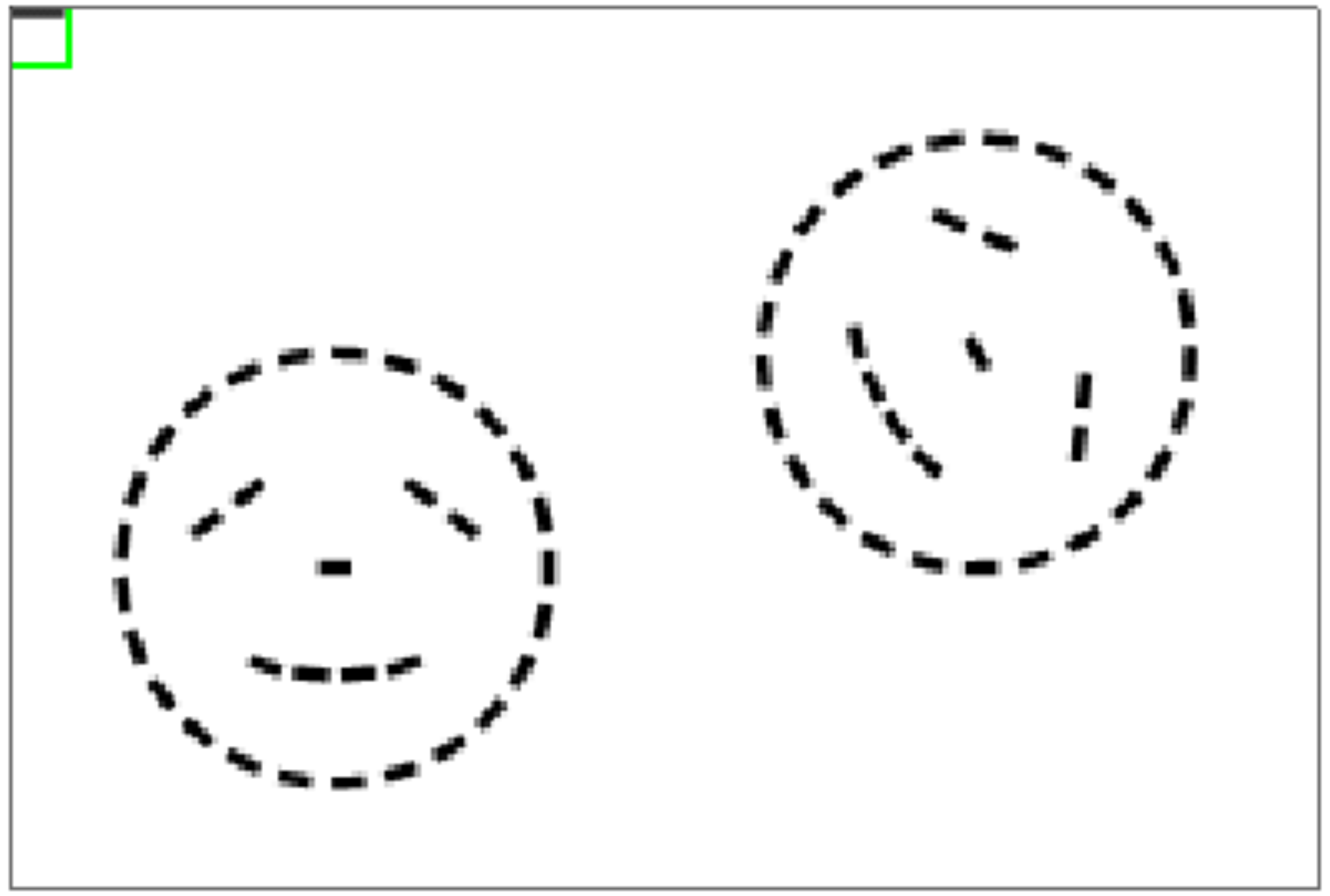
SE(2) equivariant cross-correlations

Representation of the roto-translation group!

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

translation *rotation*

$\star_{\mathbb{R}^2}$



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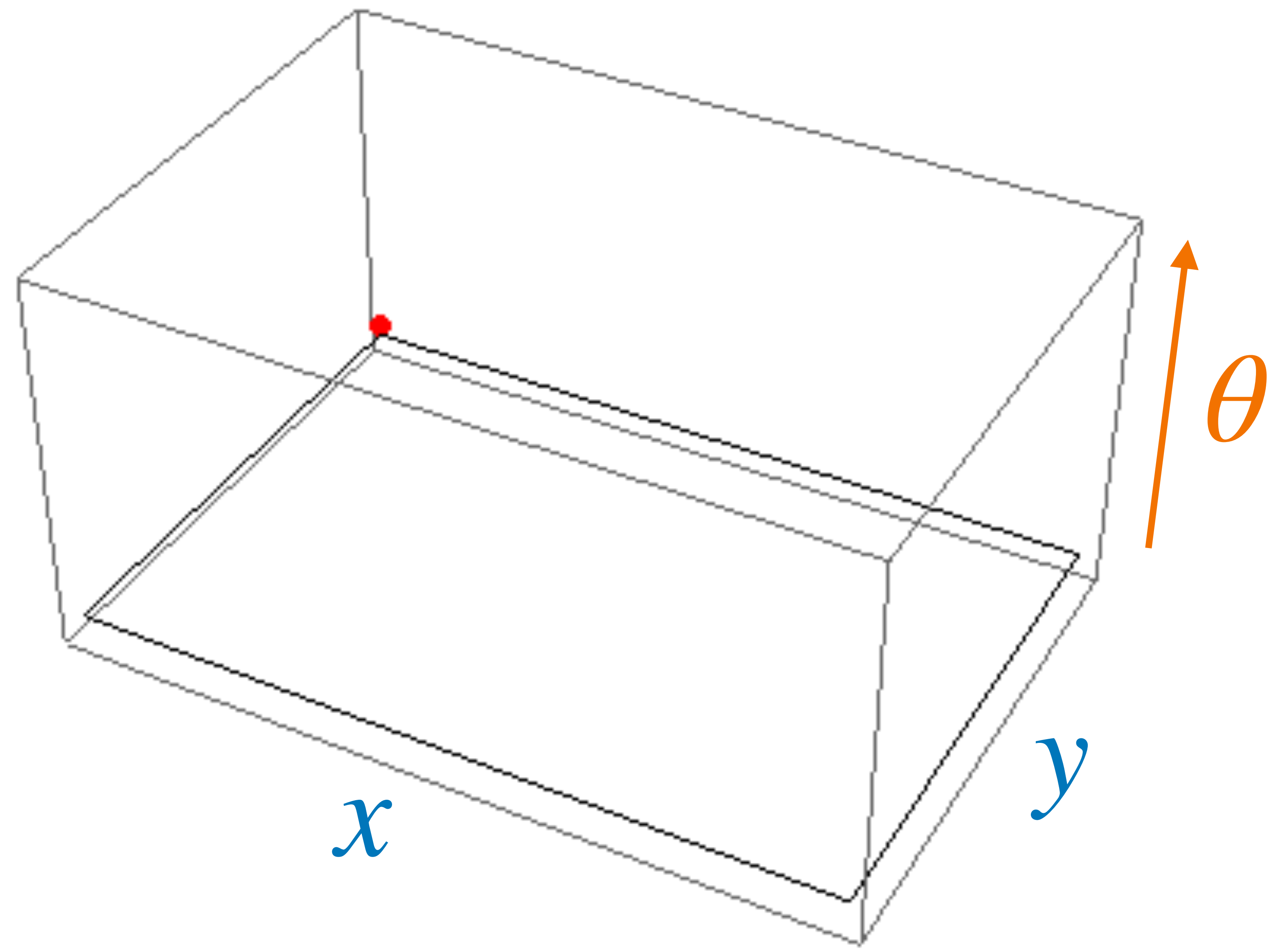


$\mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(\mathbb{R}^2)} k$

Rotated 2D convolution kernel

f^{in}

2D feature map

f^{out}

3D (*SE(2)*) feature map (after ReLU)

SE(2) equivariant cross-correlations

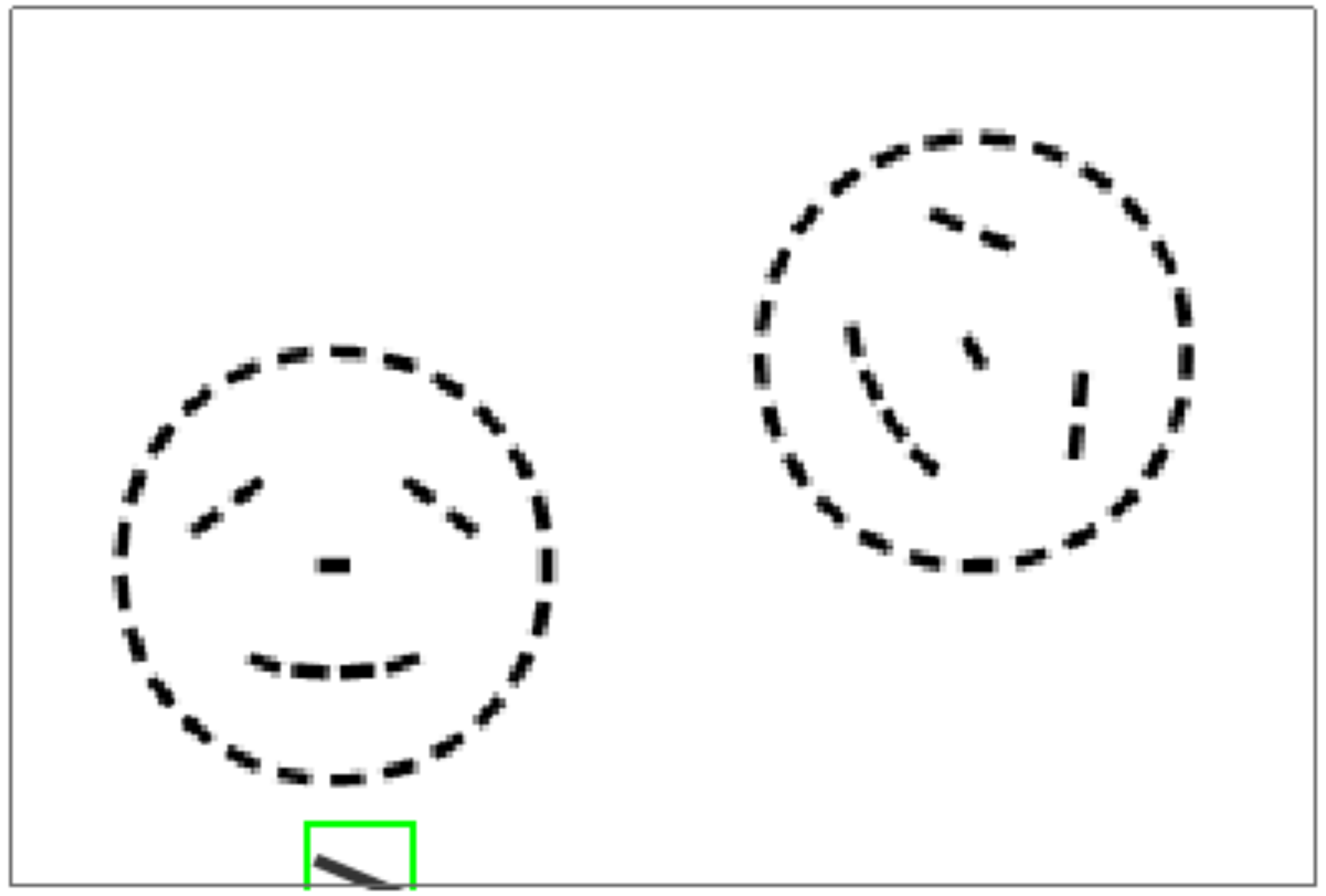
Representation of the roto-translation group!

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

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

translation *rotation*

$\star_{\mathbb{R}^2}$



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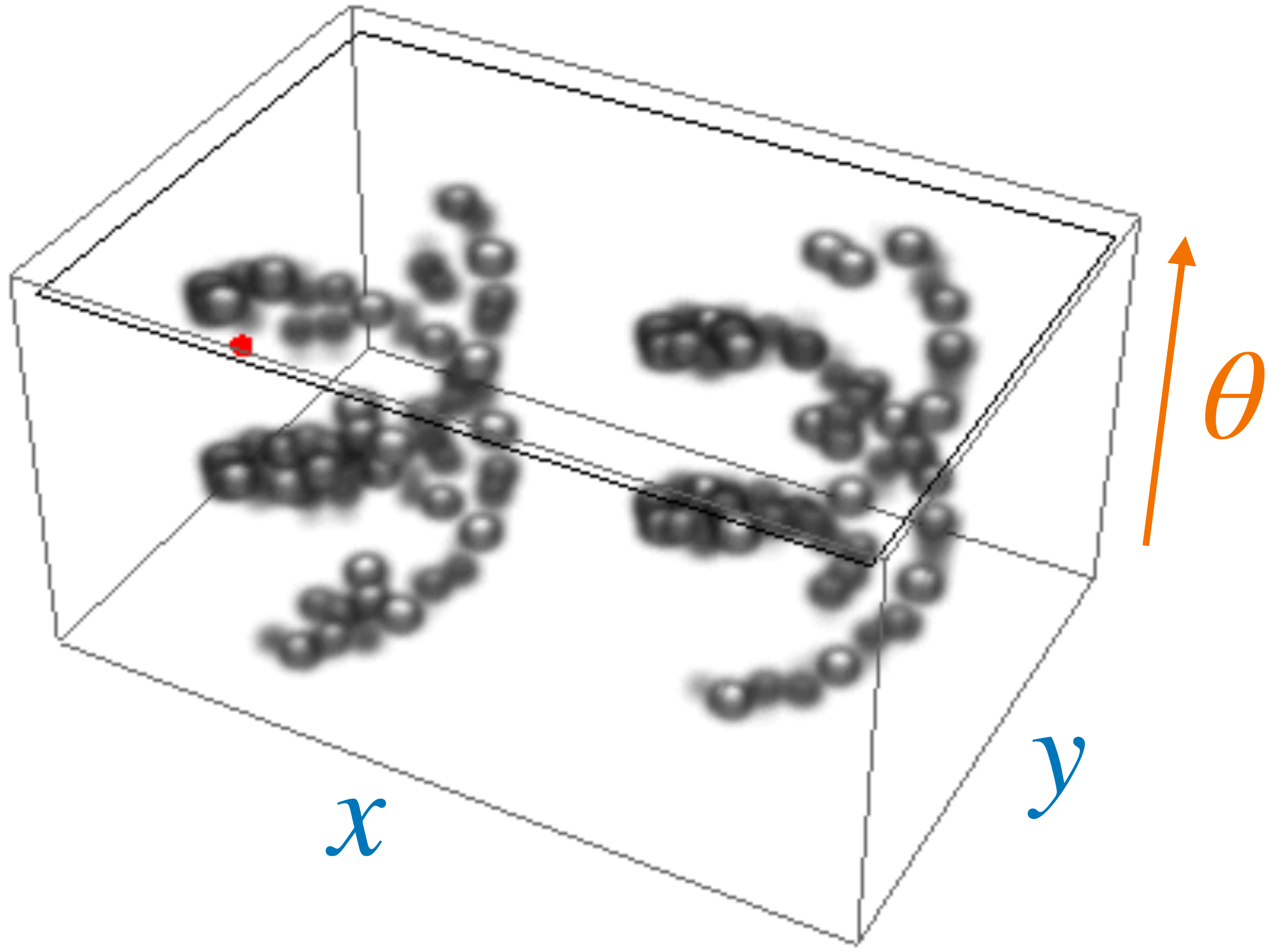


$\mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(\mathbb{R}^2)} k$
Rotated 2D convolution kernel

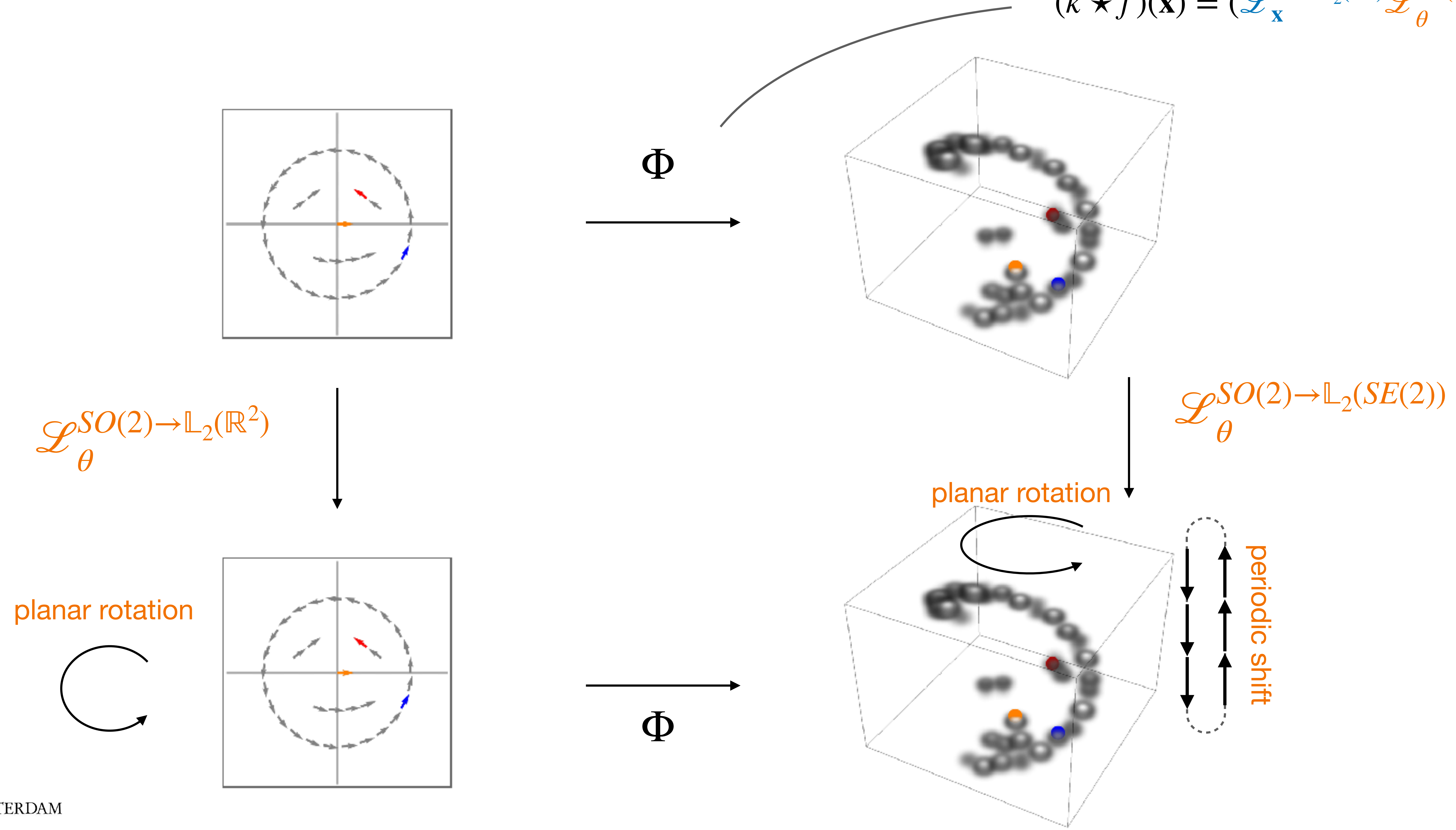
f^{in}
2D feature map

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

Group **equivariance**

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

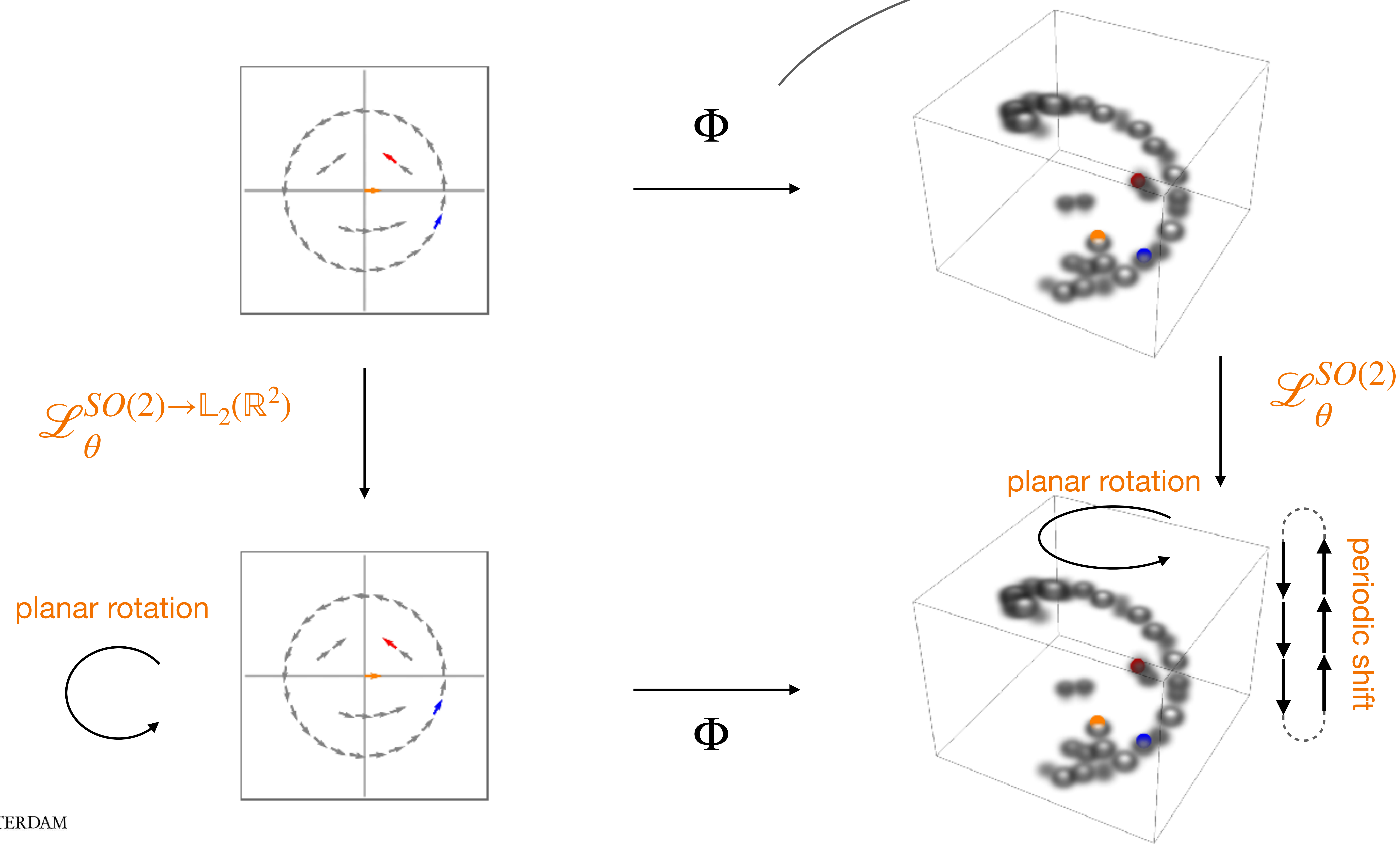
$$(k \,\tilde{\star}\, f)(\mathbf{x}) = (\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2\to\mathbb{L}_2(\mathbb{R}^2)} \mathscr{L}_{\theta}^{SO(2)\to\mathbb{L}_2(\mathbb{R}^2)} k \,,\, f)_{\mathbb{L}_2(\mathbb{R}^2)}$$



Group **equivariance**

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

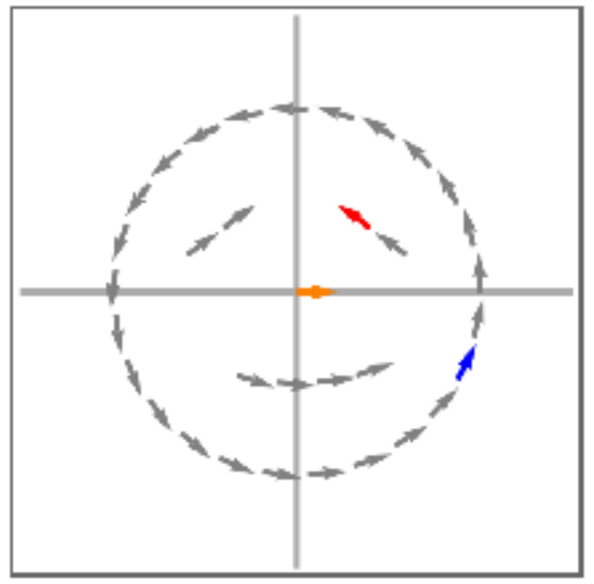
$$(k \,\tilde{\star}\, f)(\mathbf{x}) = (\mathscr{L}_{\mathbf{x}}^{\mathbf{R}^2\to\mathbb{L}_2(\mathbb{R}^2)} \mathscr{L}_{\theta}^{SO(2)\to\mathbb{L}_2(\mathbb{R}^2)} k \,,\, f)_{\mathbb{L}_2(\mathbb{R}^2)}$$



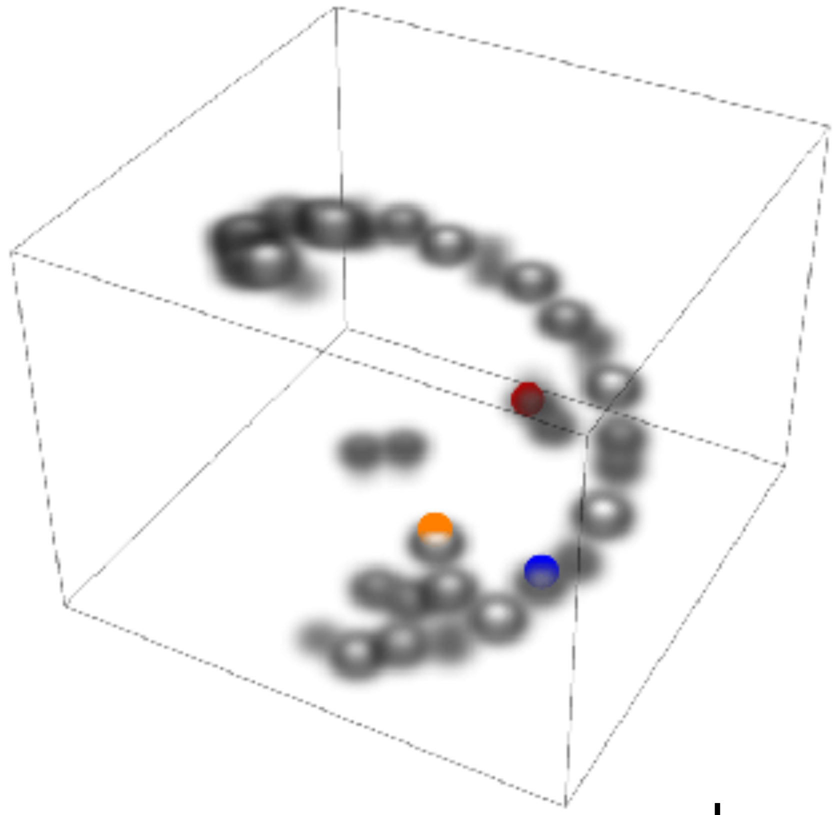
Group equivariance

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

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



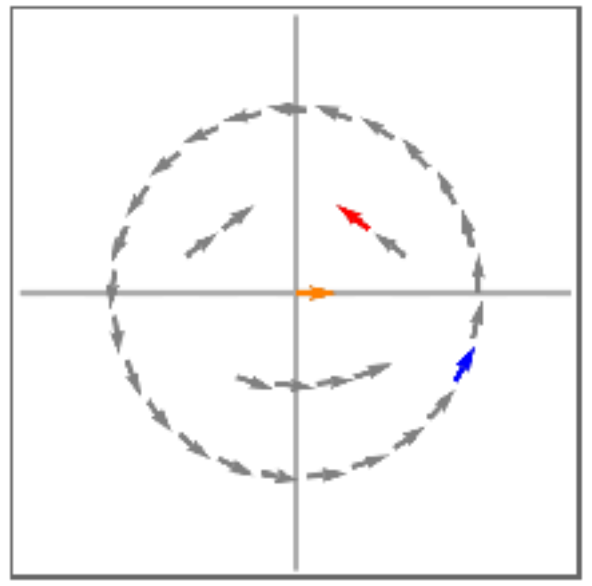
$\xrightarrow{\Phi}$



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

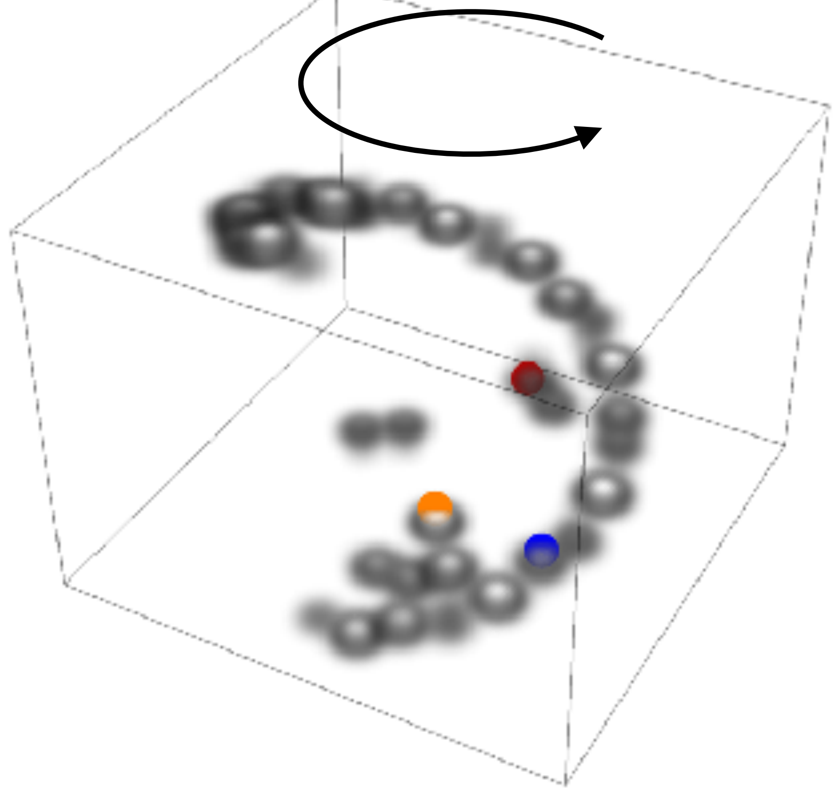
$\mathscr{L}_{\theta}^{SO(2)\to\mathbb{L}_2(SE(2))}$

planar rotation



$\xrightarrow{\Phi}$

planar rotation



periodic shift

What about subsequent layers?

SE(2) equivariant cross-correlations

Group correlations:

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

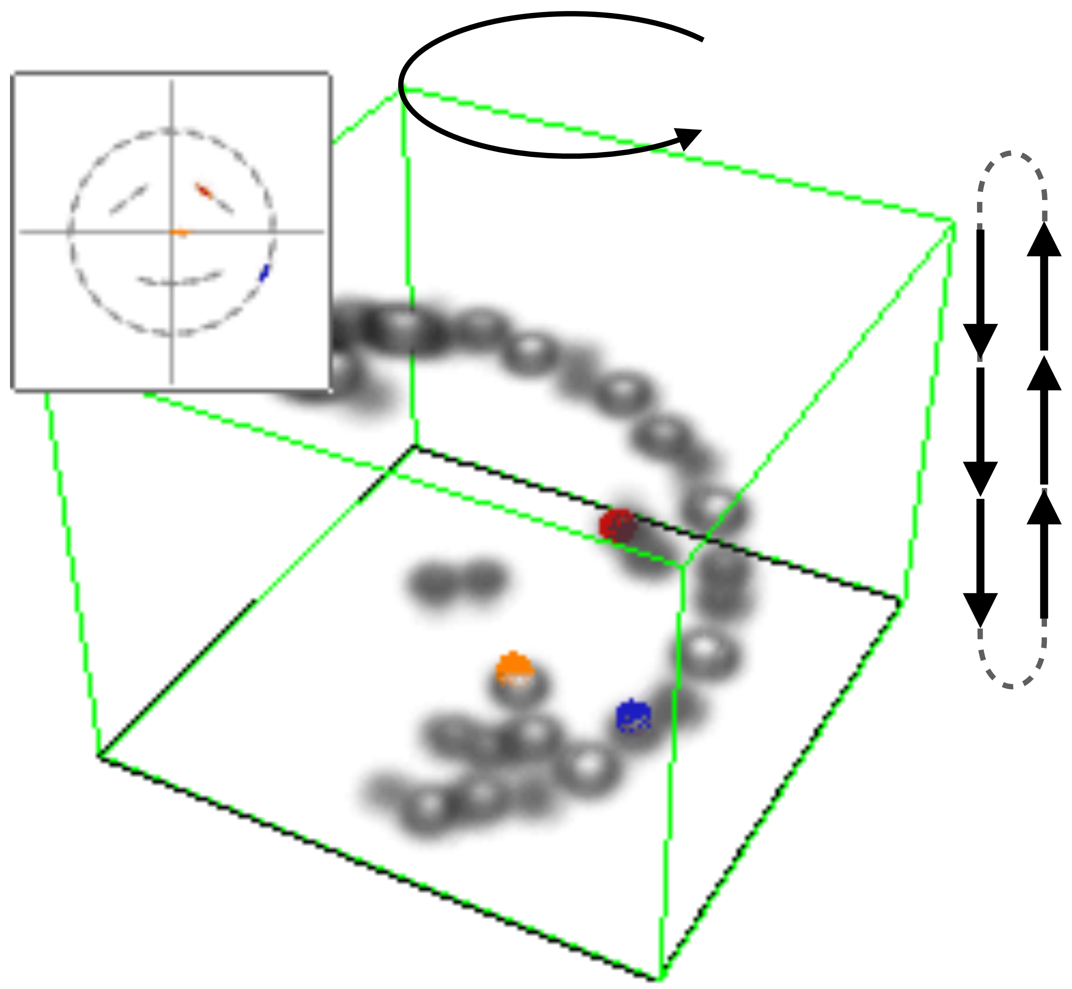
translation *rotation*

SE(2) equivariant cross-correlations

Group correlations:

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

translation *rotation*



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

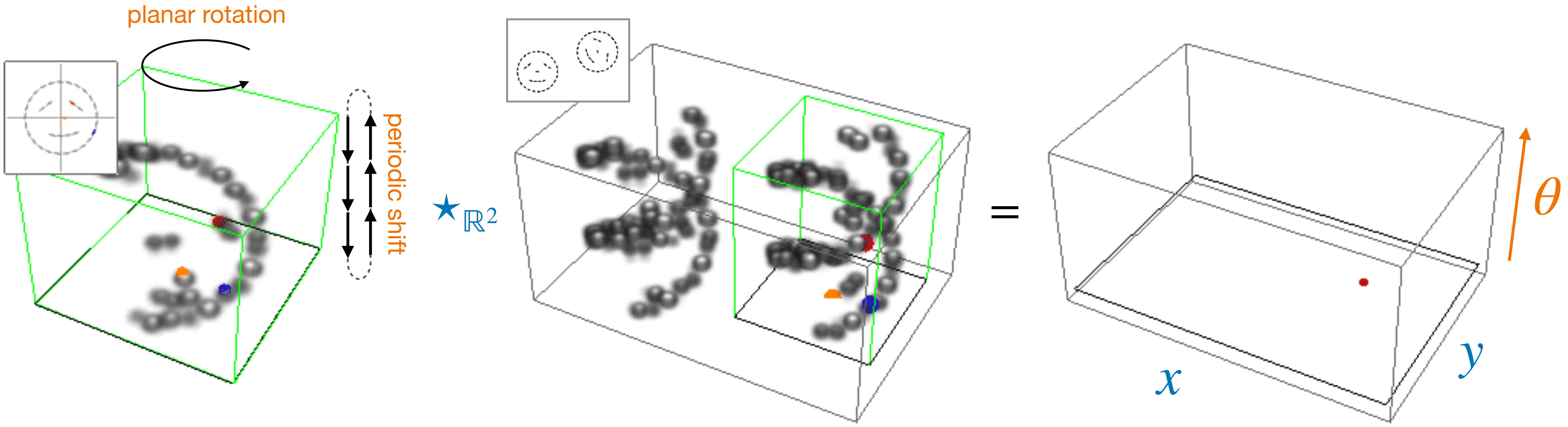
Rotated SE(2) convolution kernel

SE(2) equivariant cross-correlations

Group correlations:

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

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)

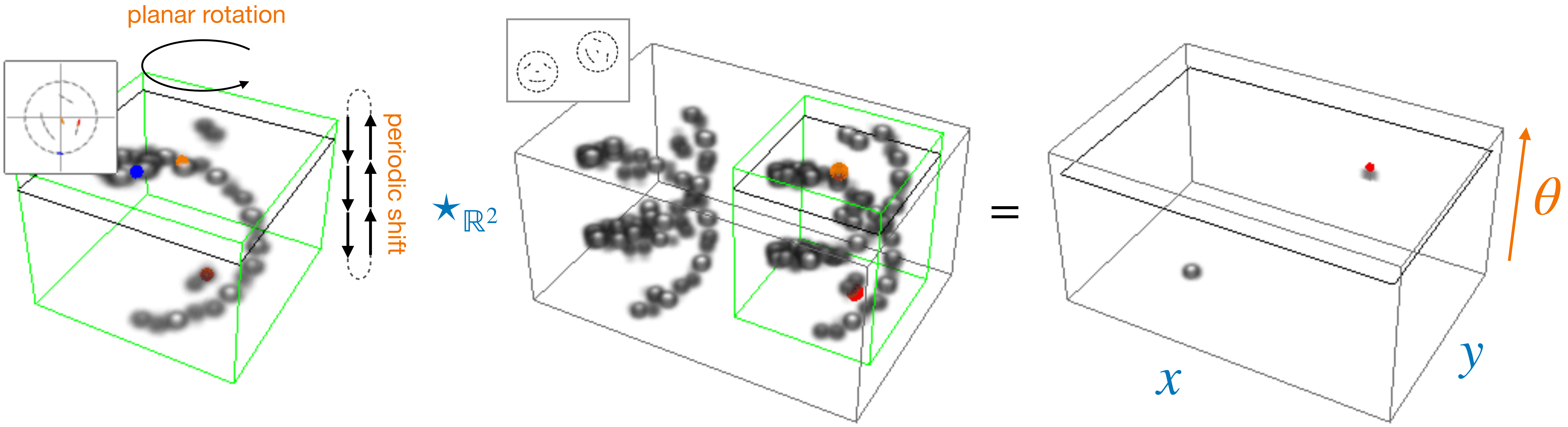
SE(2) equivariant cross-correlations

Group correlations:

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

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

translation *rotation*



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

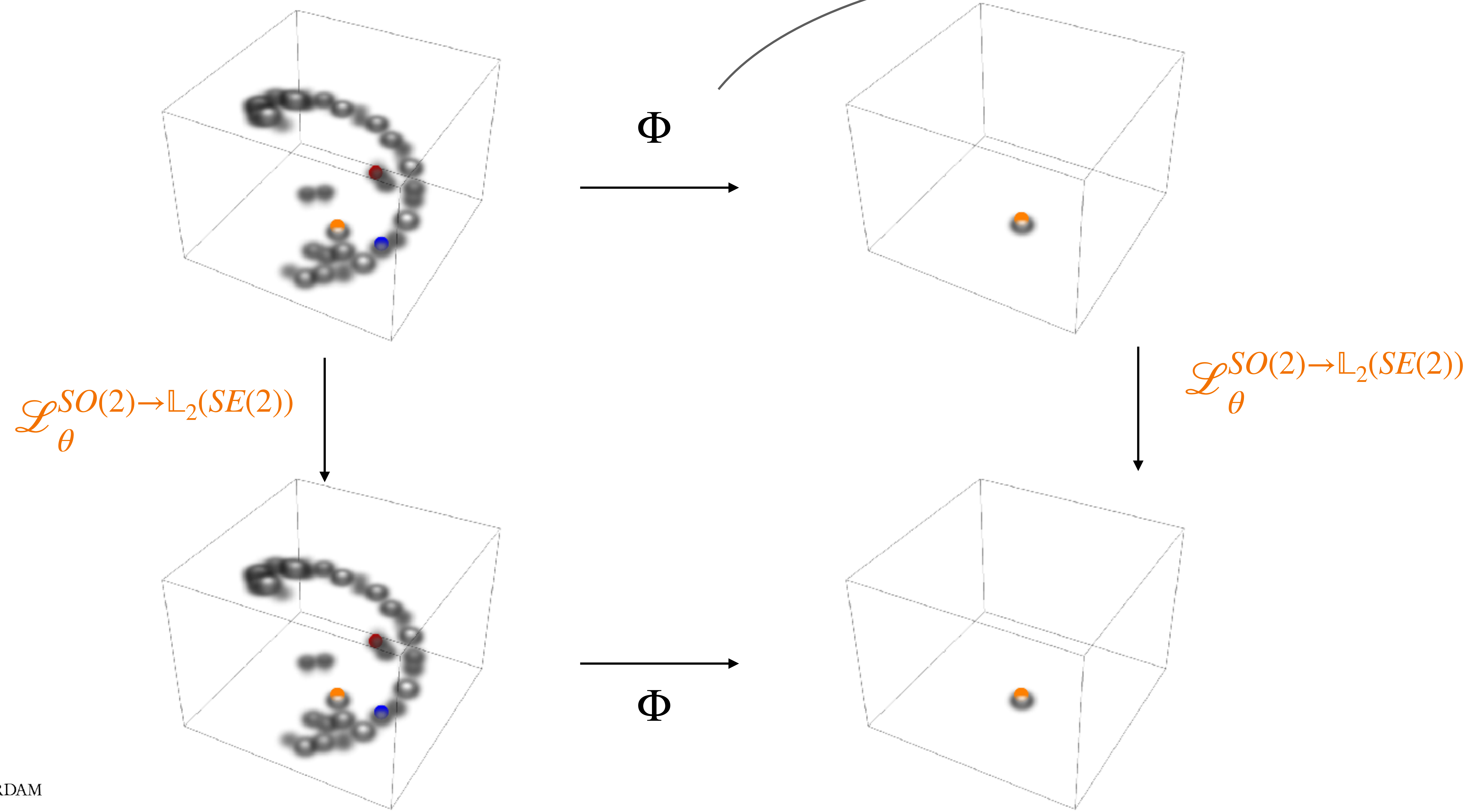
f^{in}
SE(2) feature map

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

Group equivariance

SE(2) group convolutions are roto-translation equivariant

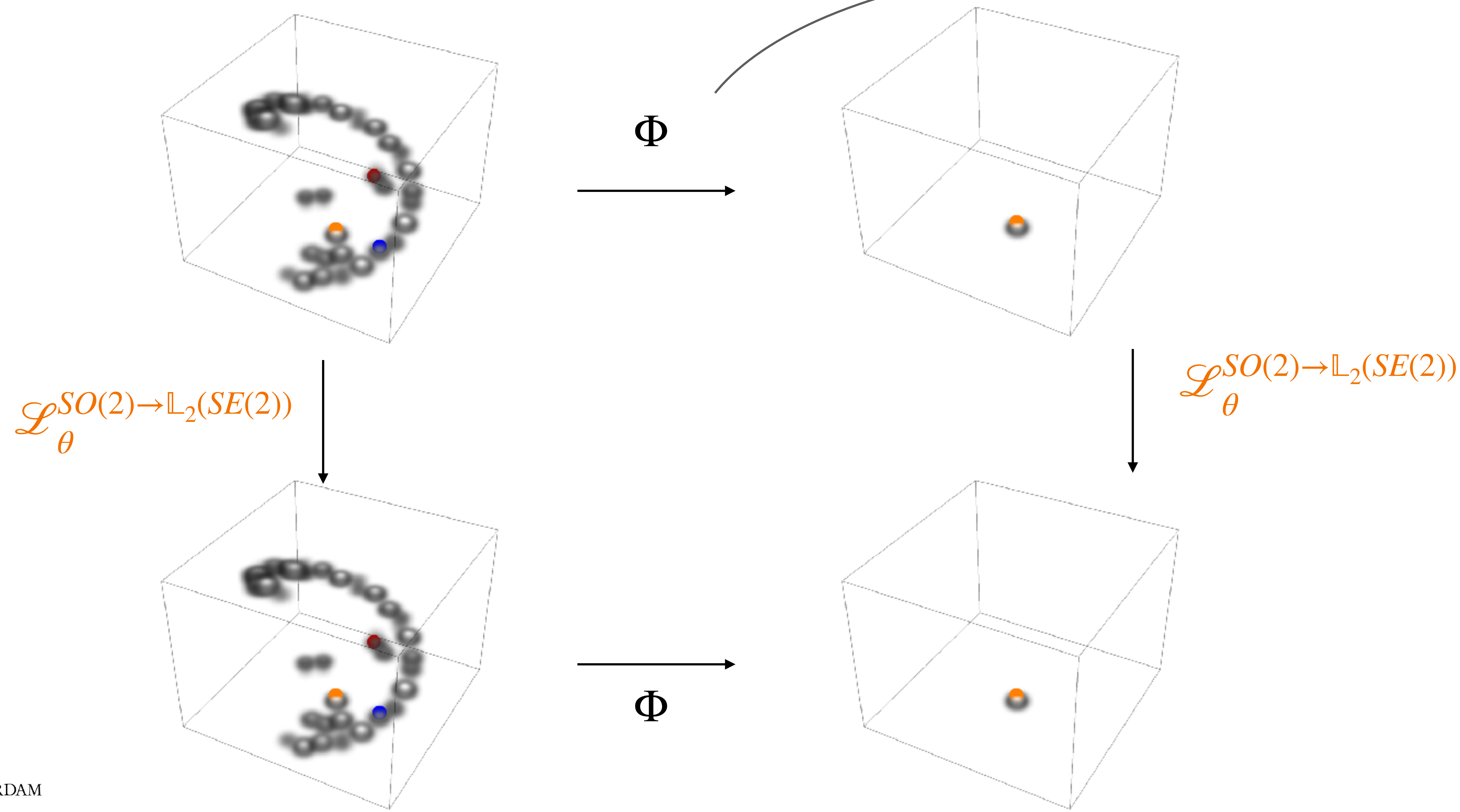
$$(k \star f)(\mathbf{x}) = (\mathcal{L}_{\mathbf{x}}^{\mathbb{R}^2\to\mathbb{L}_2(SE(2))}\mathcal{L}_{\theta}^{SO(2)\to\mathbb{L}_2(SE(2))}\, k\, ,\, f)_{\mathbb{L}_2(SE(2))}$$



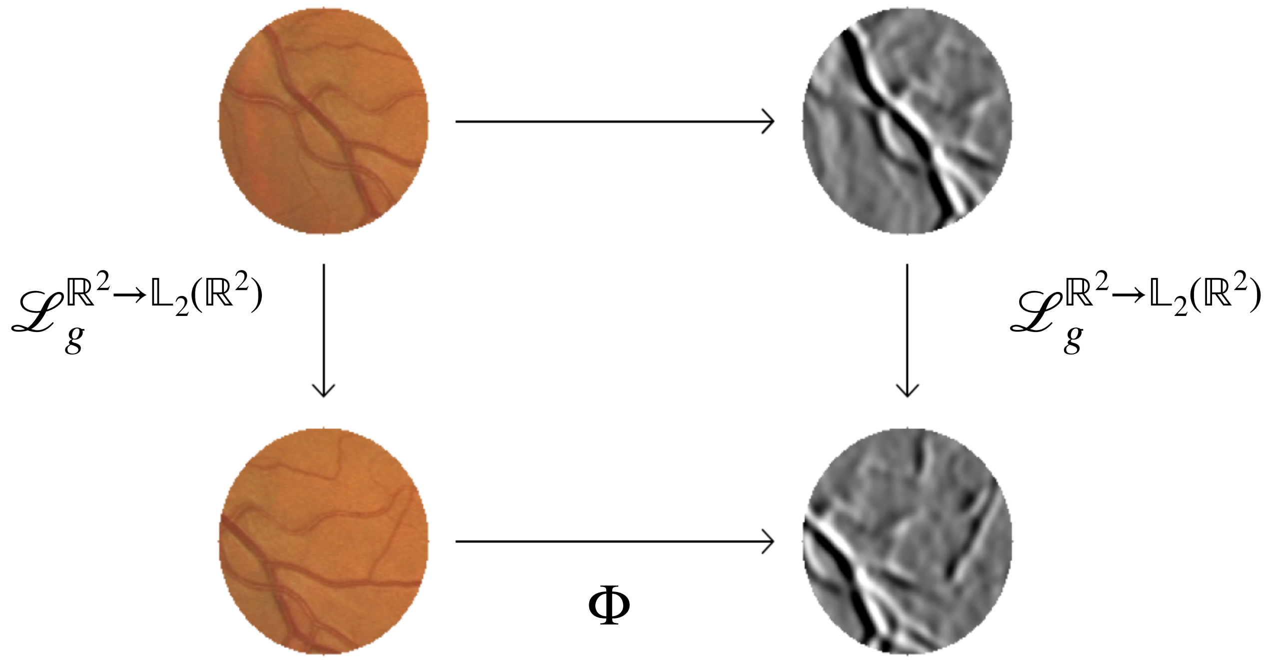
Group **equivariance**

SE(2) group convolutions are roto-translation equivariant

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



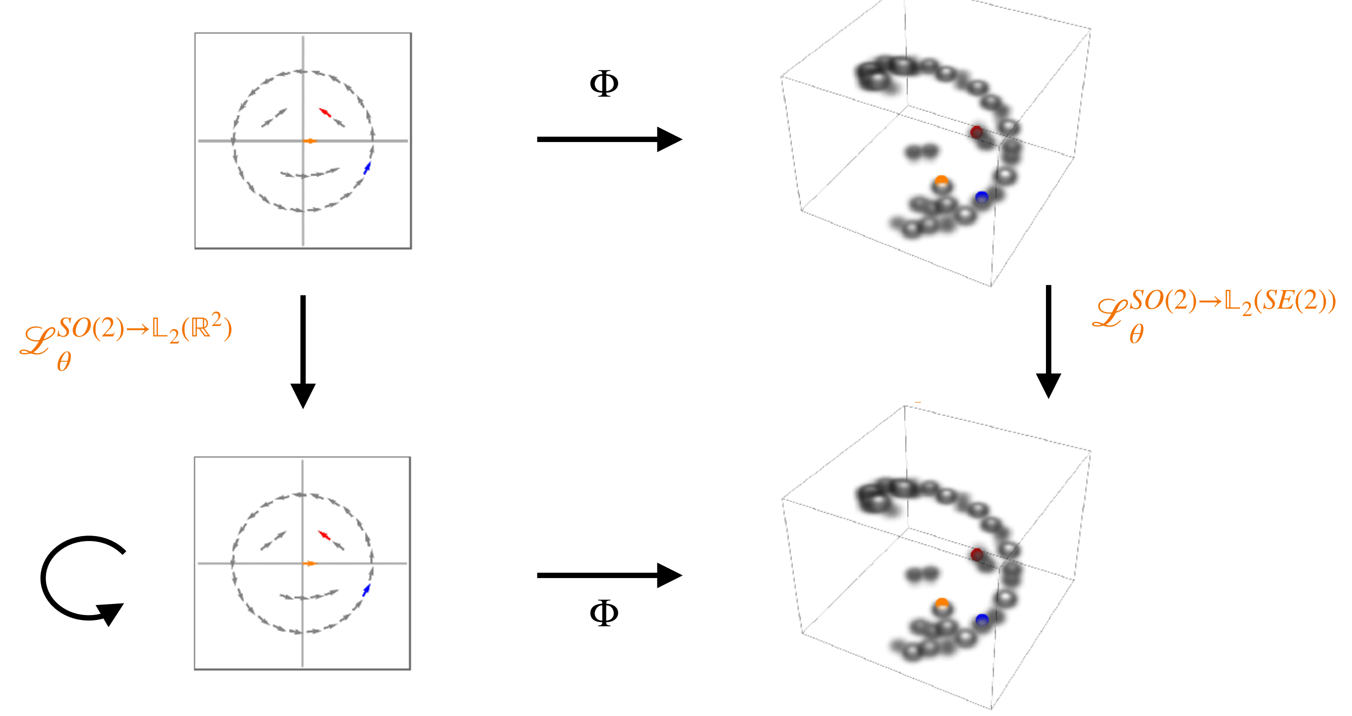
2D cross-correlation (translation equivariant)



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

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

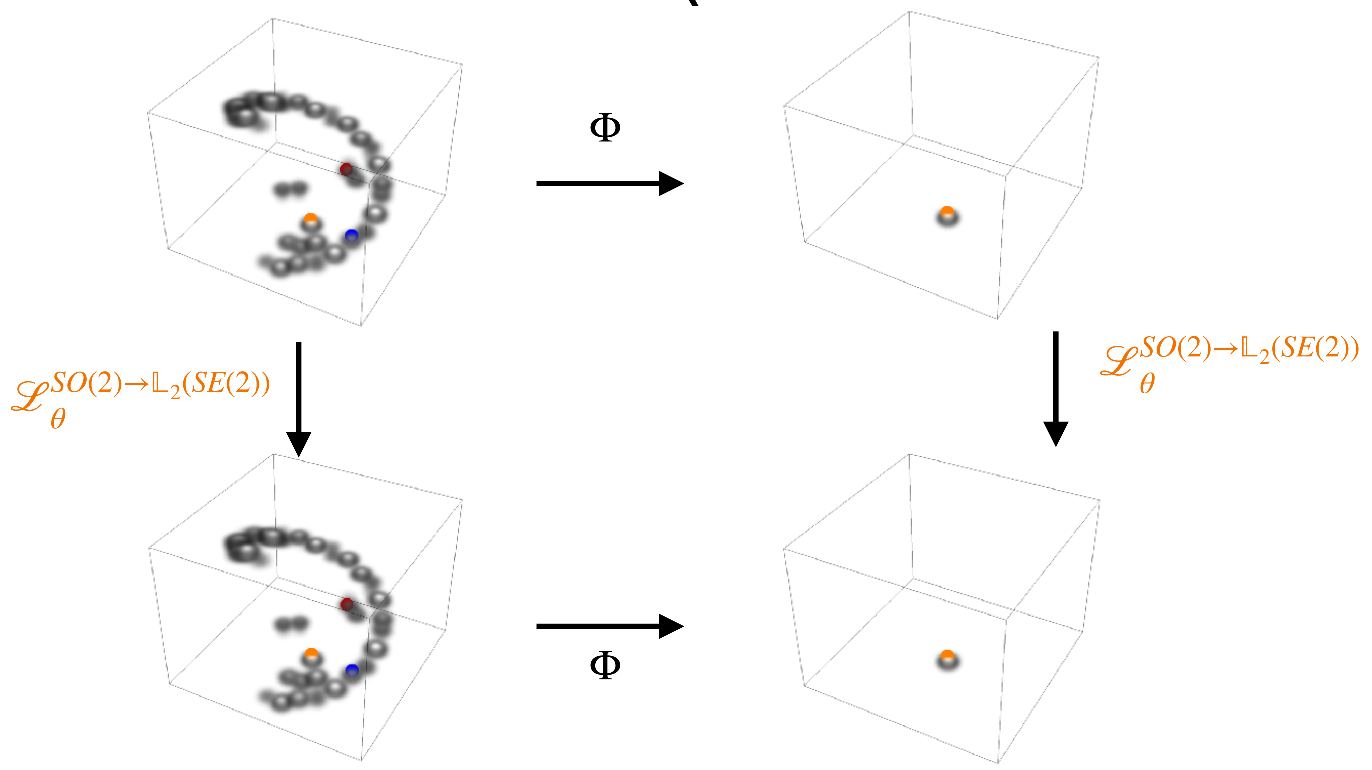
SE(2) lifting correlations (roto-translation equivariant)



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

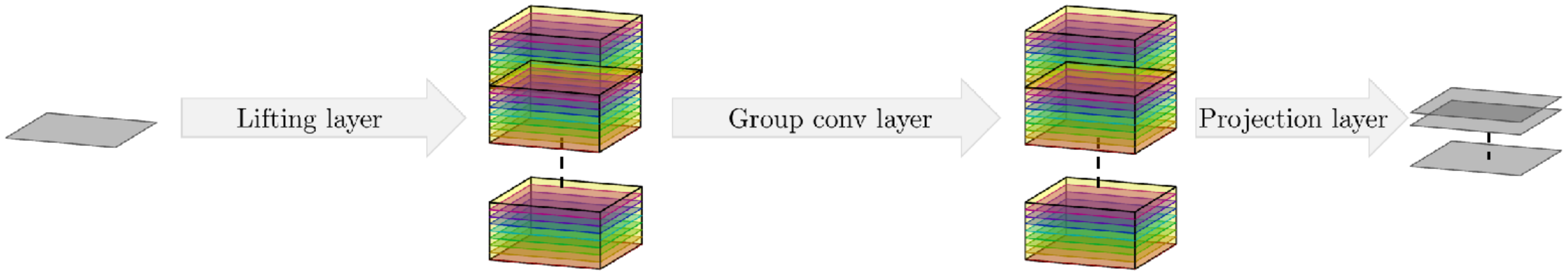
$$= \int_{\mathbb{R}^2} k(\mathbf{R}_\theta^{-1}(\mathbf{x}' - \mathbf{x})) f(\mathbf{x}') d\mathbf{x}'$$

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

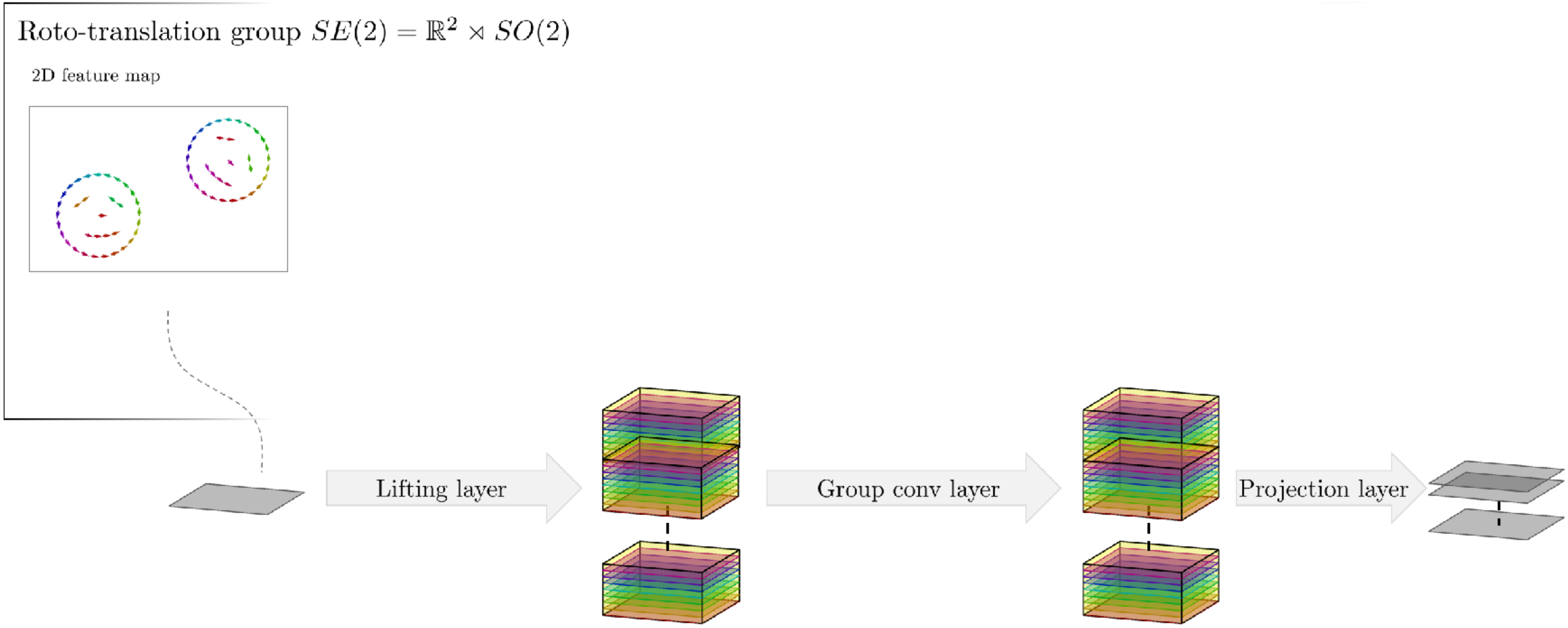


$$(k \tilde{\star} f)(\mathbf{x}) = (\mathcal{L}_g^{SE(2)\to\mathbb{L}_2(SE(2))} k , f)_{\mathbb{L}_2(SE(2))}$$

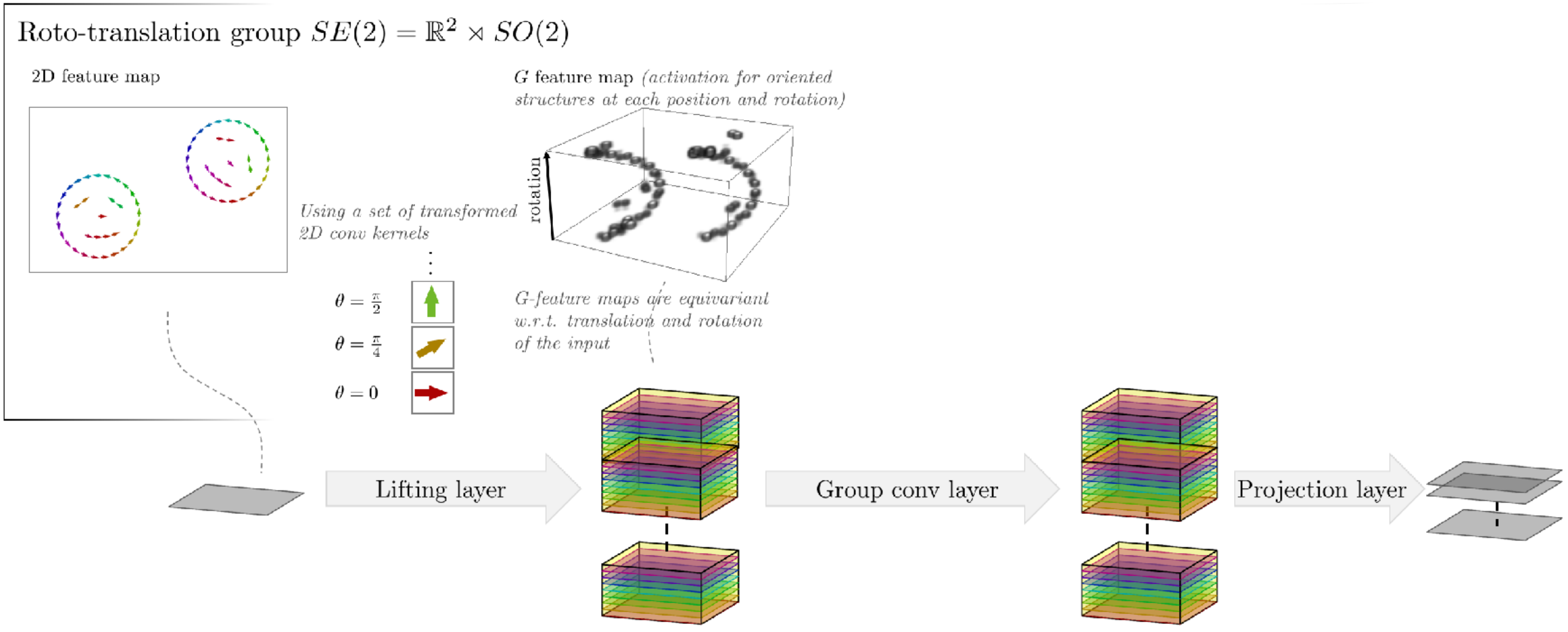
$$= \int_{\mathbb{R}^2} \int_{S^1} k(\mathbf{R}_\theta^{-1}(\mathbf{x}' - \mathbf{x}), \theta' - \theta \mod 2\pi) f(\mathbf{x}', \theta') d\mathbf{x}'$$



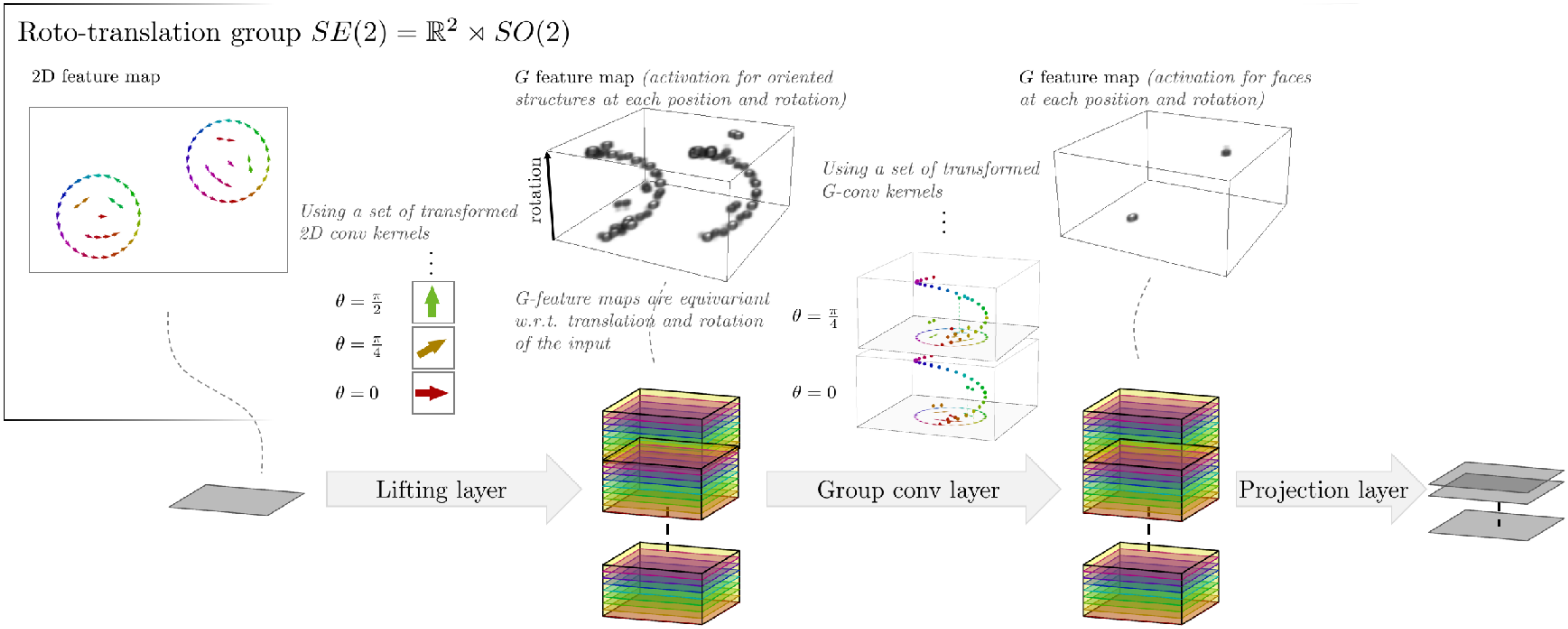
Lifting layer
Group conv layer
Projection layer



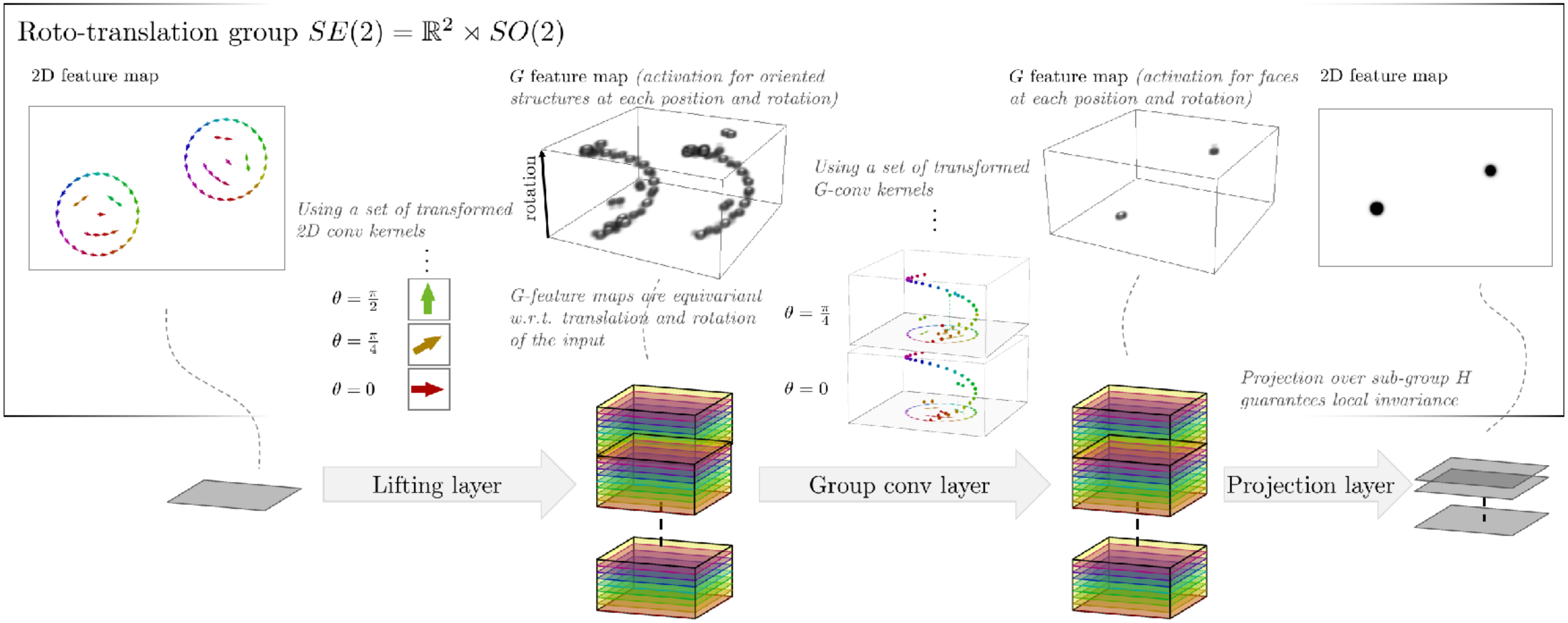
Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
Lifting layer
Group conv layer
Projection layer

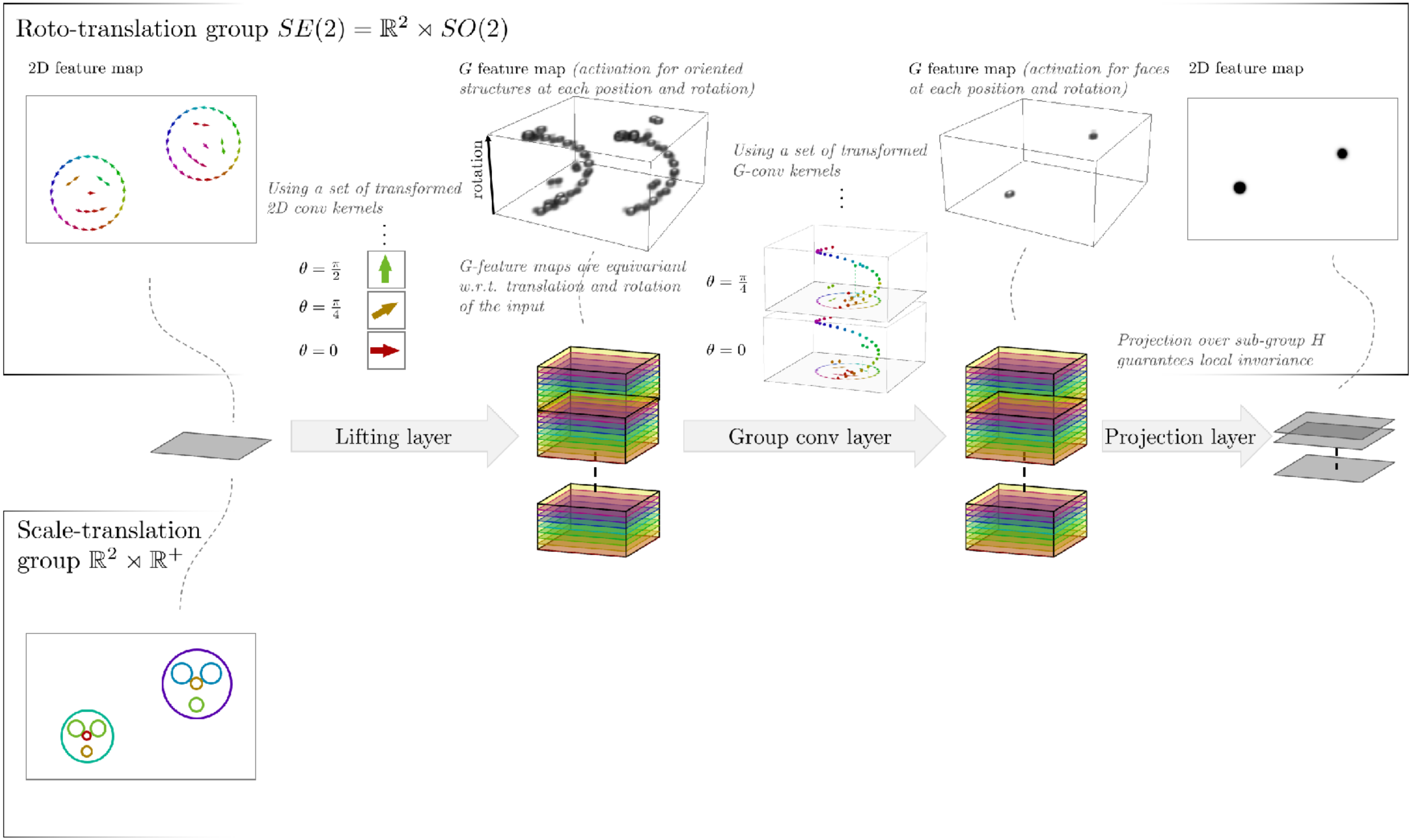


Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
G feature map *(activation for oriented structures at each position and rotation)*
rotation
Using a set of transformed 2D conv kernels
$\theta = \frac{\pi}{2}$
$\theta = \frac{\pi}{4}$
$\theta = 0$
G-feature maps are equivariant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

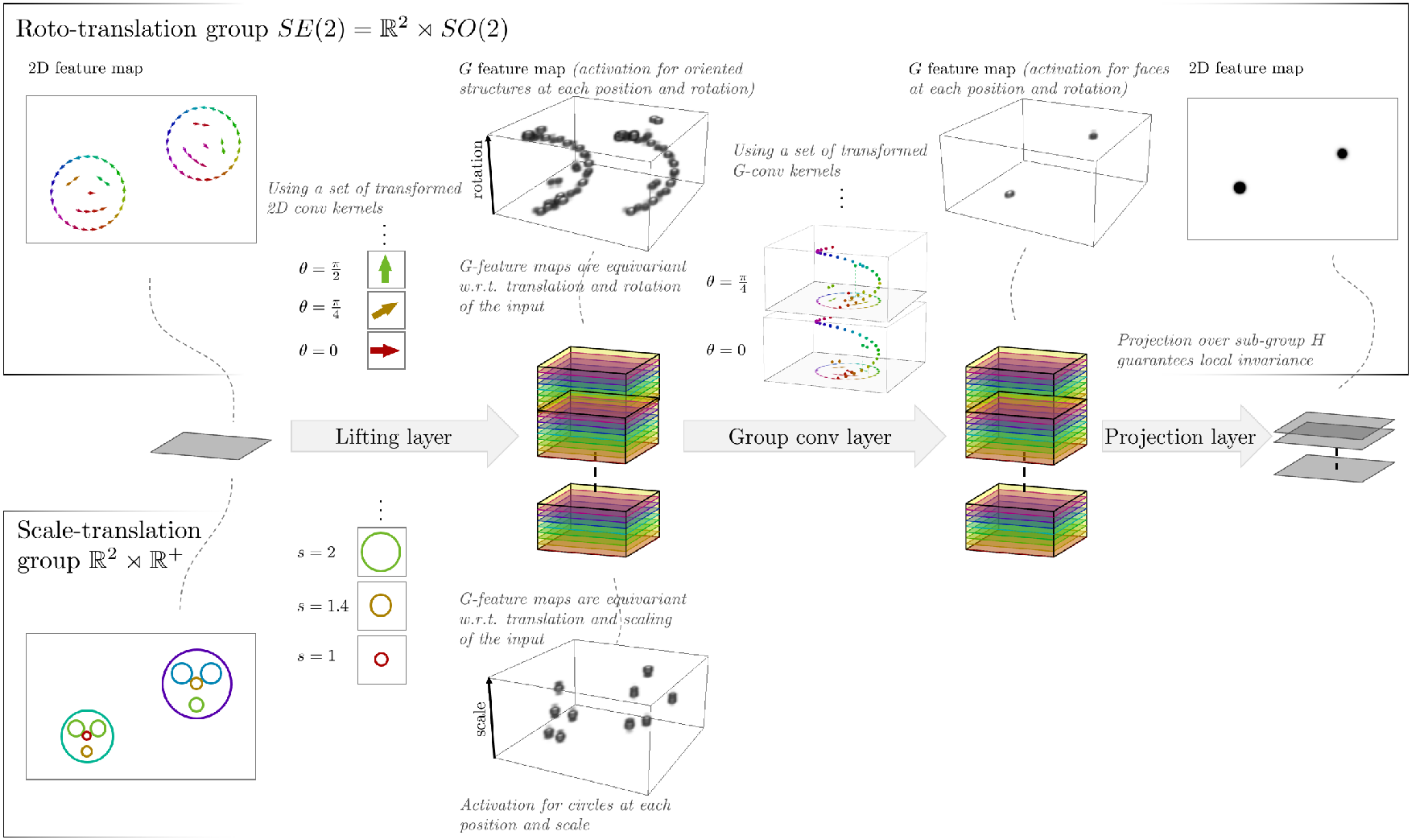


Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
G feature map (activation for oriented structures at each position and rotation)
G feature map (activation for faces at each position and rotation)
rotation
Using a set of transformed 2D conv kernels
Using a set of transformed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

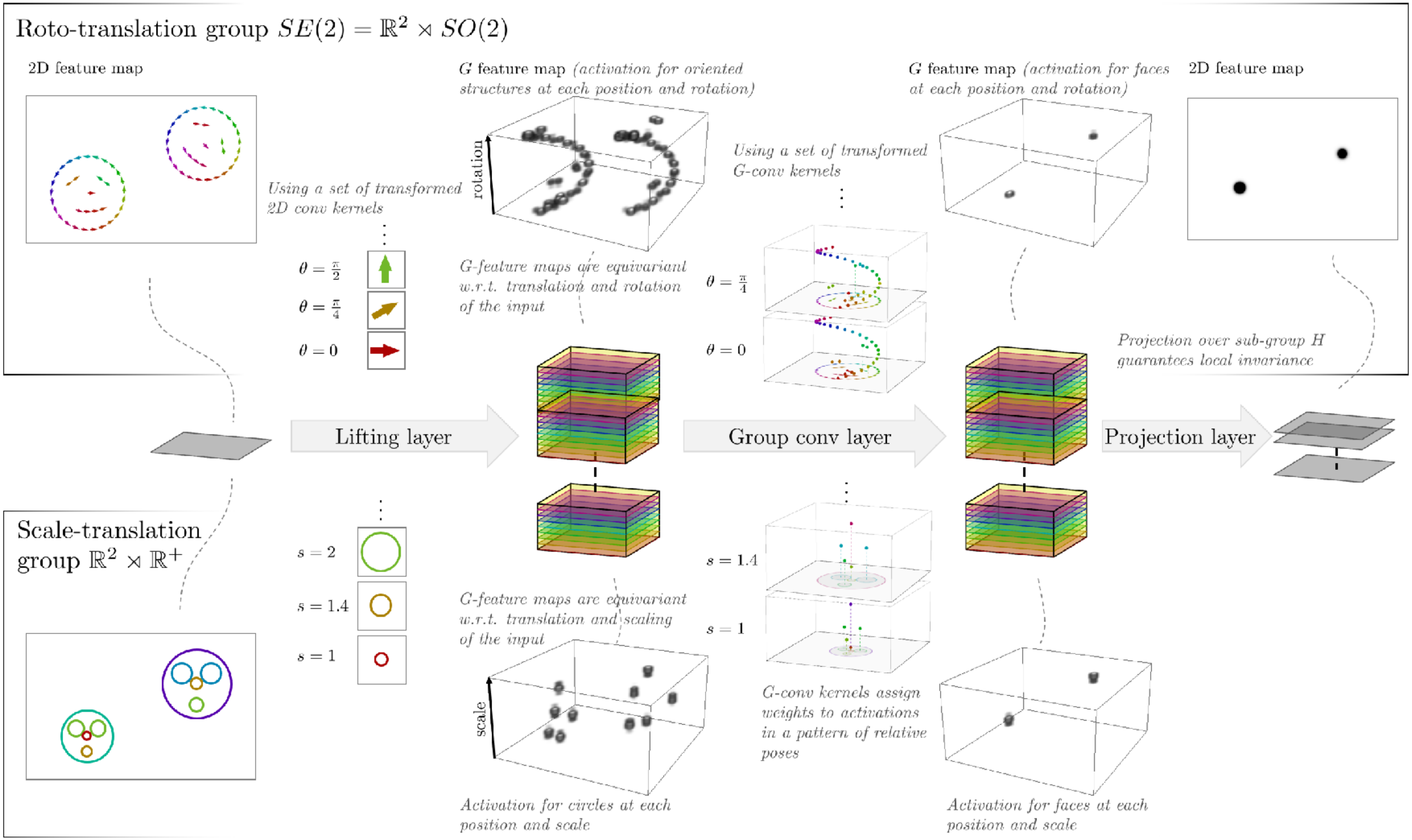

Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
G feature map *(activation for oriented structures at each position and rotation)*
rotation
Using a set of transformed 2D conv kernels
$\theta = \frac{\pi}{2}$
$\theta = \frac{\pi}{4}$
$\theta = 0$
G-feature maps are equivariant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



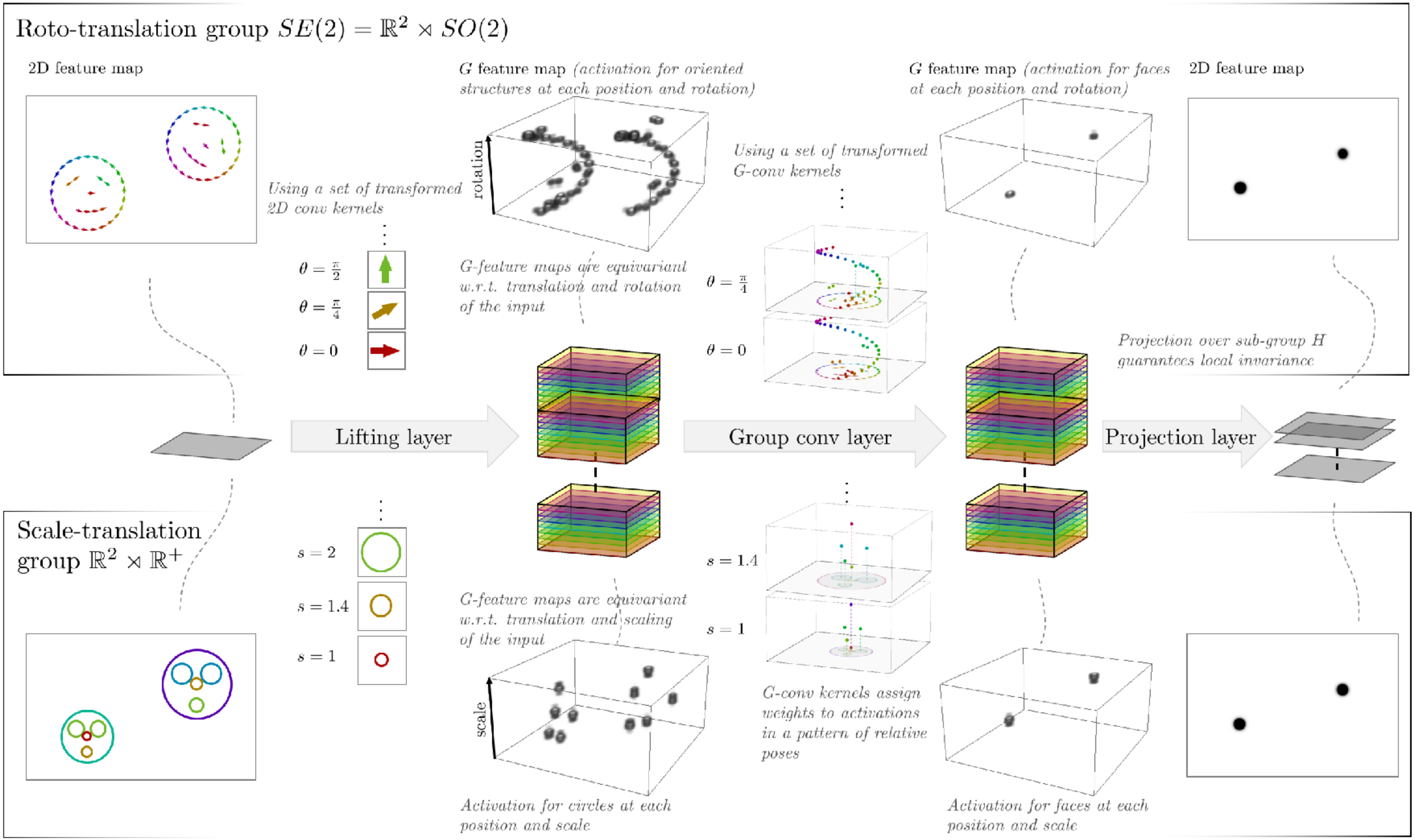
Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
2D feature map
Using a set of transformed 2D conv kernels
$\theta = \frac{\pi}{2}$
$\theta = \frac{\pi}{4}$
$\theta = 0$
G feature map (activation for oriented structures at each position and rotation)
rotation
G-feature maps are equivariant 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
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
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
G feature map (activation for oriented structures at each position and rotation)
rotation
G feature map (activation for faces at each position and rotation)
2D feature map
Using a set of transformed 2D conv kernels
Using a set of transformed G-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
$\theta = \frac{\pi}{4}$
$\theta = 0$
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
$s = 1.4$
$s = 1$
scale
G-conv kernels assign weights to activations in a pattern of relative poses
Activation for circles at each position and scale
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

Content of this talk

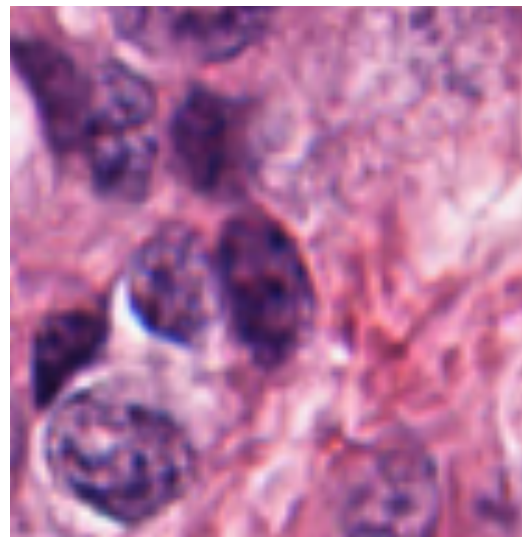
1. Why do we want equivariant learning models?
   - Geometric guarantees + weight sharing/sample efficiency

2. A group theoretical view on **recognition by components** (capsule nets)
   - Group theoretical prerequisites (**group product** and **representations**)
   - **Group convolutions** perform pattern recognition by components

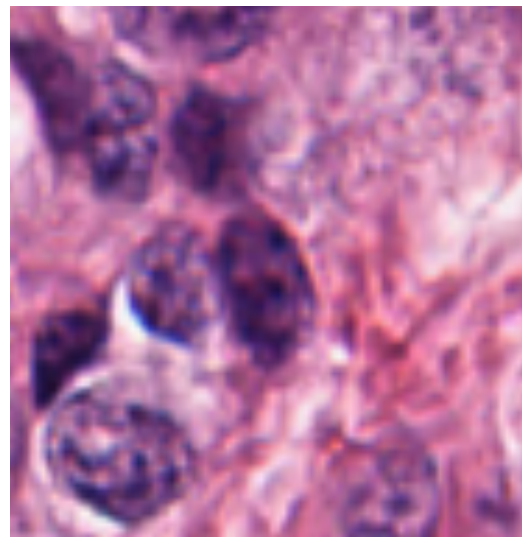
3. Experimental examples

4. Theorem: Linear maps between feature maps are equivariant iff they are group convolutions

Architecture for rotation invariant mitotic cell detection

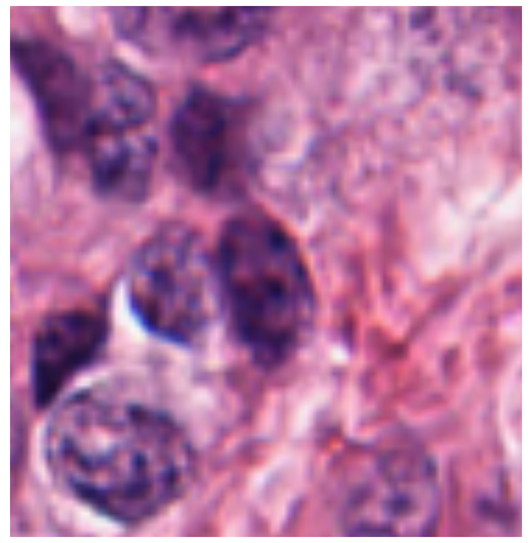


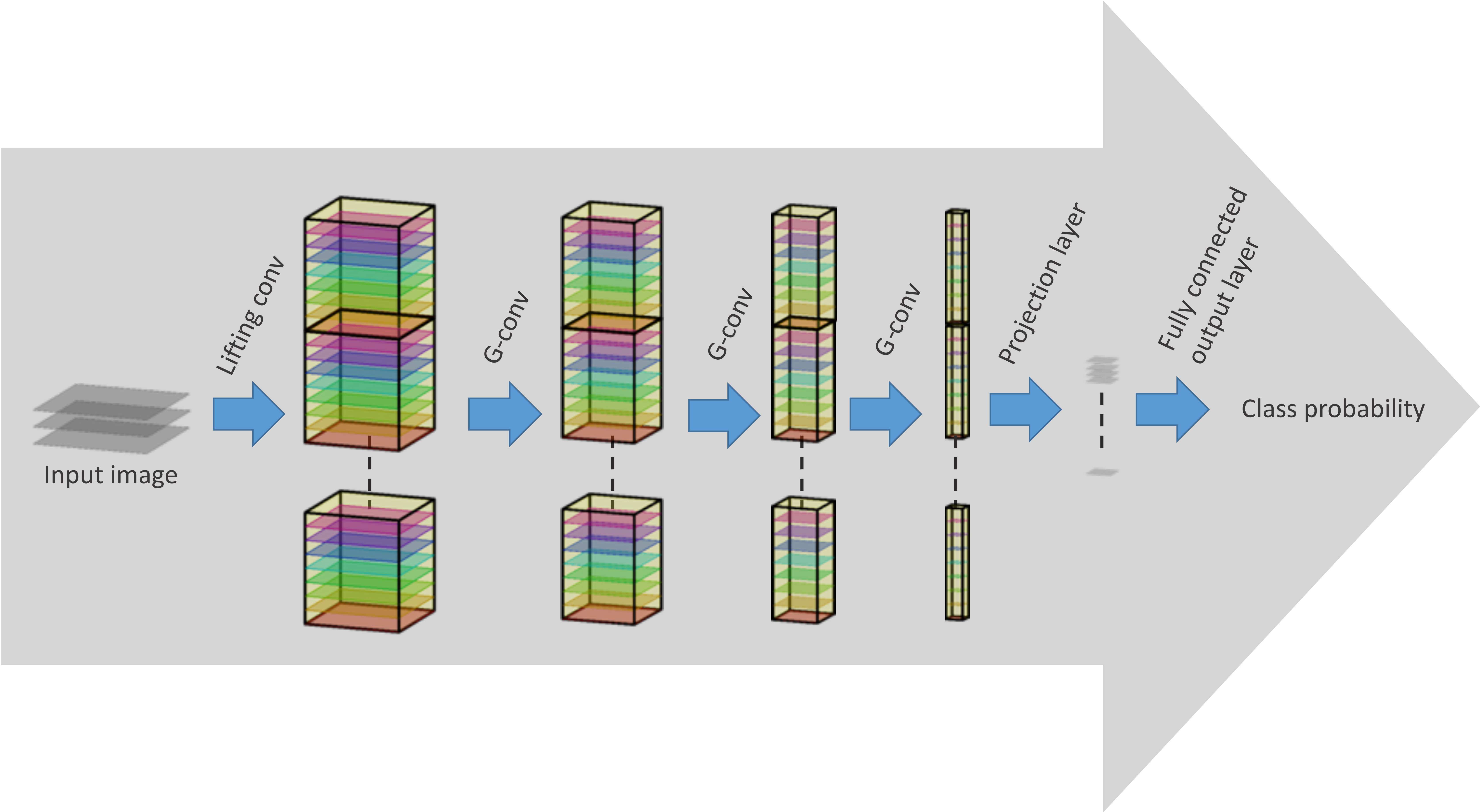
Architecture for rotation invariant mitotic cell detection



“normal” (0)
vs
“mitotic” (1)

Architecture for rotation invariant mitotic cell detection





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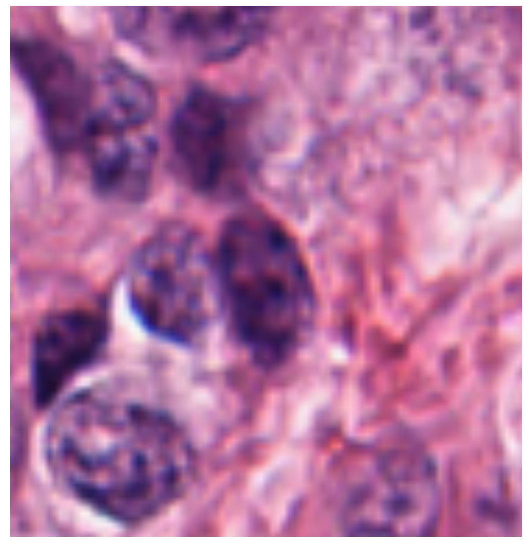

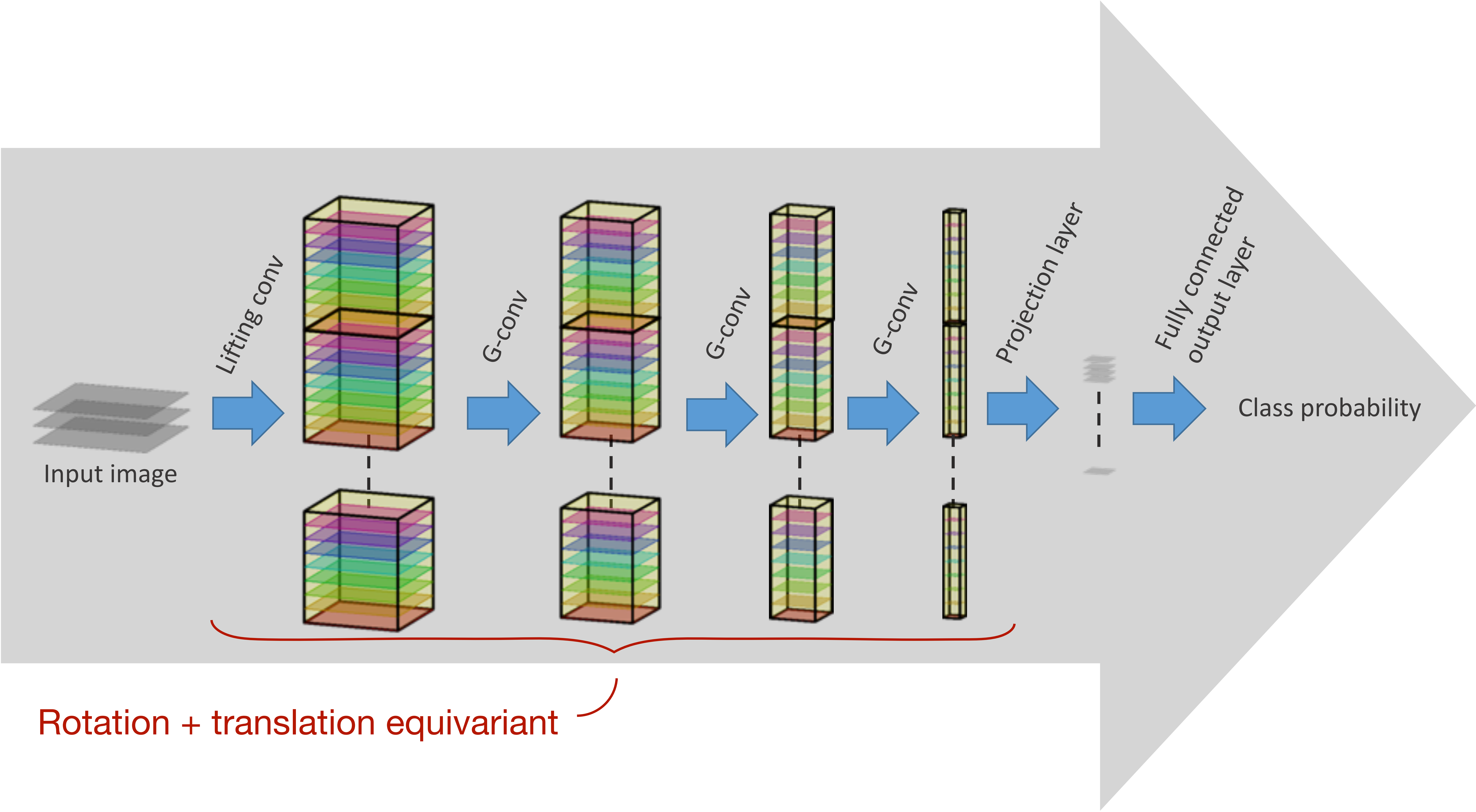

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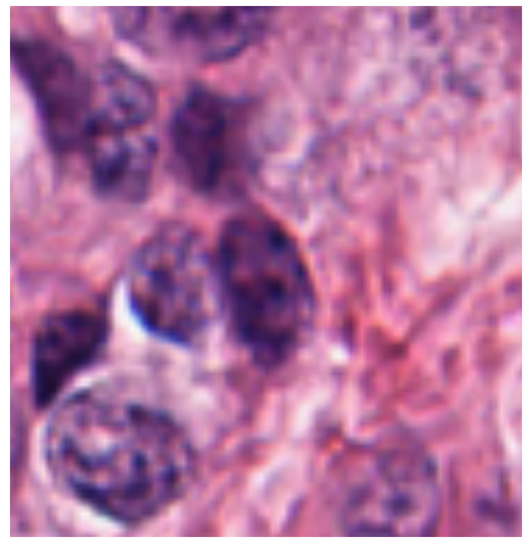

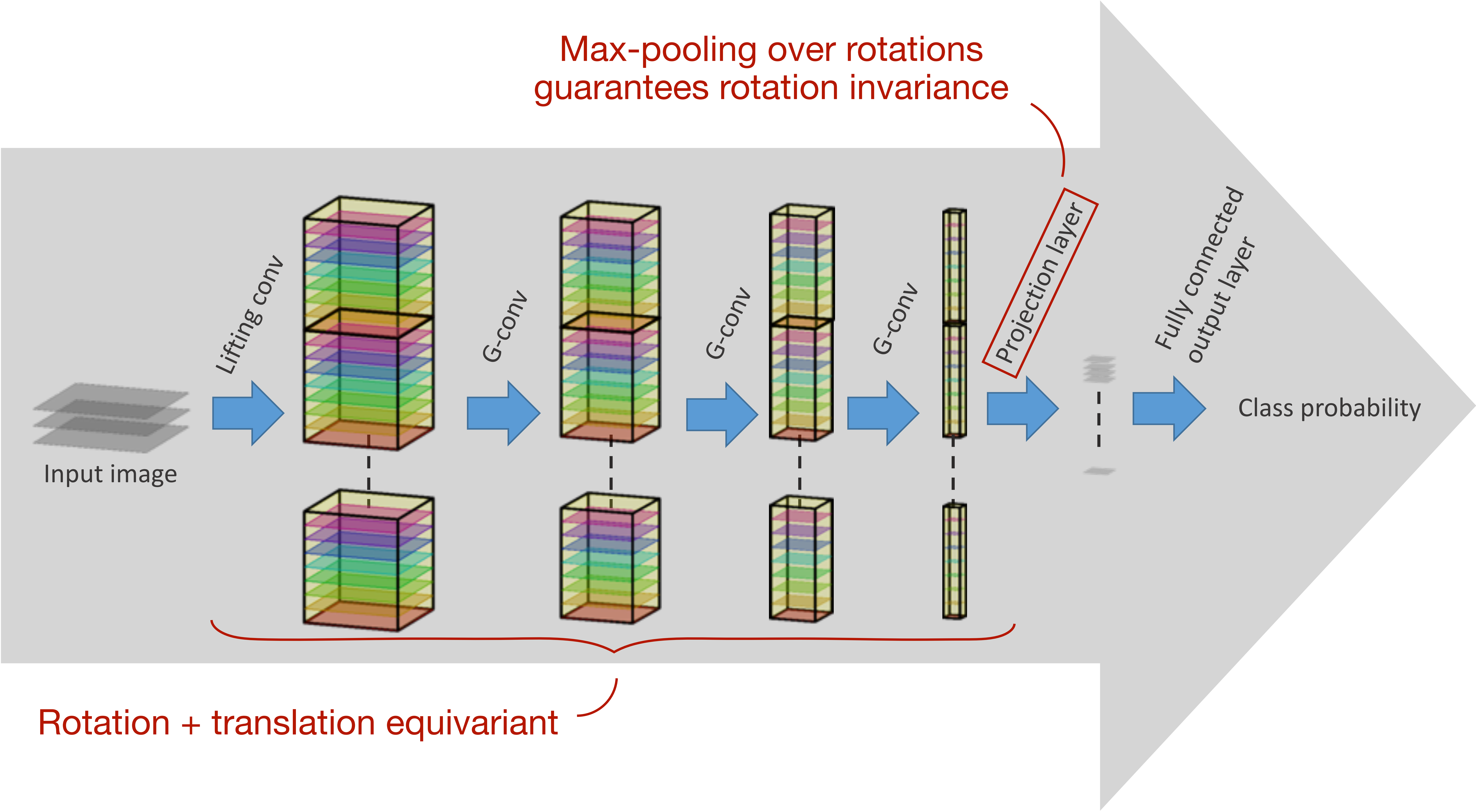

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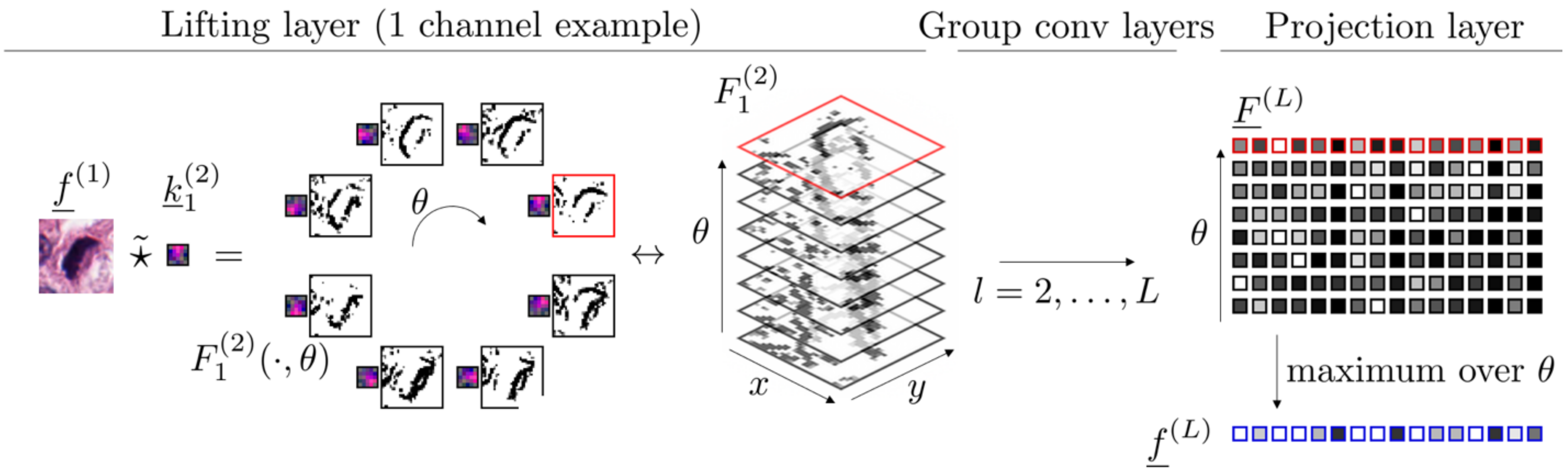

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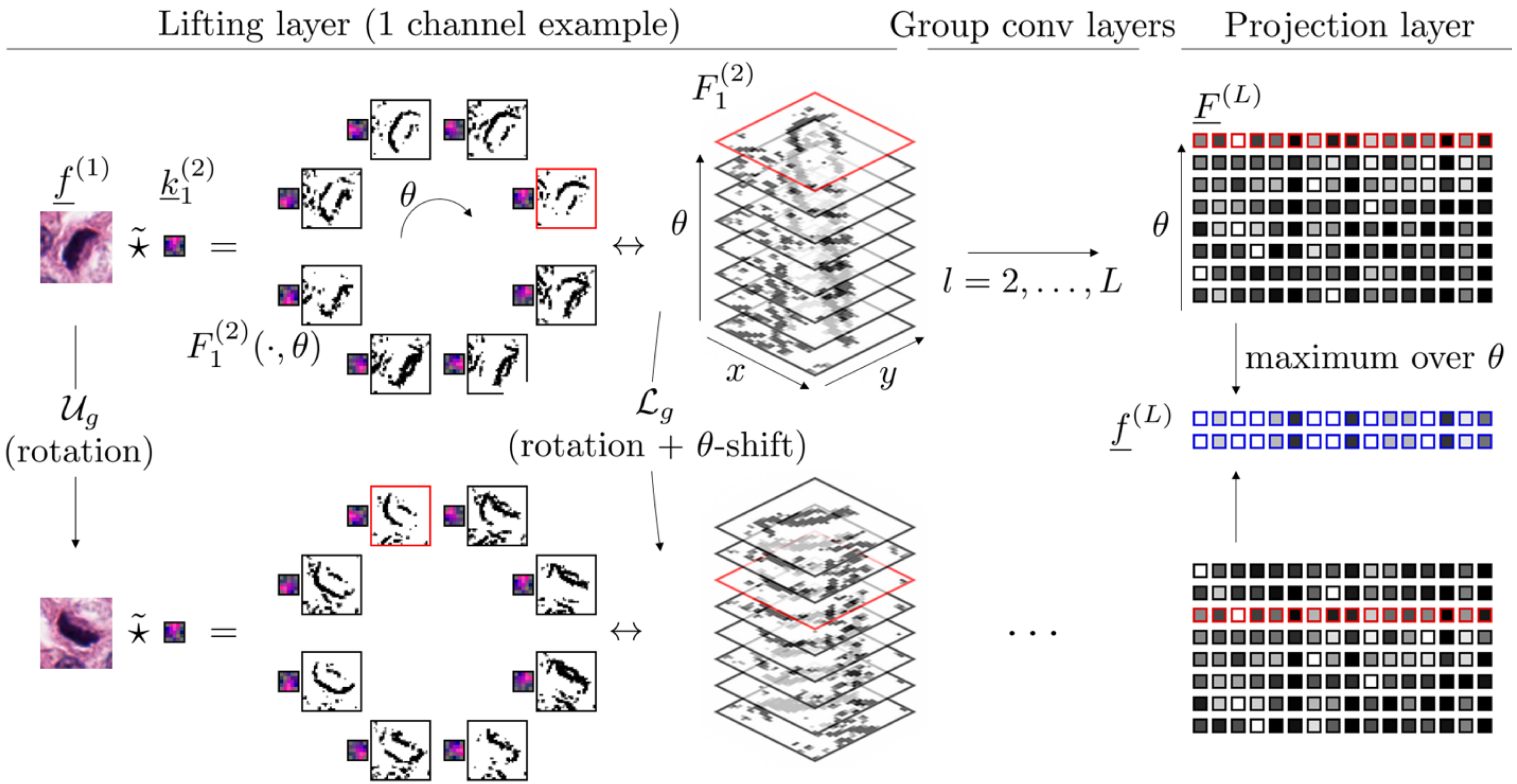
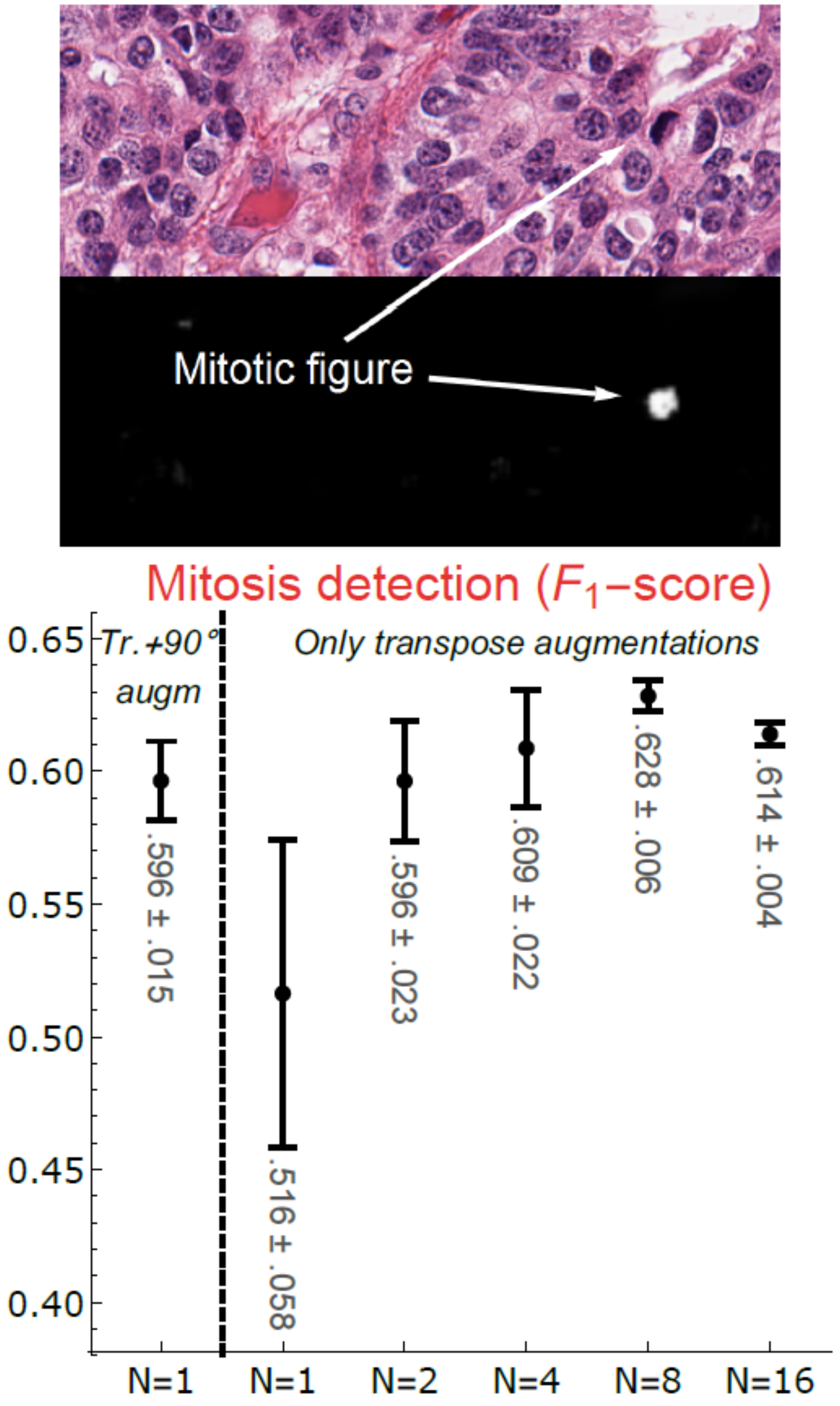


Architecture for rotation invariant mitotic cell detection

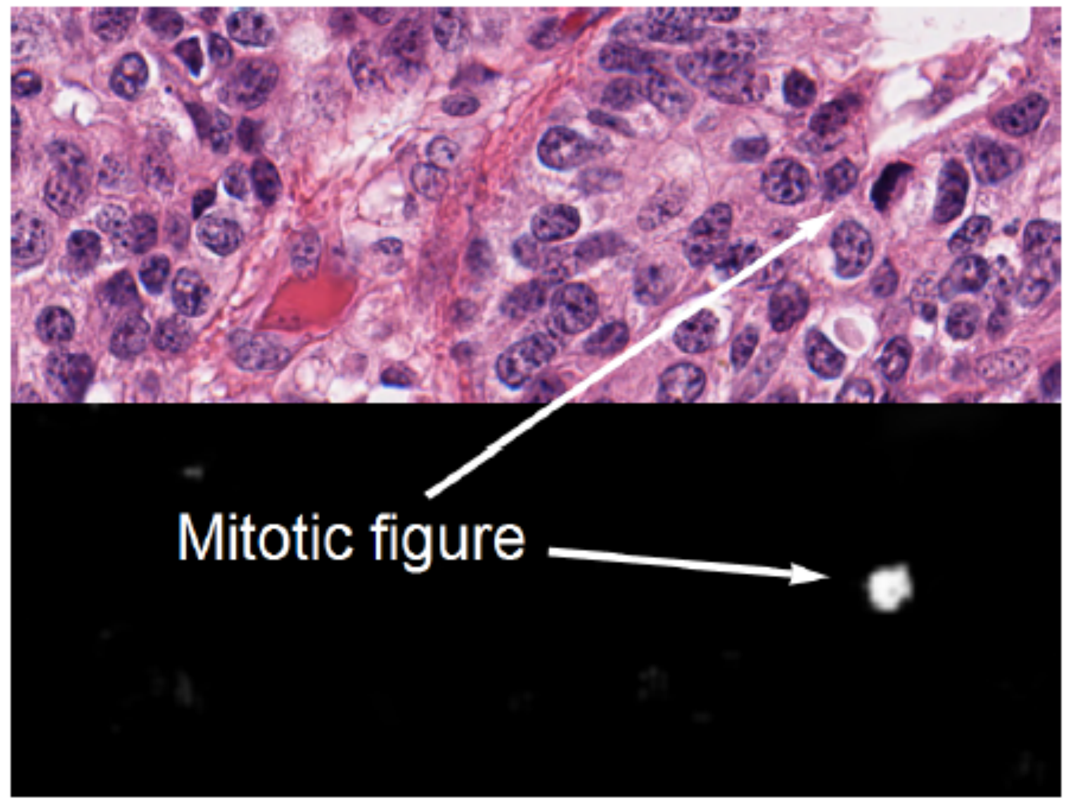
Bekkers & Lafarge et al. MICCAI 2018

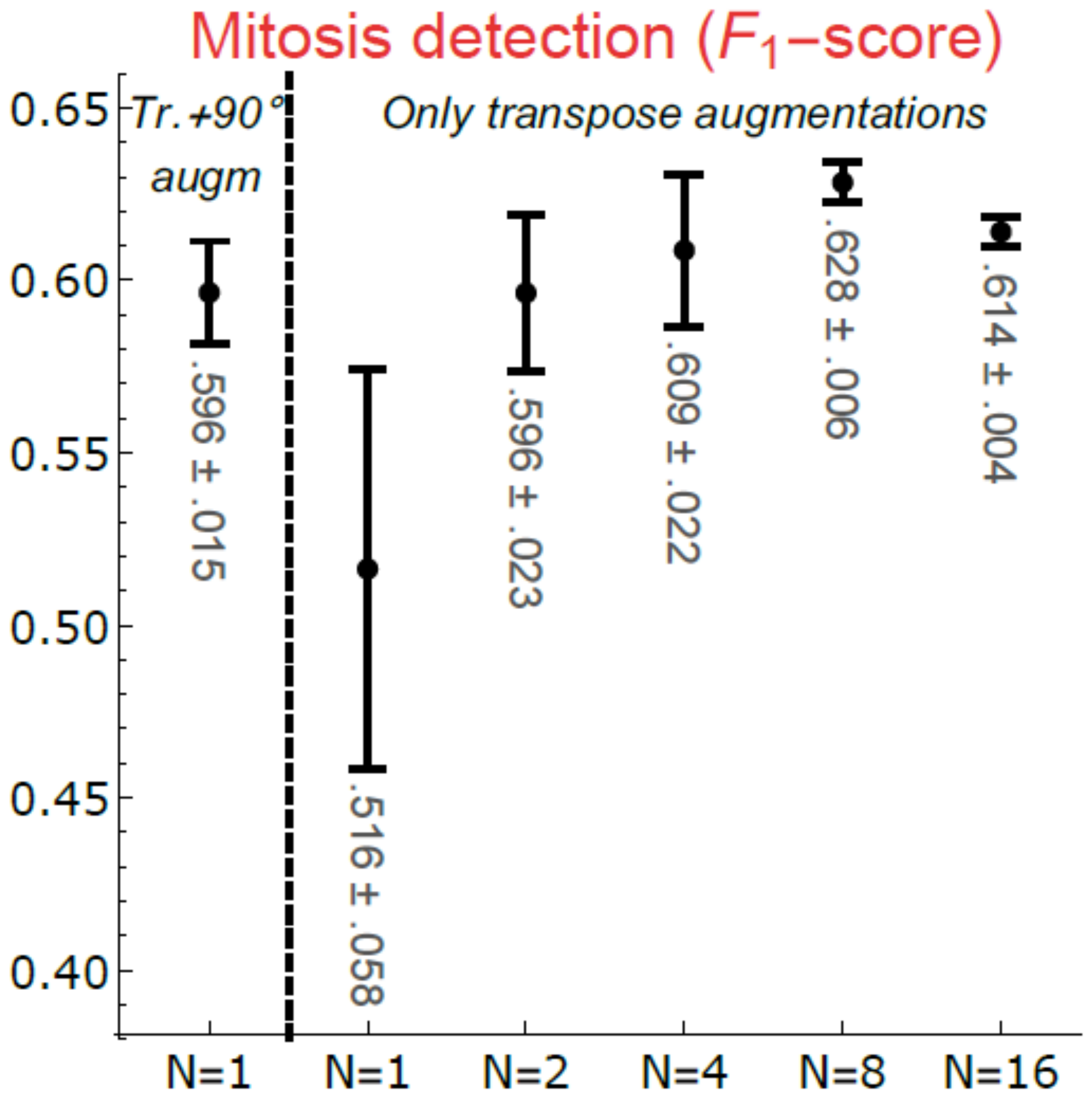


G-CNNs without data-augmentation
outperform
CNNs with data-augmentation

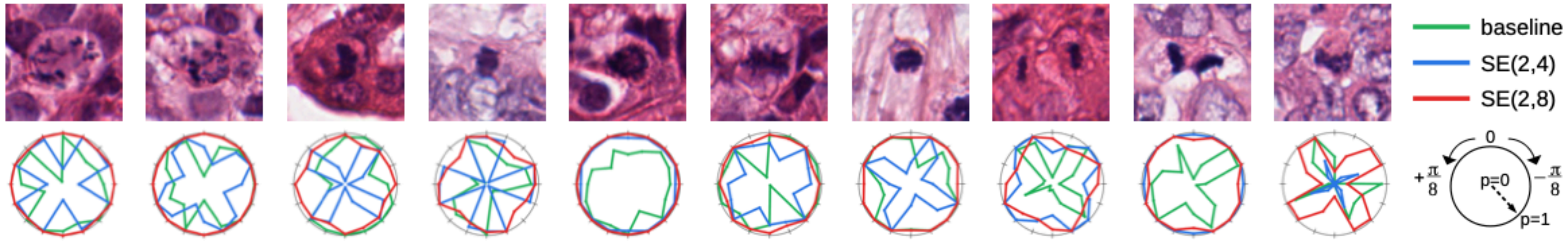
Architecture for rotation invariant mitotic cell detection

Bekkers & Lafarge et al. MICCAI 2018





Lafarge et al. MedIA 2020

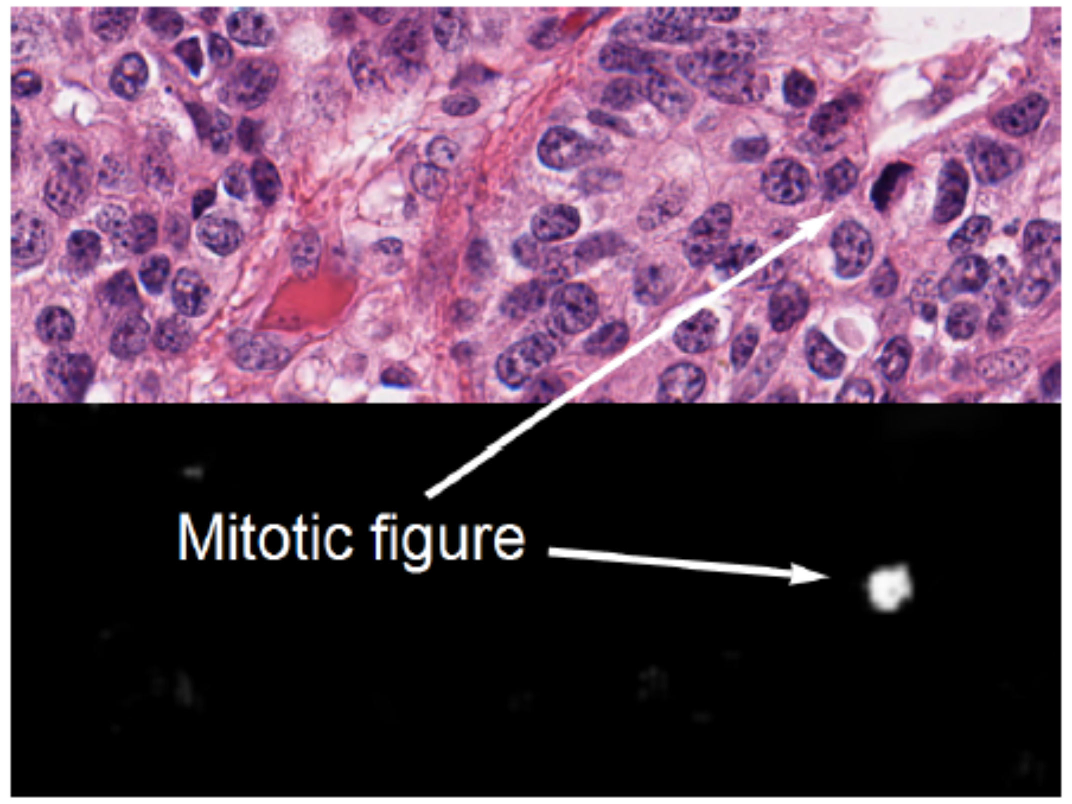


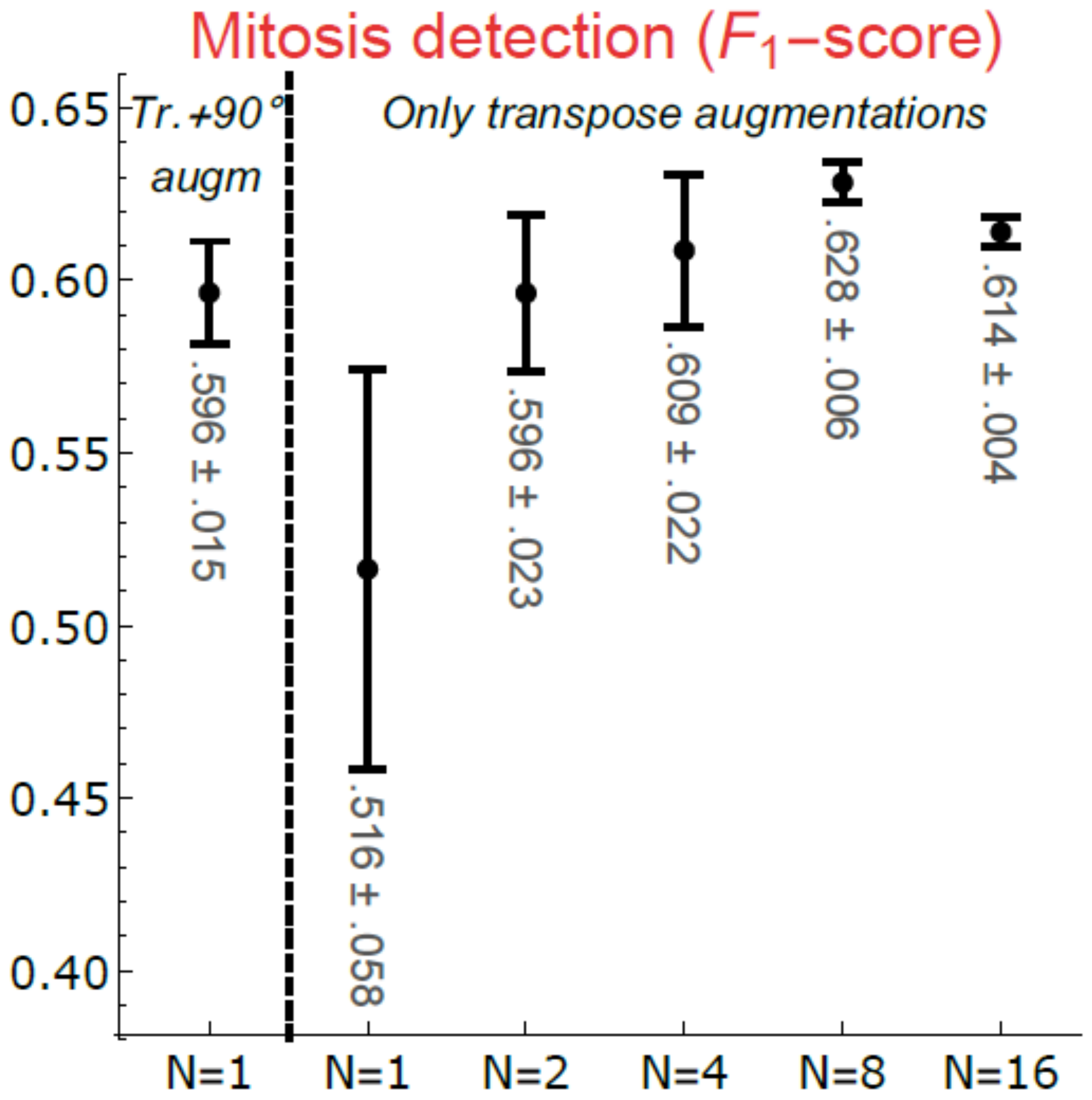
G-CNNs guarantee geometric stability. They are ***robust to input distortions****, regular CNNs aren't…*

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

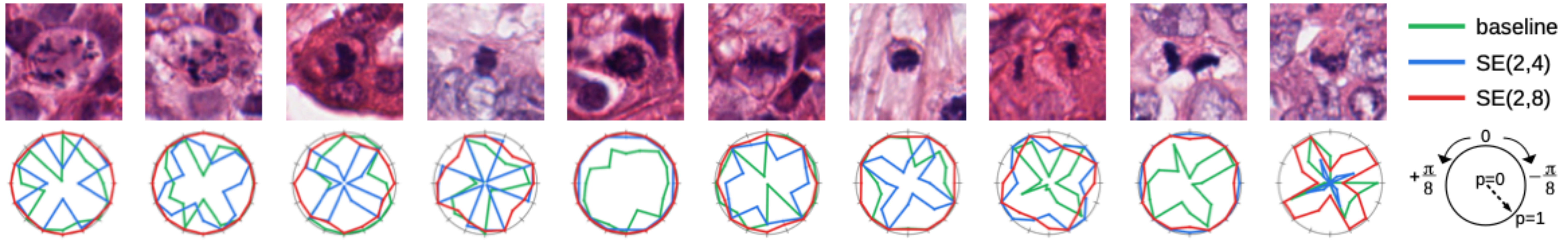
Architecture for rotation invariant mitotic cell detection

Bekkers & Lafarge et al. MICCAI 2018





Lafarge et al. MedIA 2020



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

*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

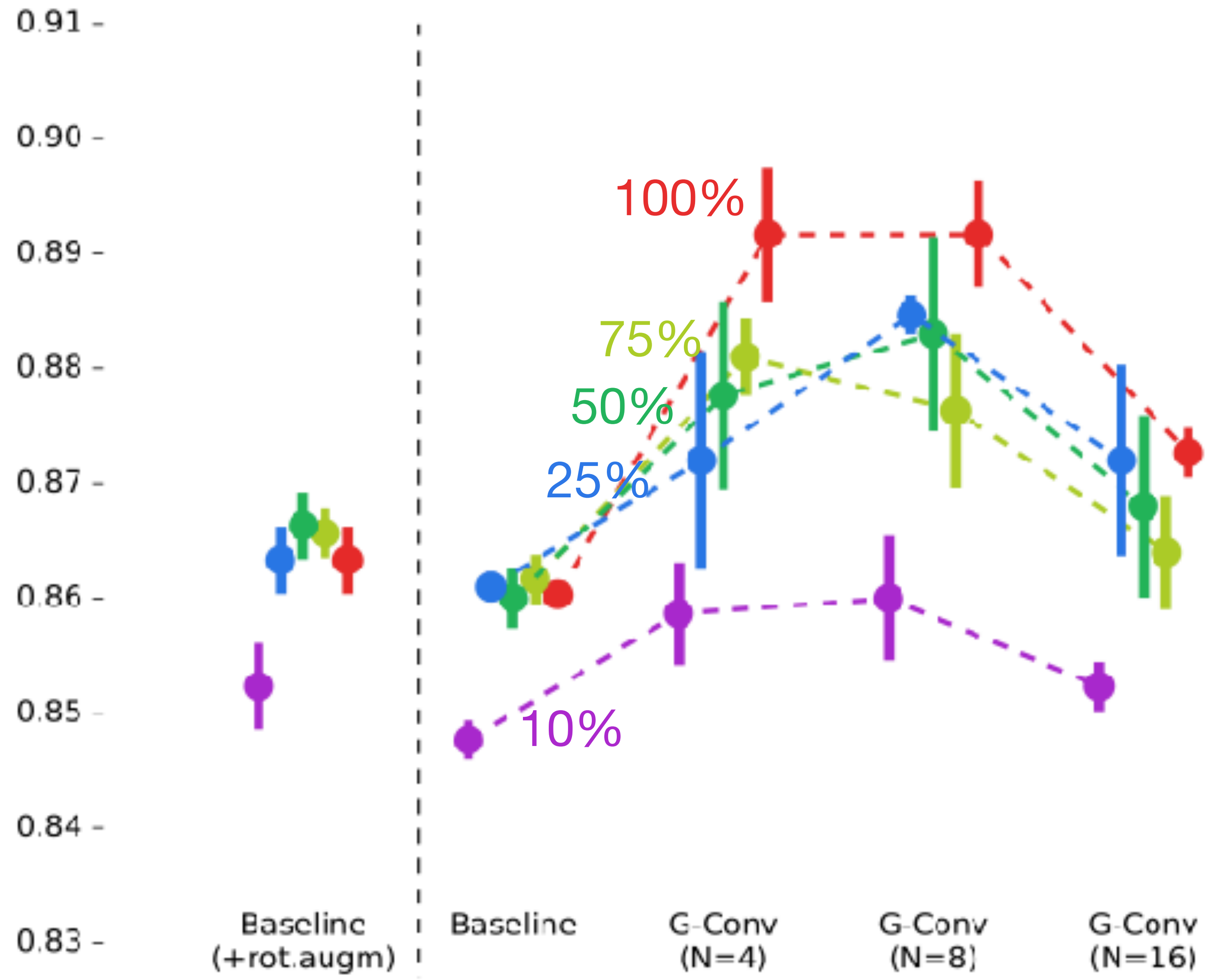
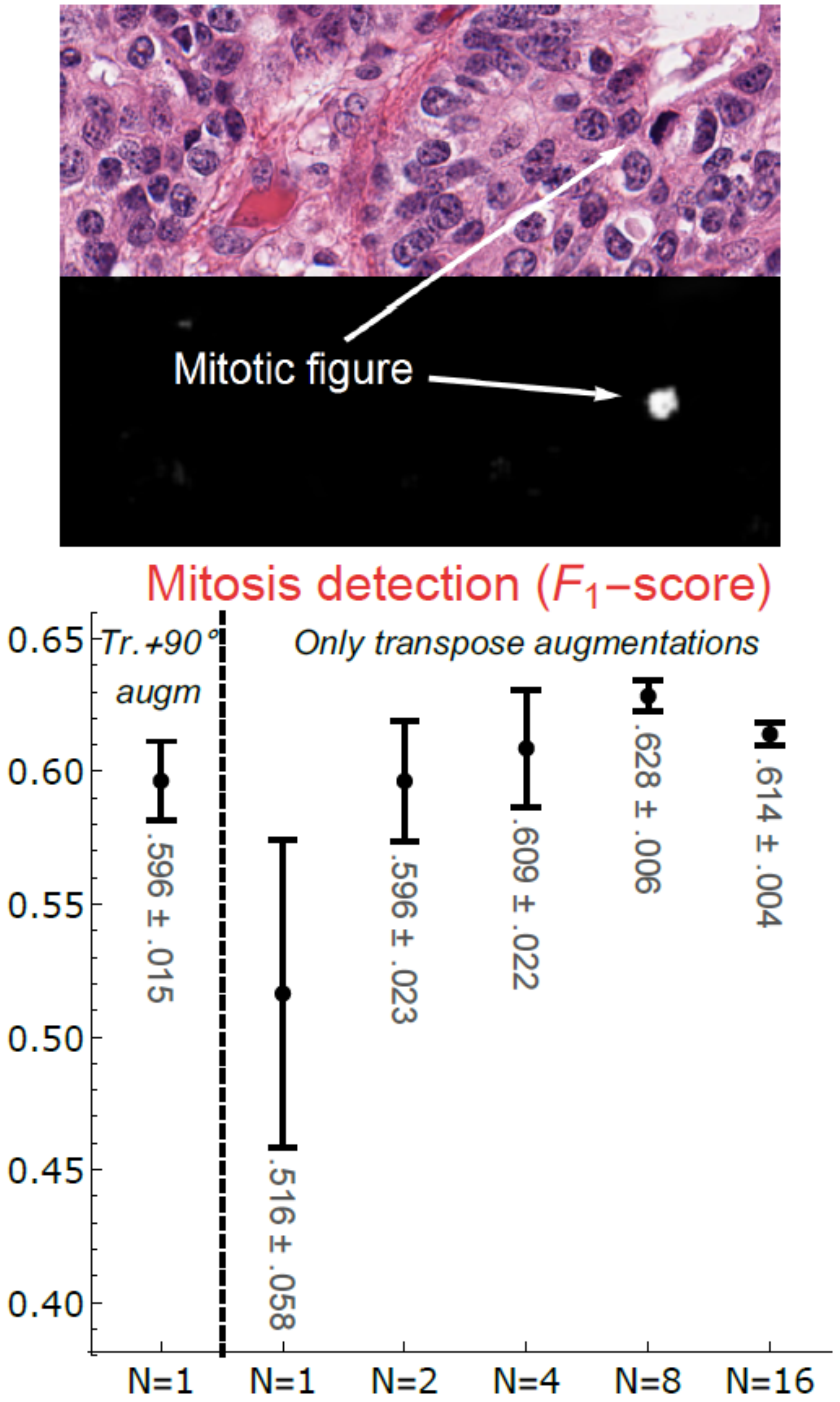
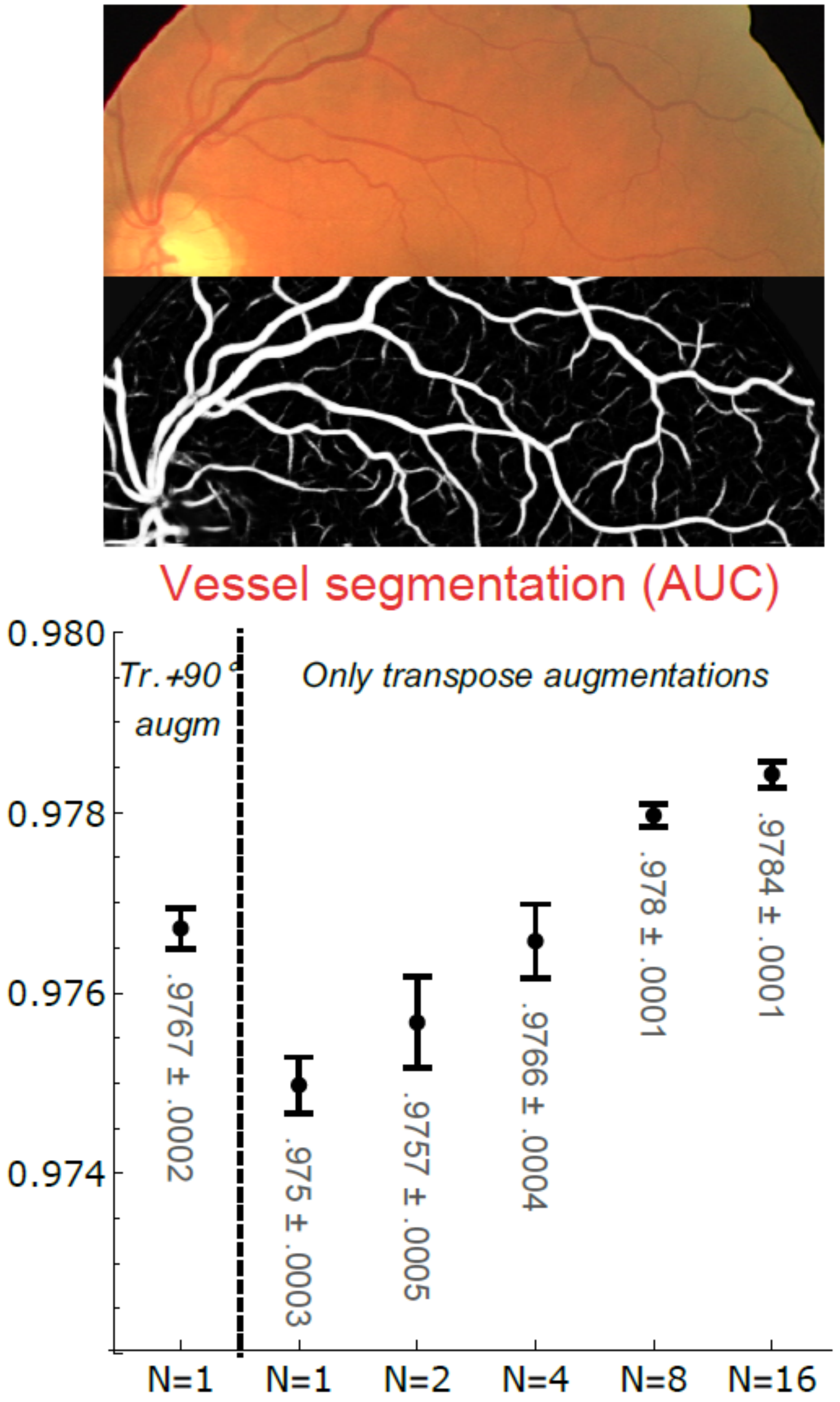


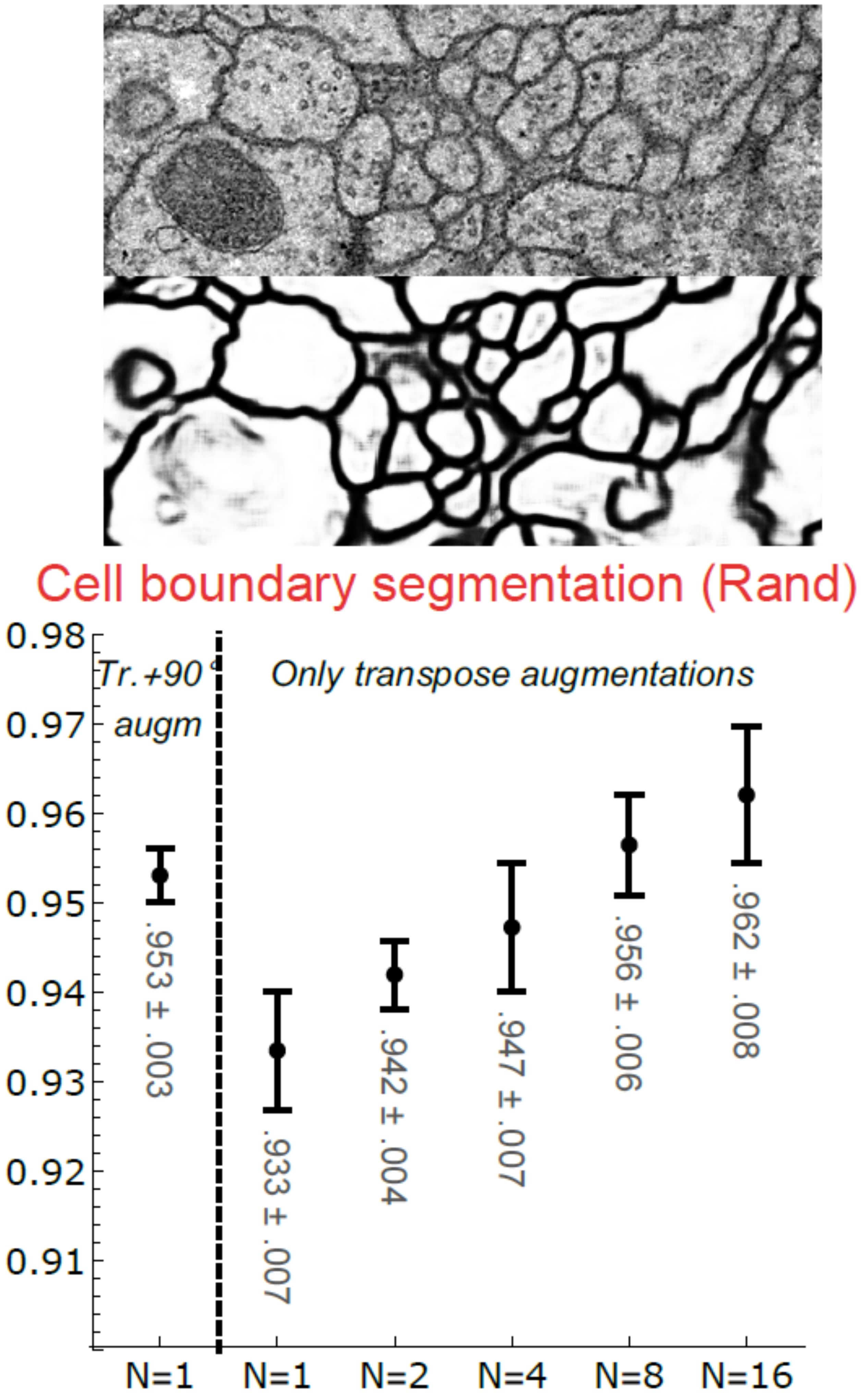
Figure 7: Mean and Standard Deviation plots summarizing the accuracy of the tumor classification models. Mean ± standard deviation is indicated. Color identifies the different data regime (red: 100%; lime: 75%; green: 50%; blue: 25%; purple: 10%).

Experiments in medical image analysis

Bekkers & Lafarge et al. MICCAI 2018



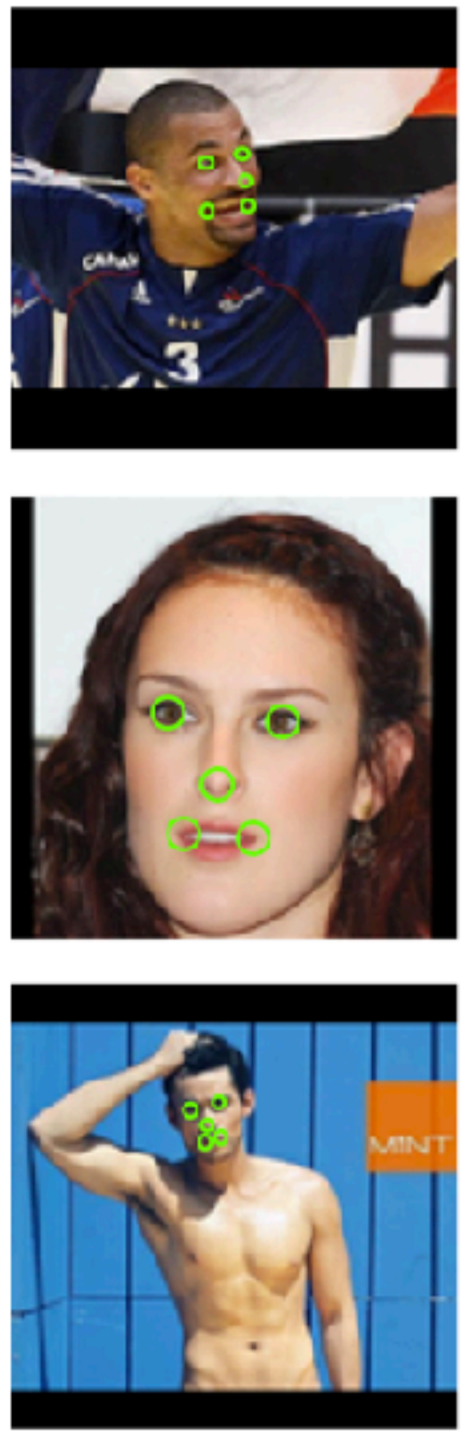


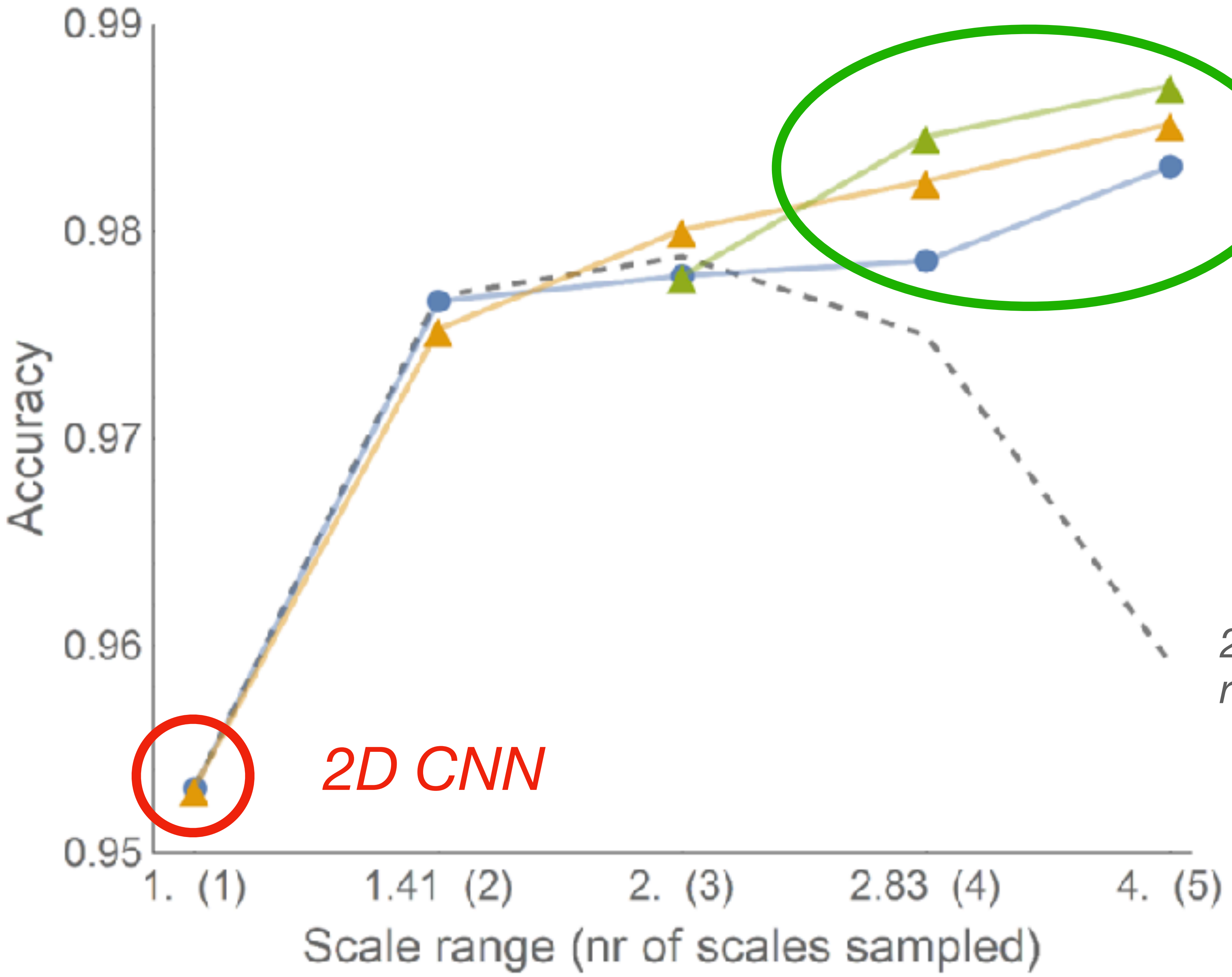


From rotation to scale equivariant CNNs

Bekkers ICLR 2020

Translation + scale equivariant G-CNNs





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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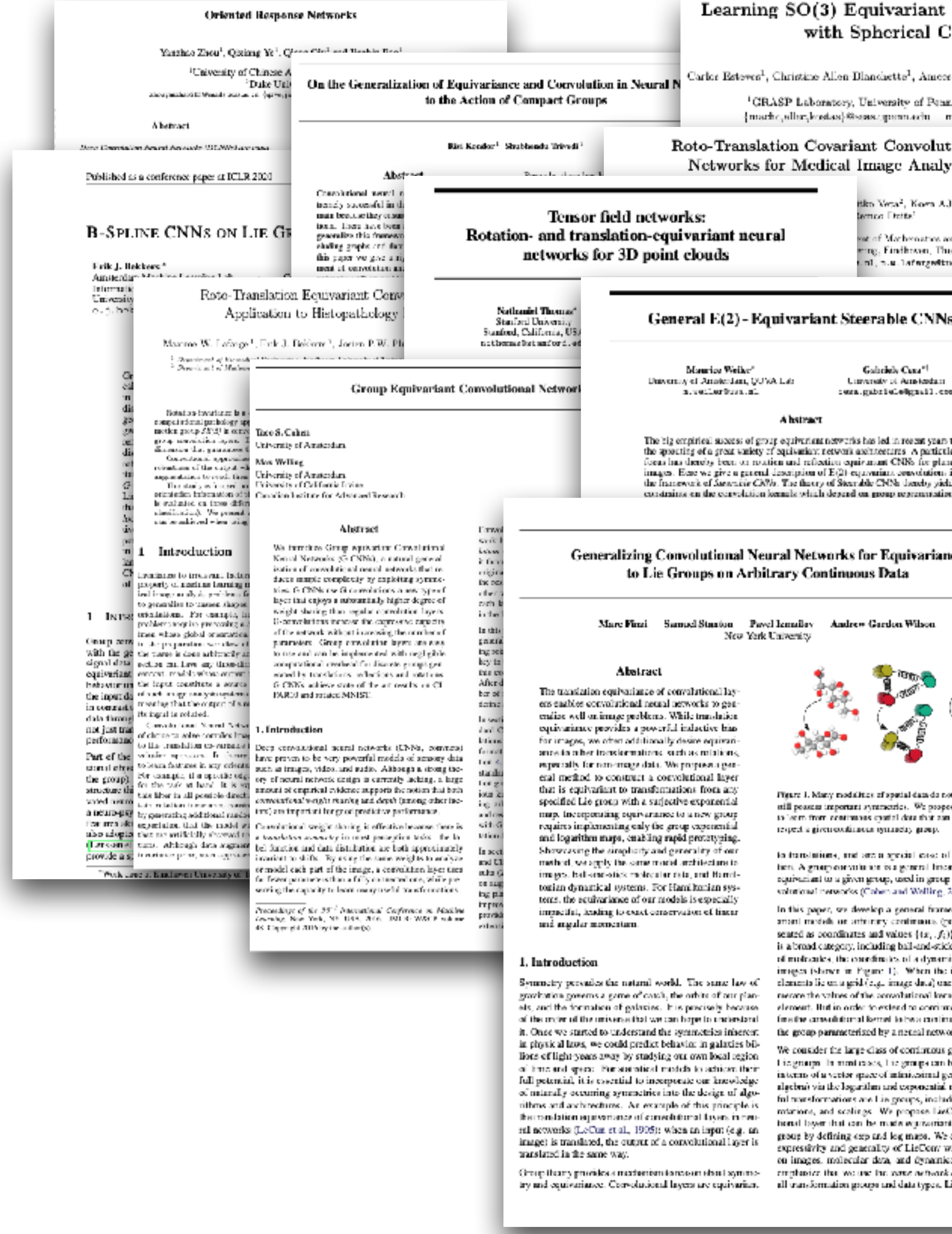
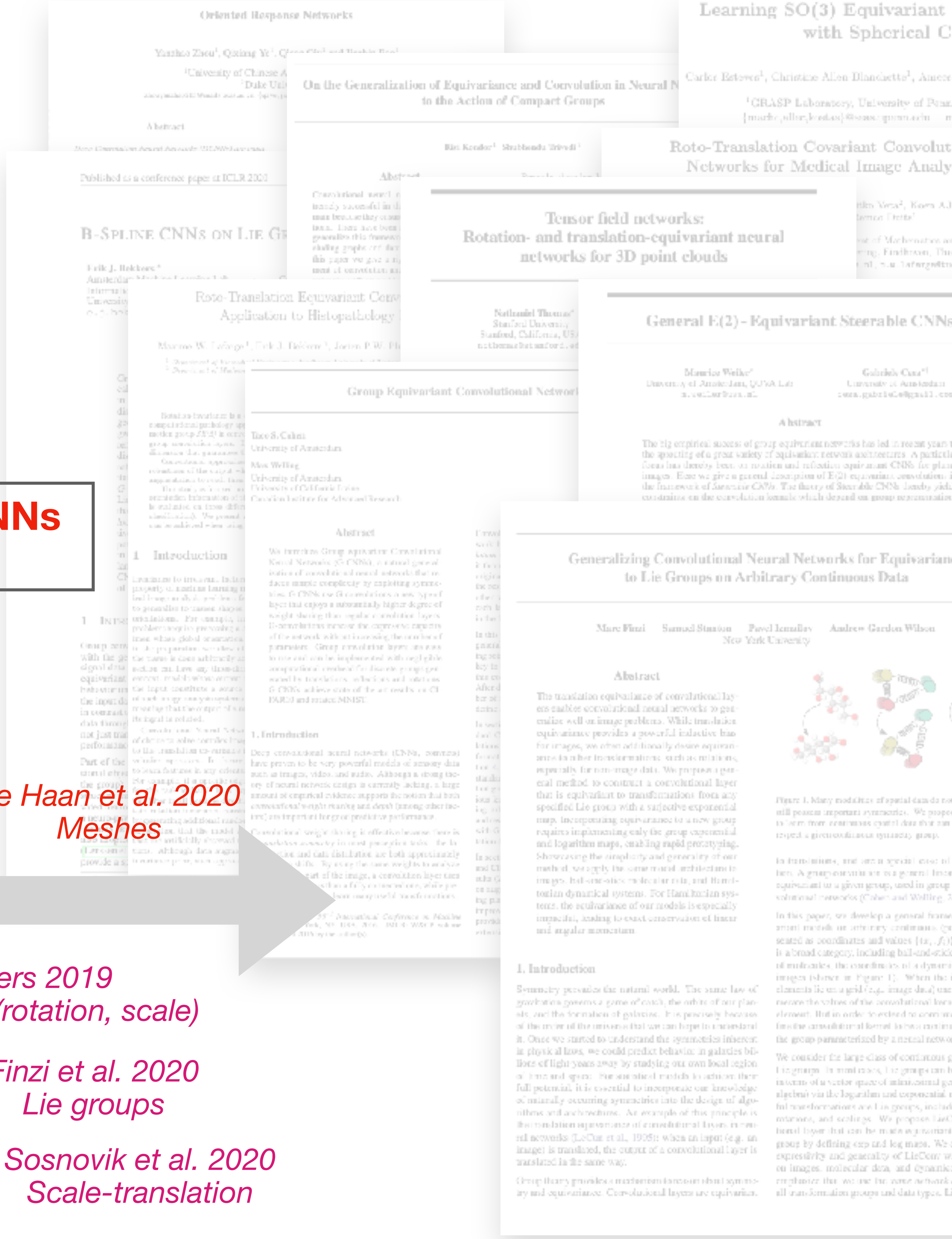


A brief history of G-CNNs



Discrete G-CNNs
(square/cube symmetries)

Gauge-equivariant CNNs
(manifolds)

Cohen-Welling 2016
p4m

Winkels-Cohen 2018
3D discrete roto-transl.

Hoogeboom et al. 2018
SE(2,6)

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Cohen et al. 2019
Icosahedron

de Haan et al. 2020
Meshes

NNs → CNNs → G-CNNs

LeCun et al. 1990

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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

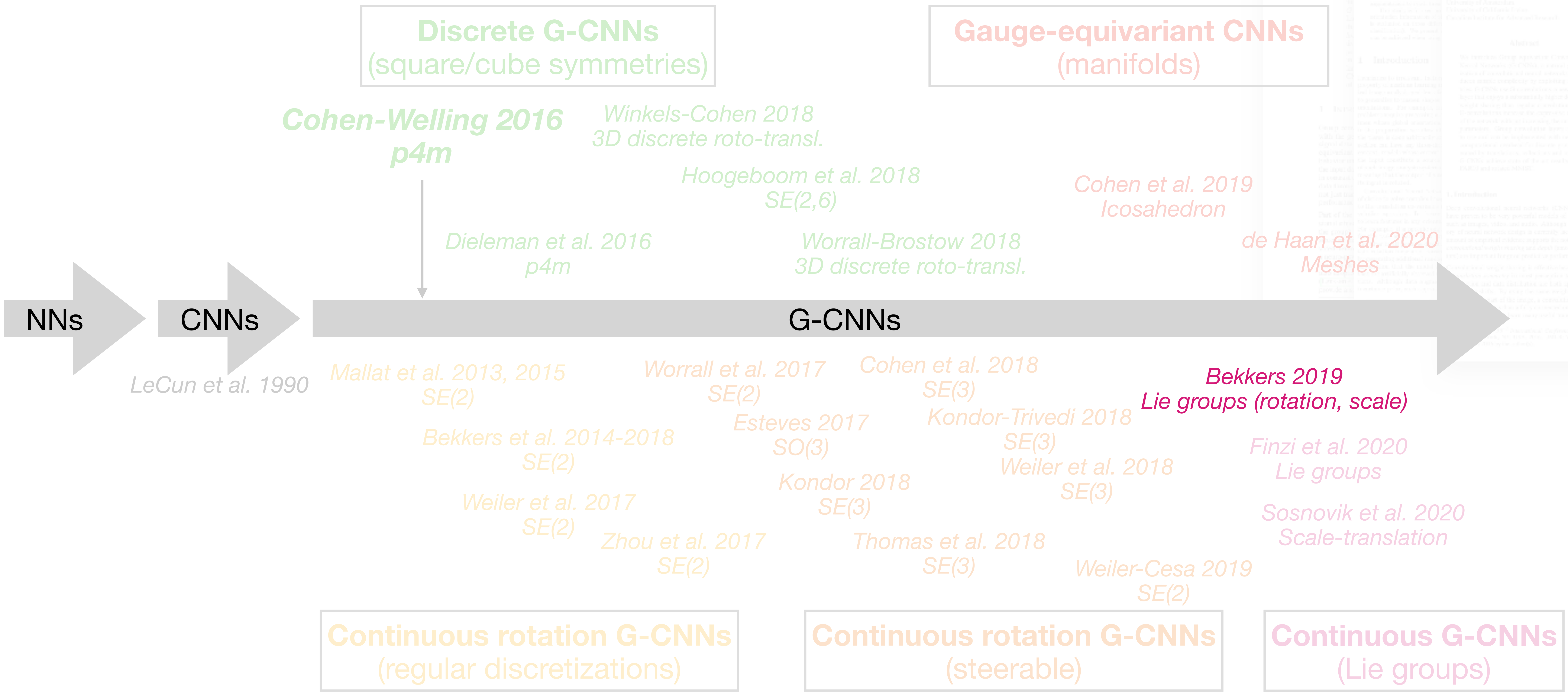
Sosnovik et al. 2020
Scale-translation

Continuous rotation G-CNNs
(regular discretizations)

Continuous rotation G-CNNs
(steerable)

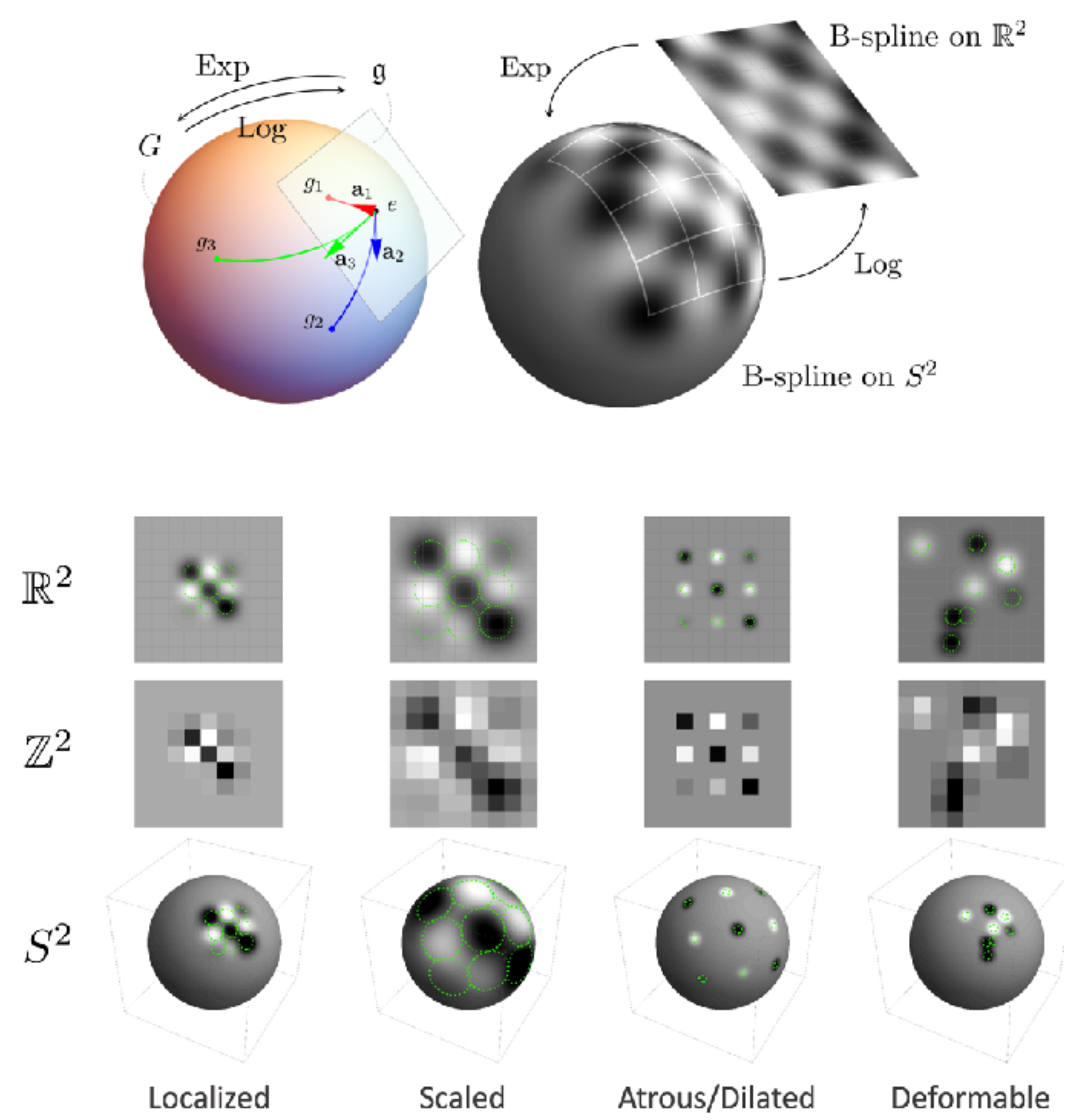
Continuous G-CNNs
(Lie groups)

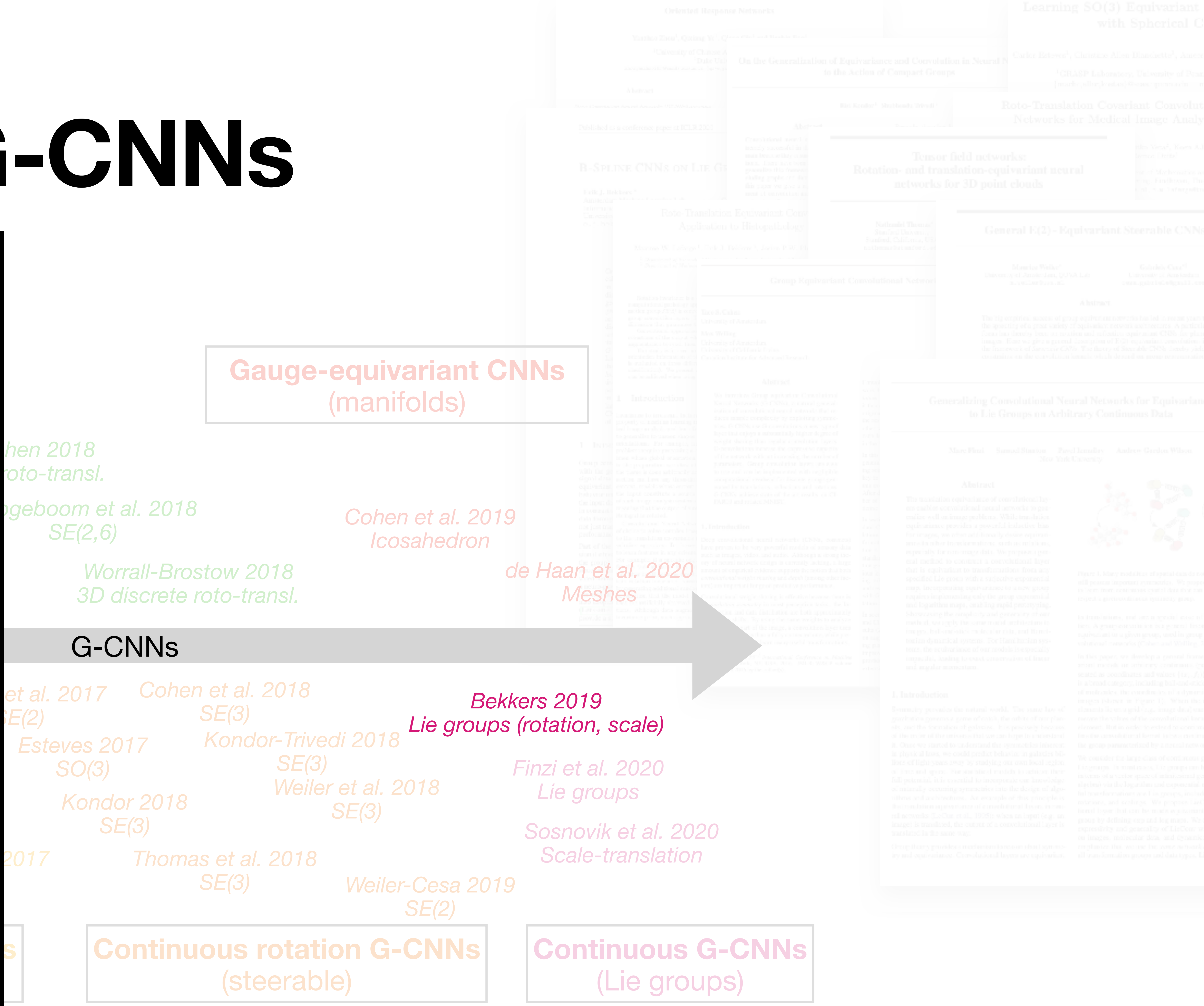
A brief history of G-CNNs



A brief history of G-CNNs

B-Spline CNNs on Lie Groups - ICLR 2020





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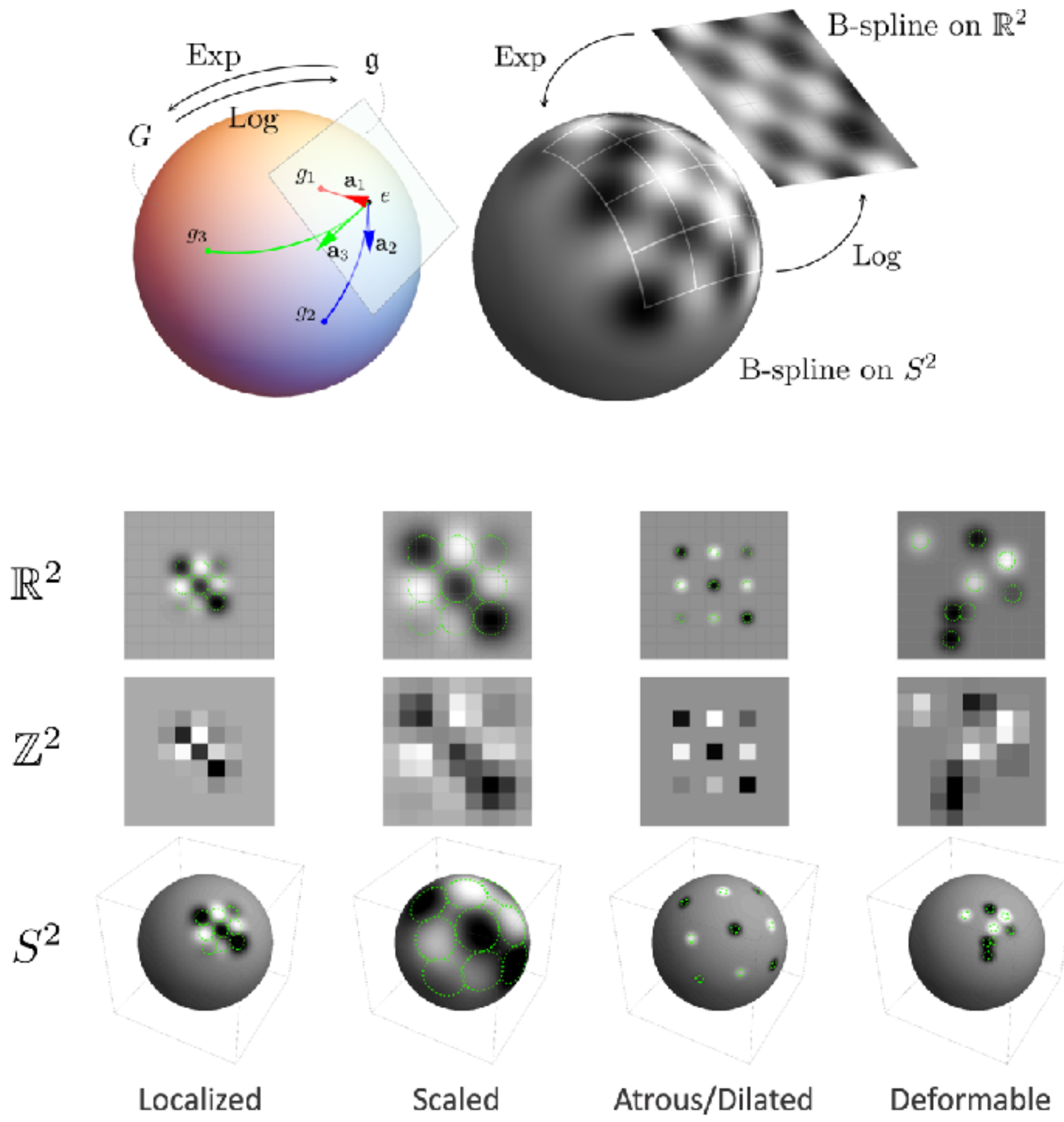
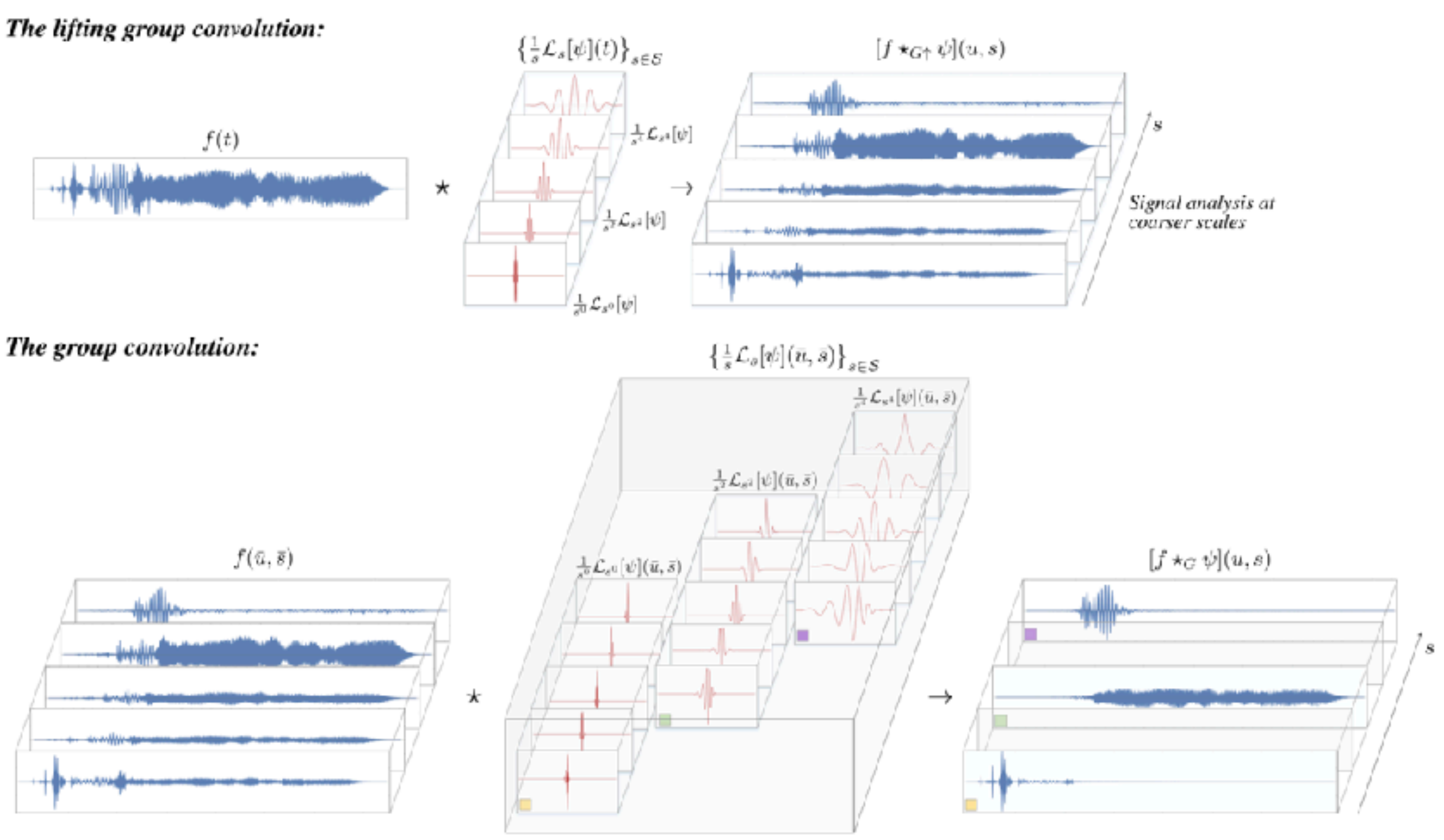


Romero, Bekkers, Tomczak, Hoogeboom
Wavelet Networks: Scale Equivariant Learning From Raw Waveforms - arXiv:2006.05259

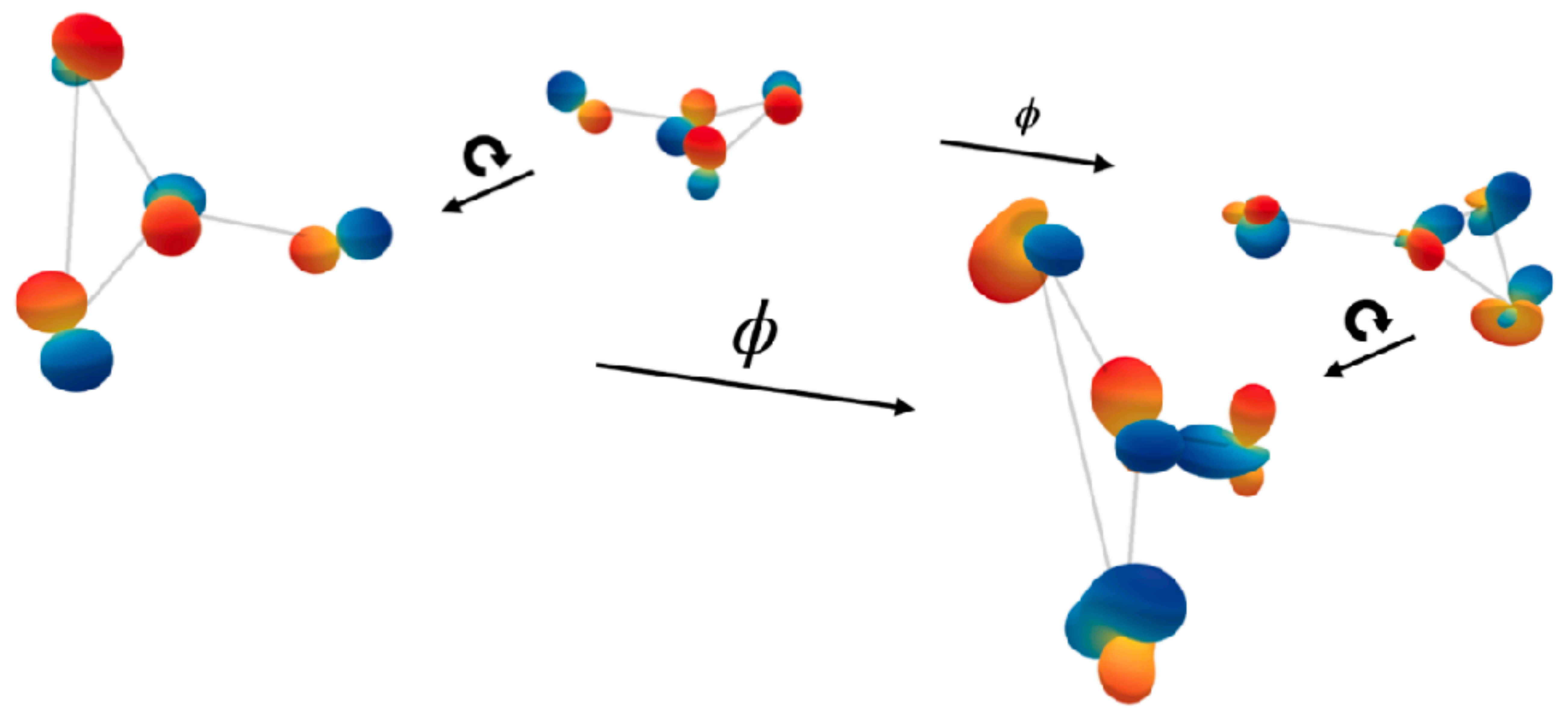


A brief history of G-CNNs

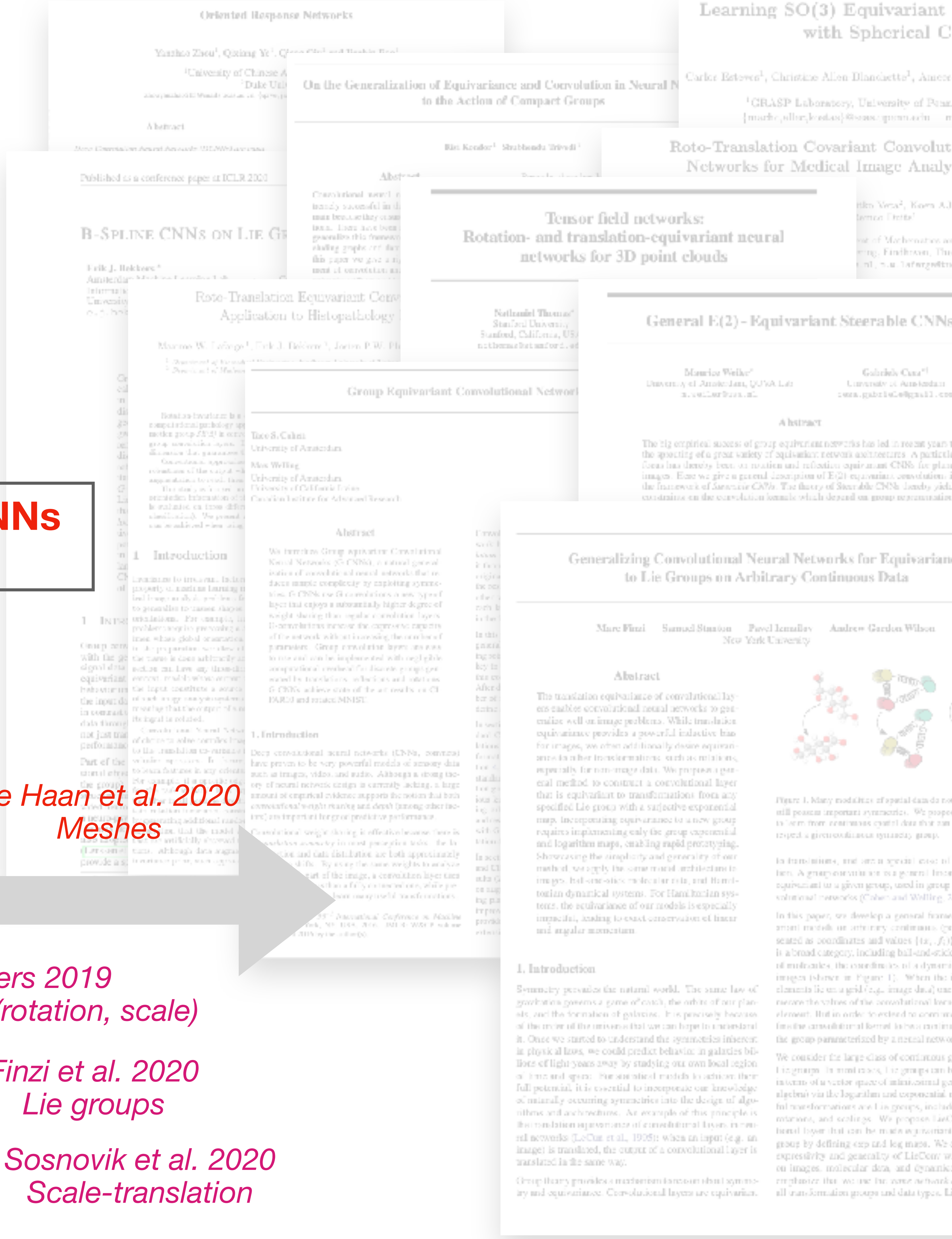
NNs

LeC

Brandstetter, Hesselink, van der Pol, Bekkers, Welling **Steerable Equivariant Message Passing on Molecular Graphs** - in review



A brief history of G-CNNs



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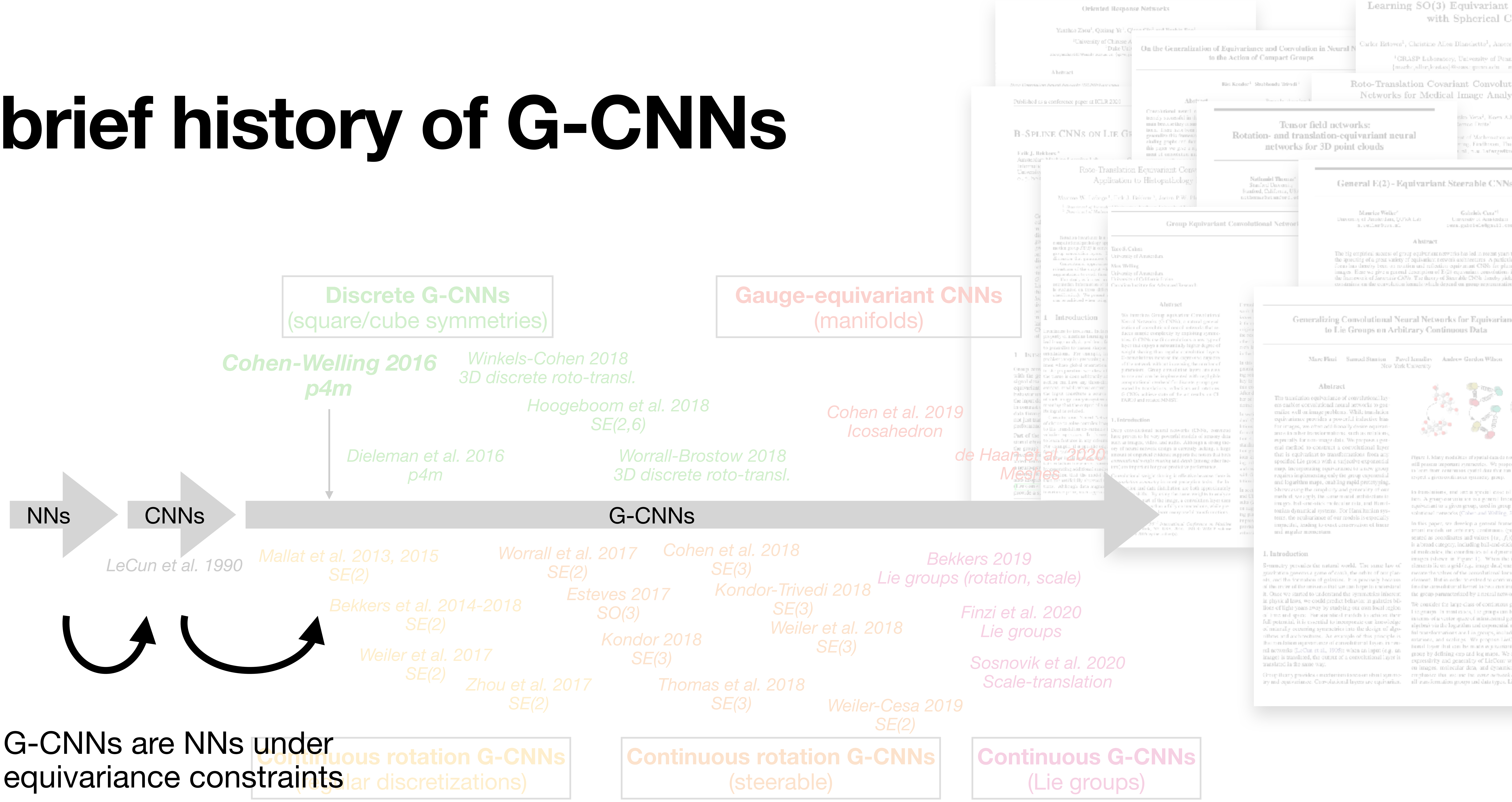
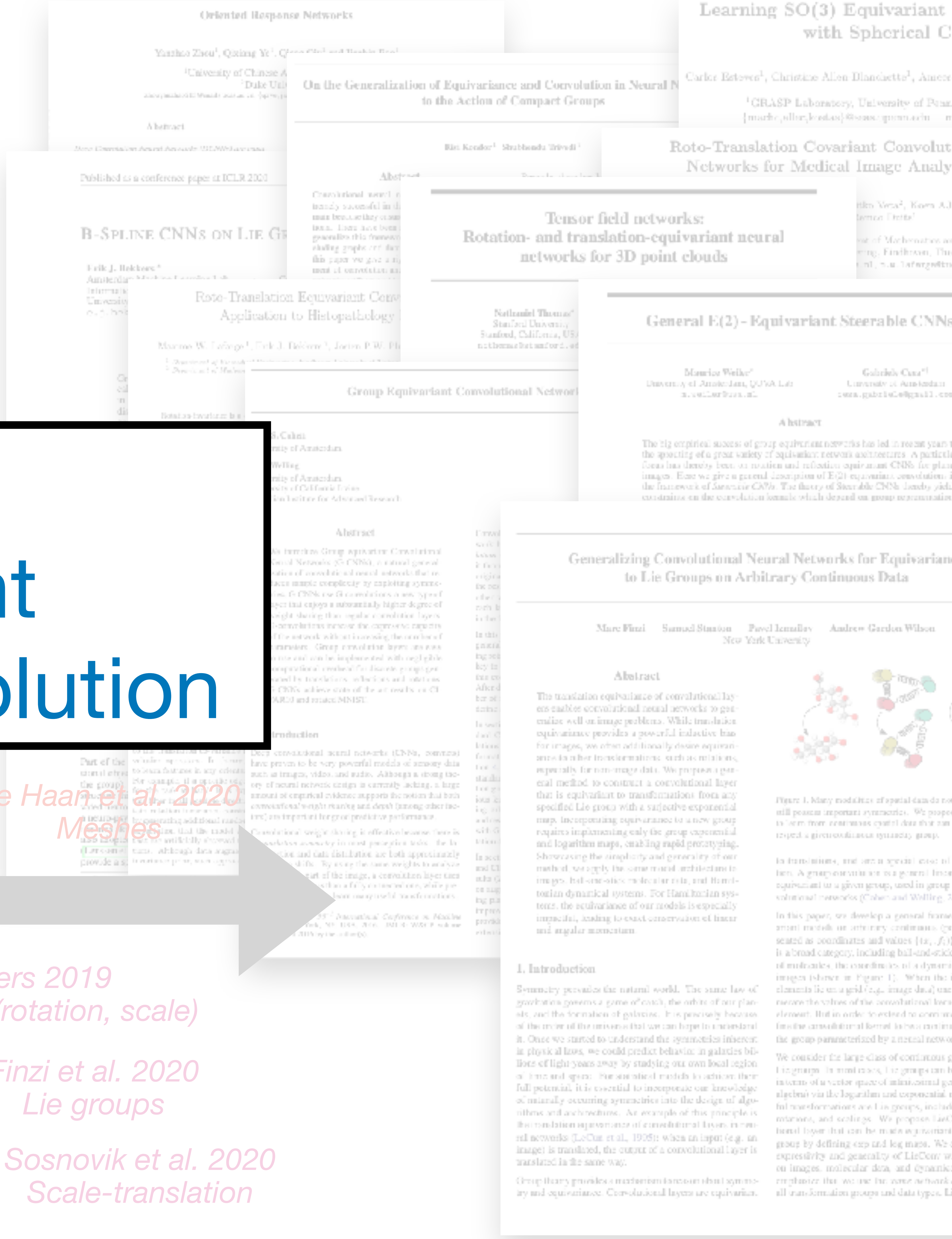


G-CNNs are NNs under equivariance constraints

A brief history of G-CNNs



Part II:
A linear map is equivariant
if and only if it is agroup convolution

Dieleman et al. 2016
p4m

Worrall-Brostow 2018
3D discrete roto-transl.

de Haan et al. 2020
Meshes

NNs | CNNs | G-CNNs

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Content

Part I: Introduction to group convolutions

* Motivation
* Introduction to group theory
* Regular group convolutional neural networks
* Applications

Part II: General theory for group equivariant deep learning

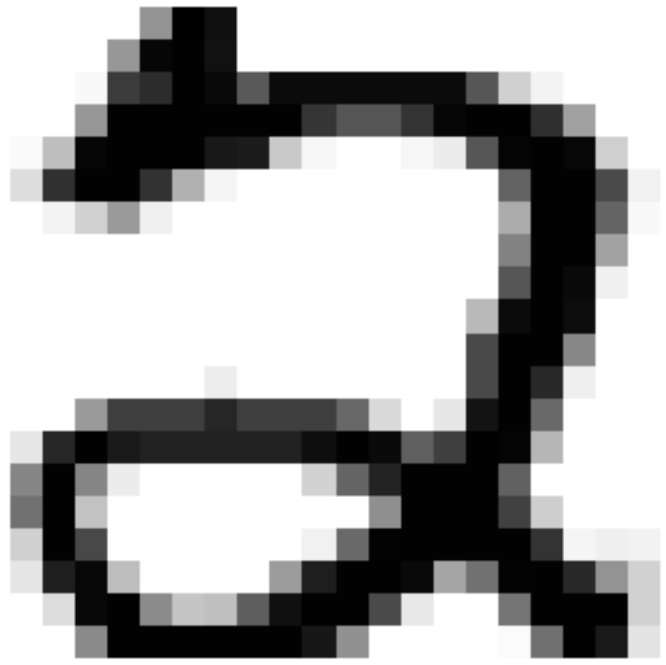
* Group convolutions are all you need!
* Deeper into group theory: representation theory, homogeneous spaces
* Characterization of types of group equivariant layers

Part III: Steerable group convolutions

* Deep dive into group theory: irreducible representations, steerable operators and vector spaces
* Examples of steerable group convolutions: Spherical data and Volumetric data/3D point clouds

Classical artificial neural networks

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



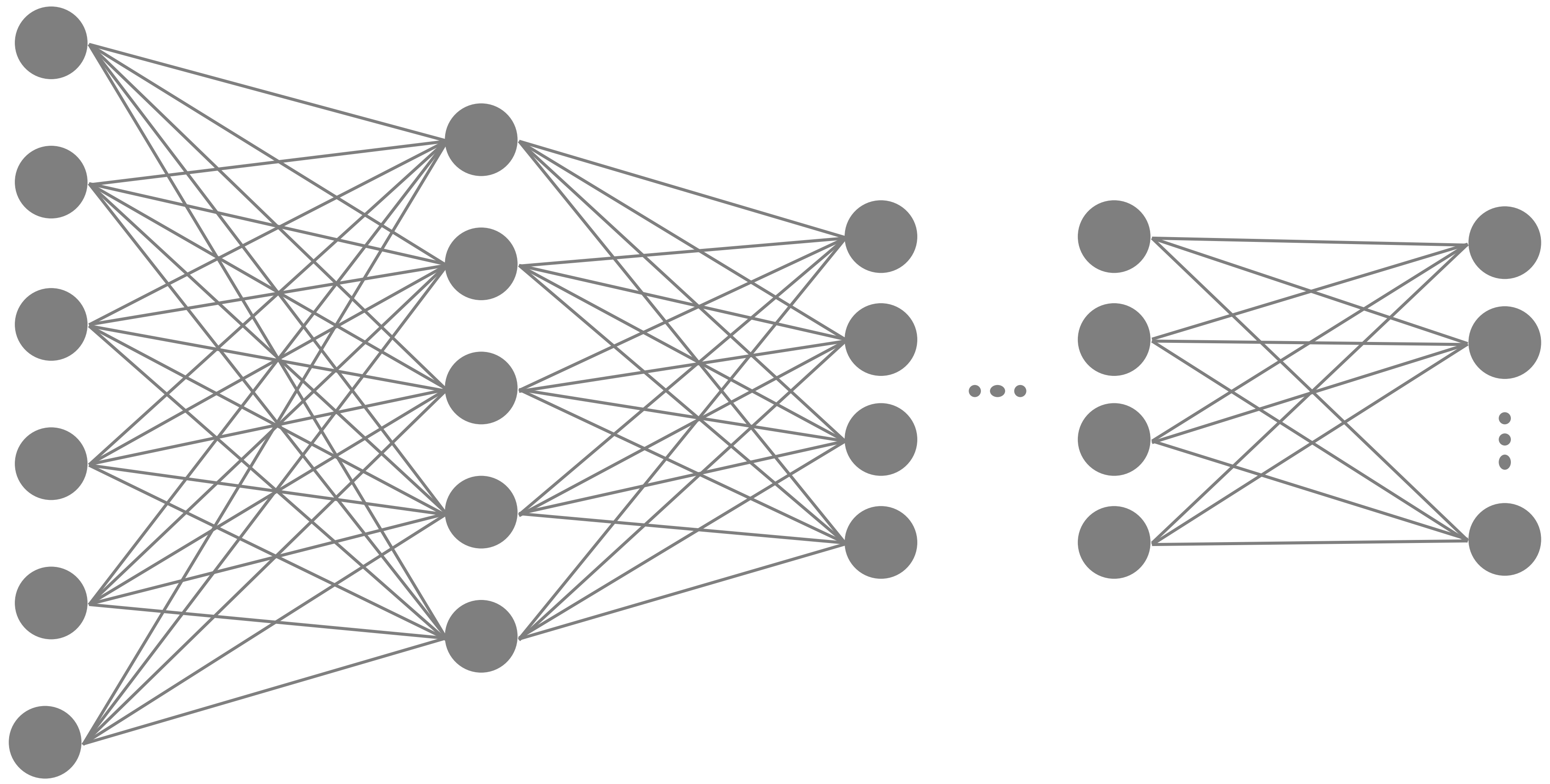


Image analyst: $\underline{x}^0 \in \mathcal{X} = \mathbb{L}_2(\mathbb{R}^2)$

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

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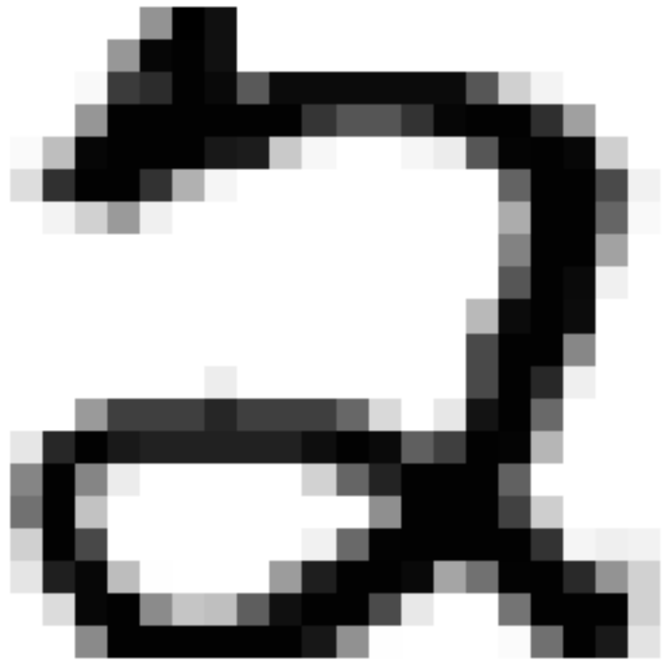

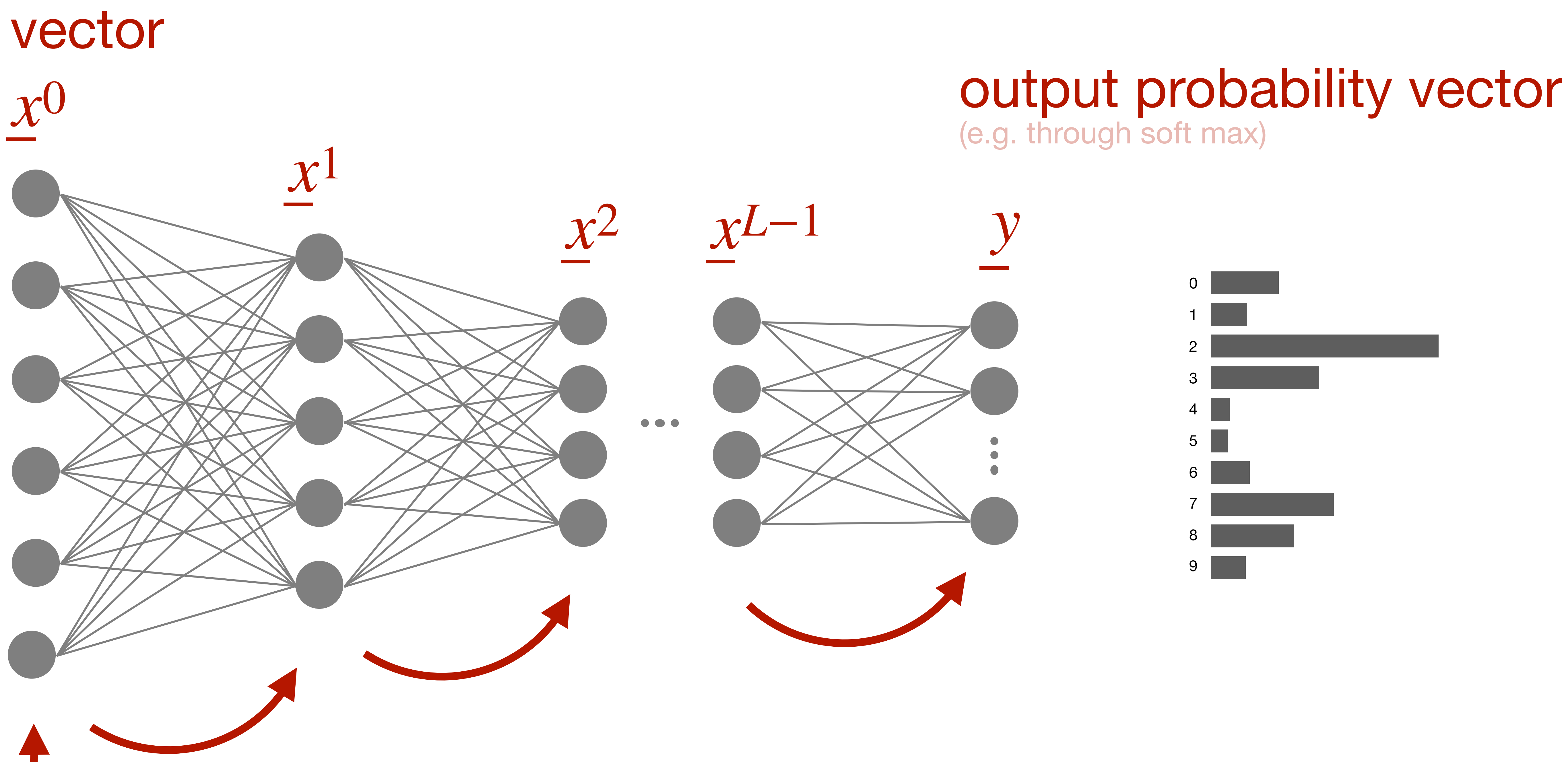

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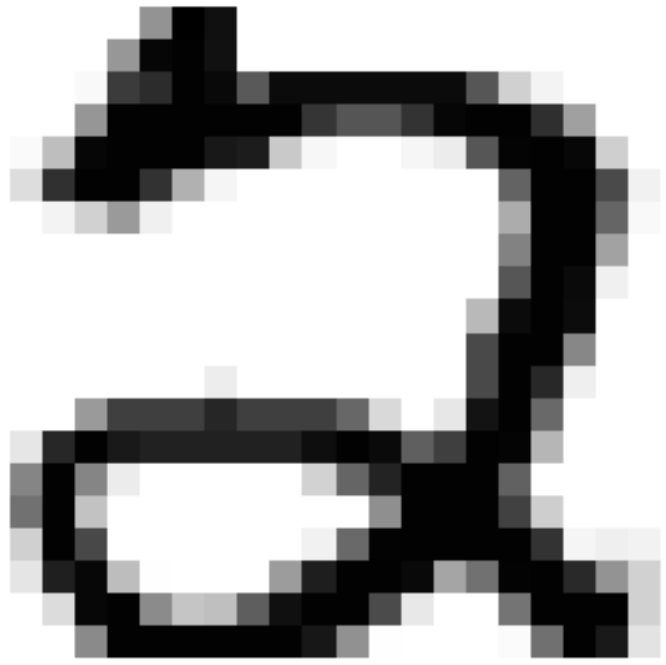
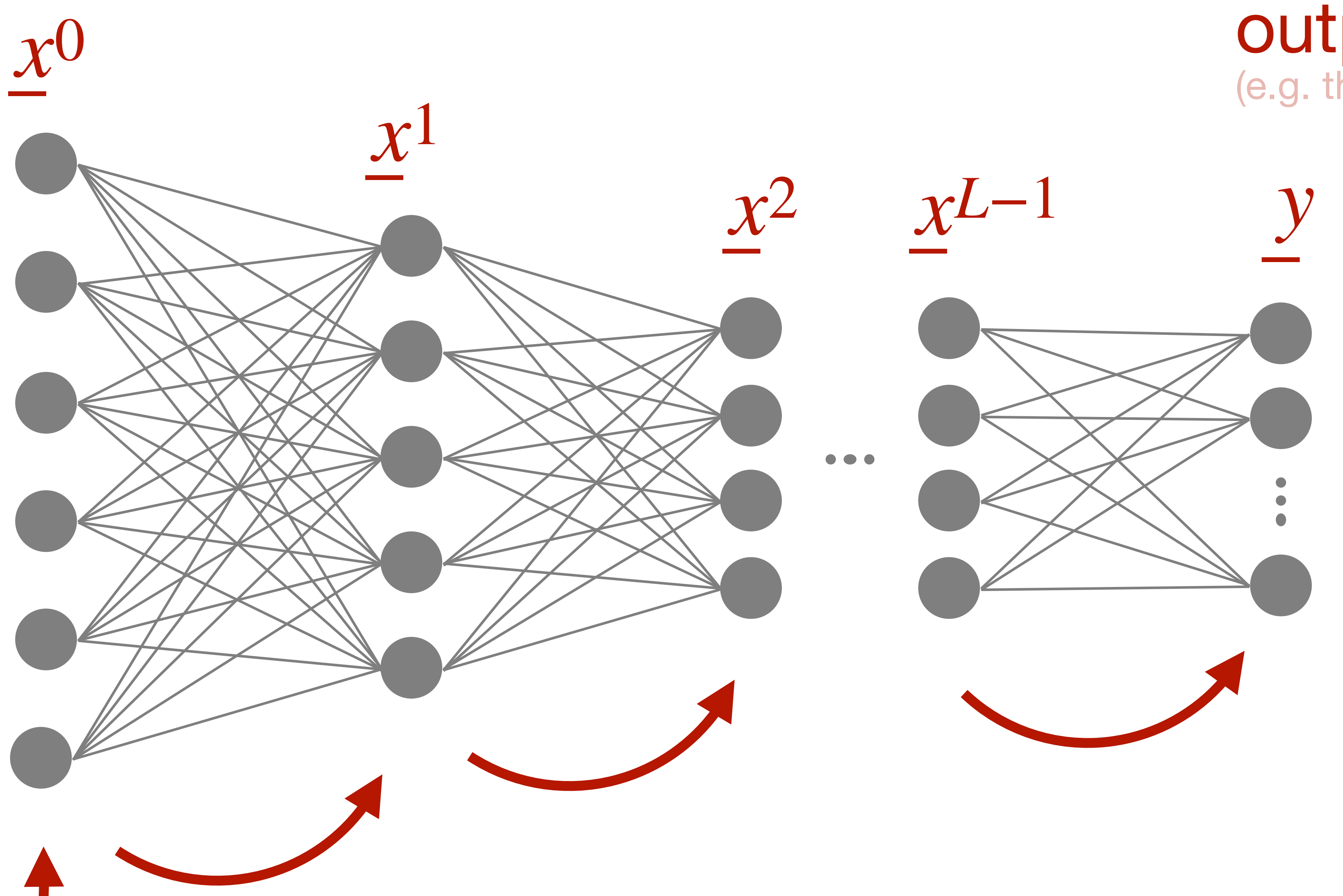
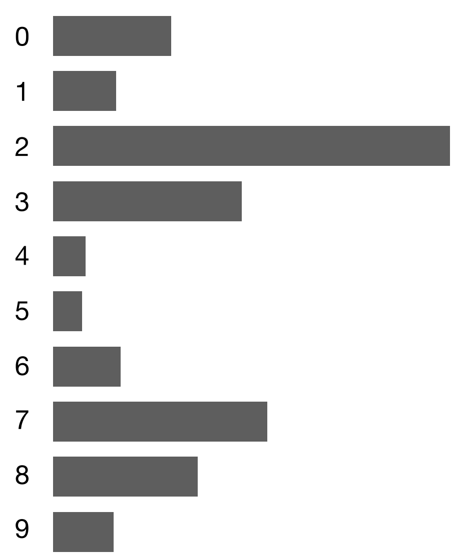


input vector

output probability vector

(e.g. through soft max)





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

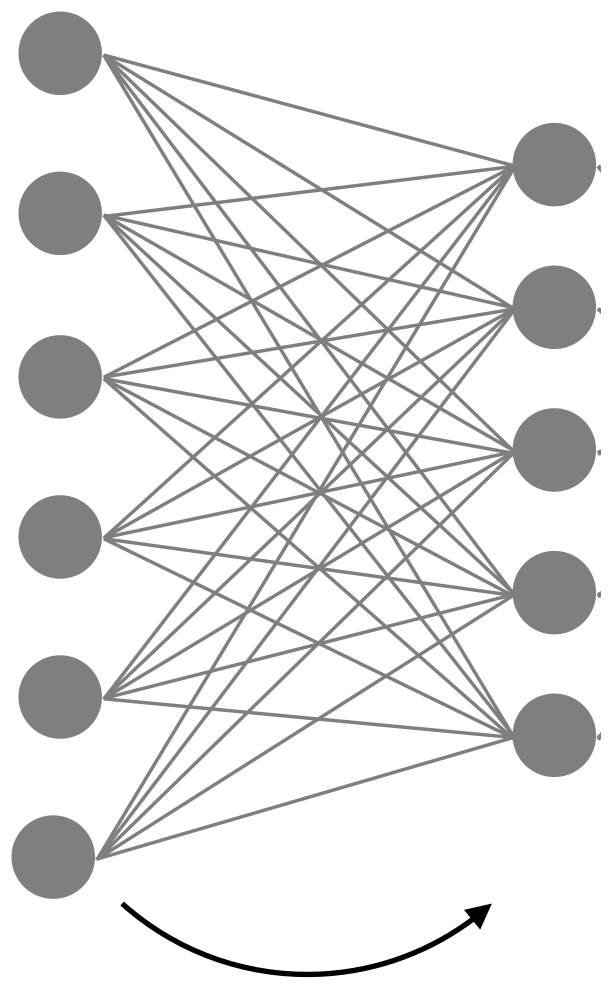
Iteratively transform the vector via

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

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

Classical artificial NNs in the continuous world

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



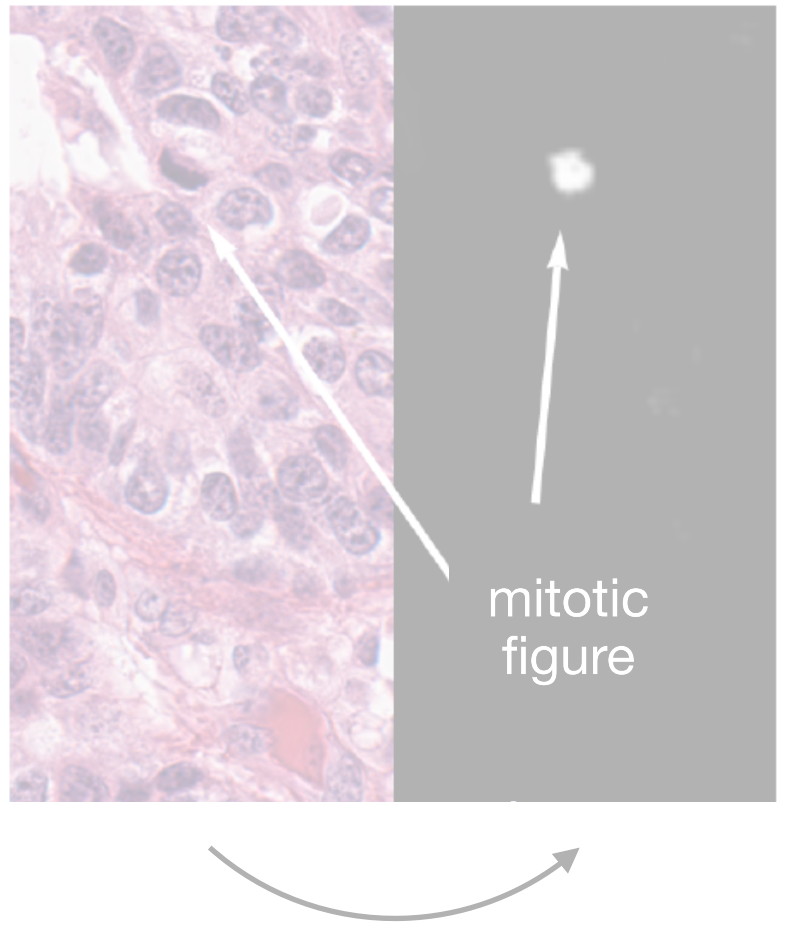
Iteratively transform the **vector** in $\mathbb{R}^{N^x}$ via

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

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 $f \in \mathcal{X} = \mathbb{L}_2(X)$



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

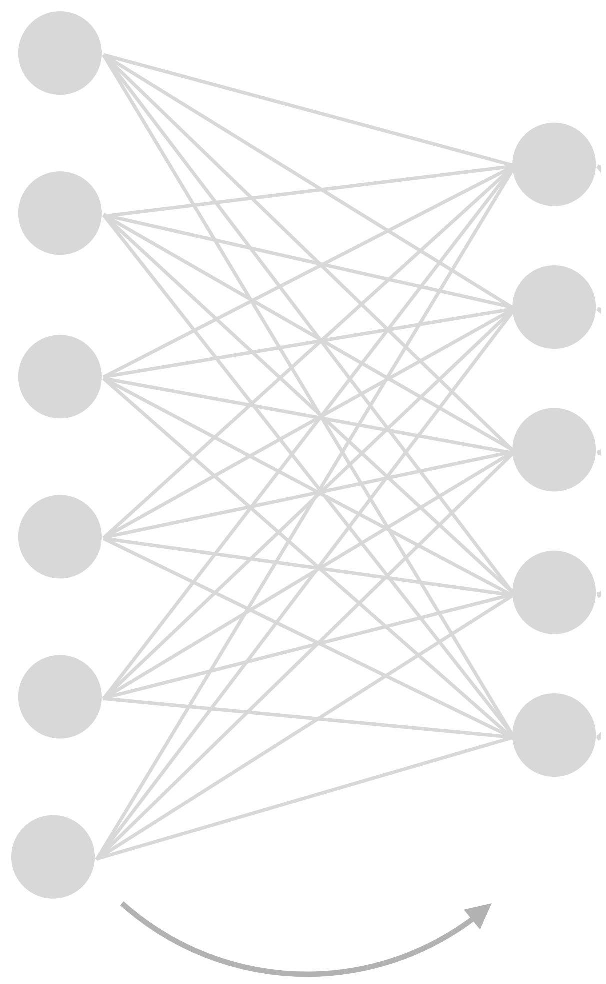
$$f^{out} = \varphi(K f^{in} + b^l)$$

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

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



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

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

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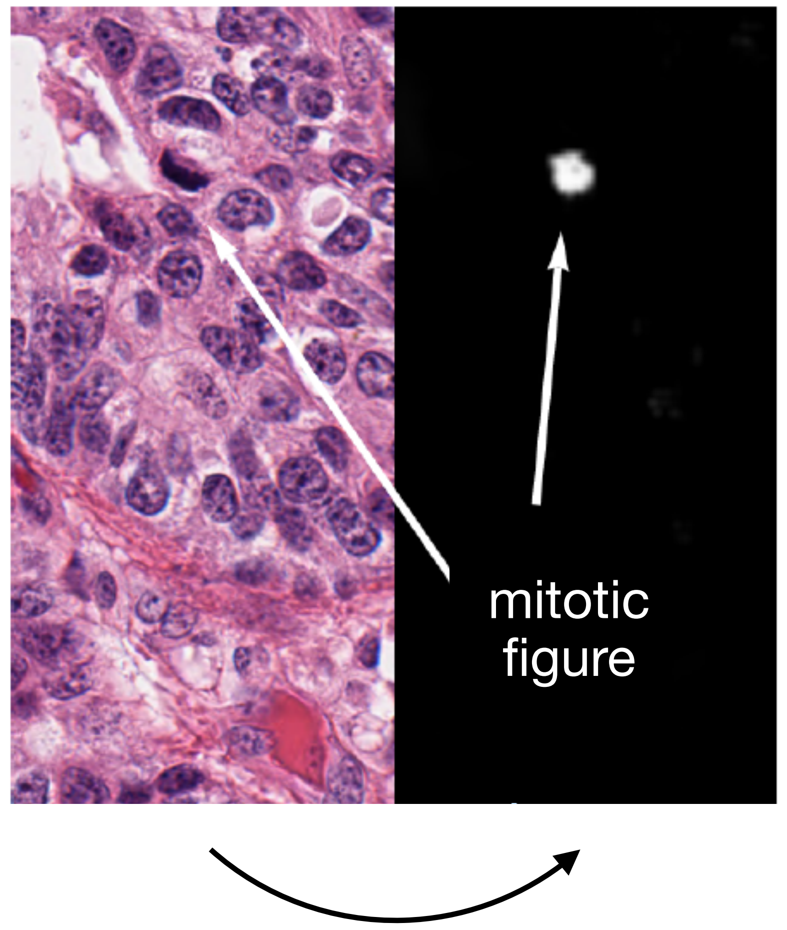
Working with feature maps $f \in \mathscr{X} = \mathbb{L}_2(X)$



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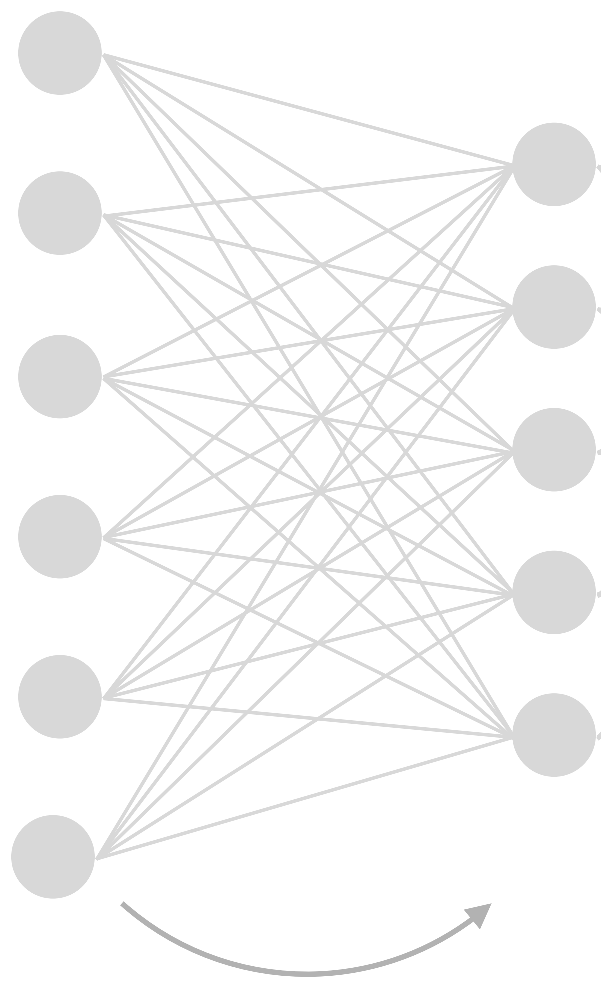
$$f^{out} = \varphi(K f^{in} + b^l)$$

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

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



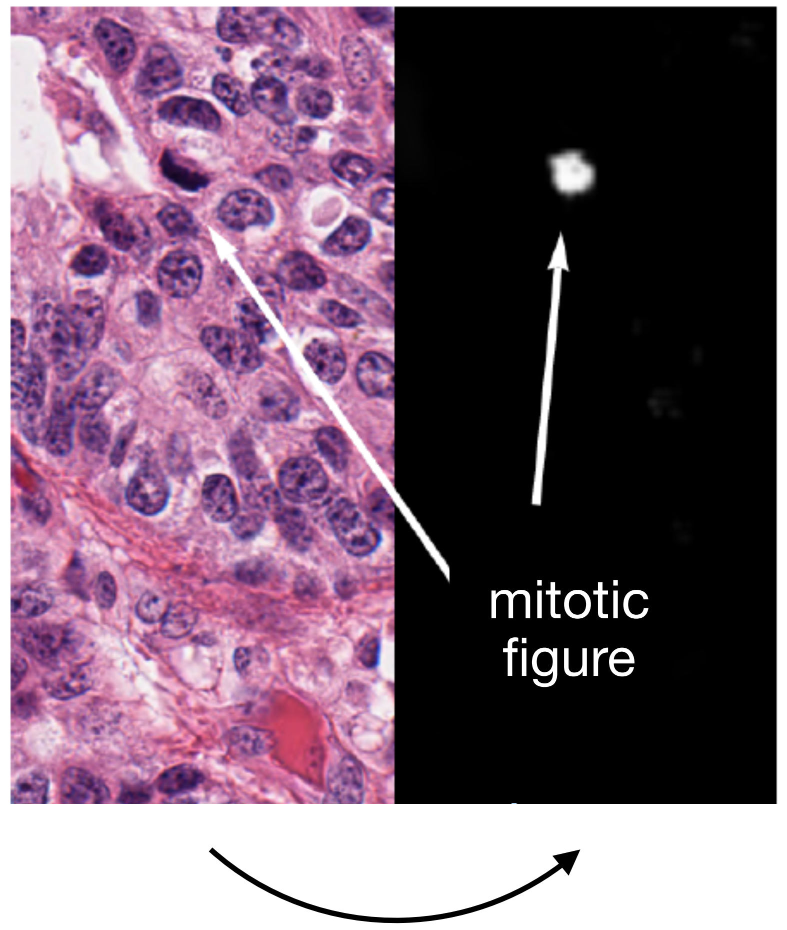
Iteratively transform the **vector** in $\mathbb{R}^{N^x}$ via

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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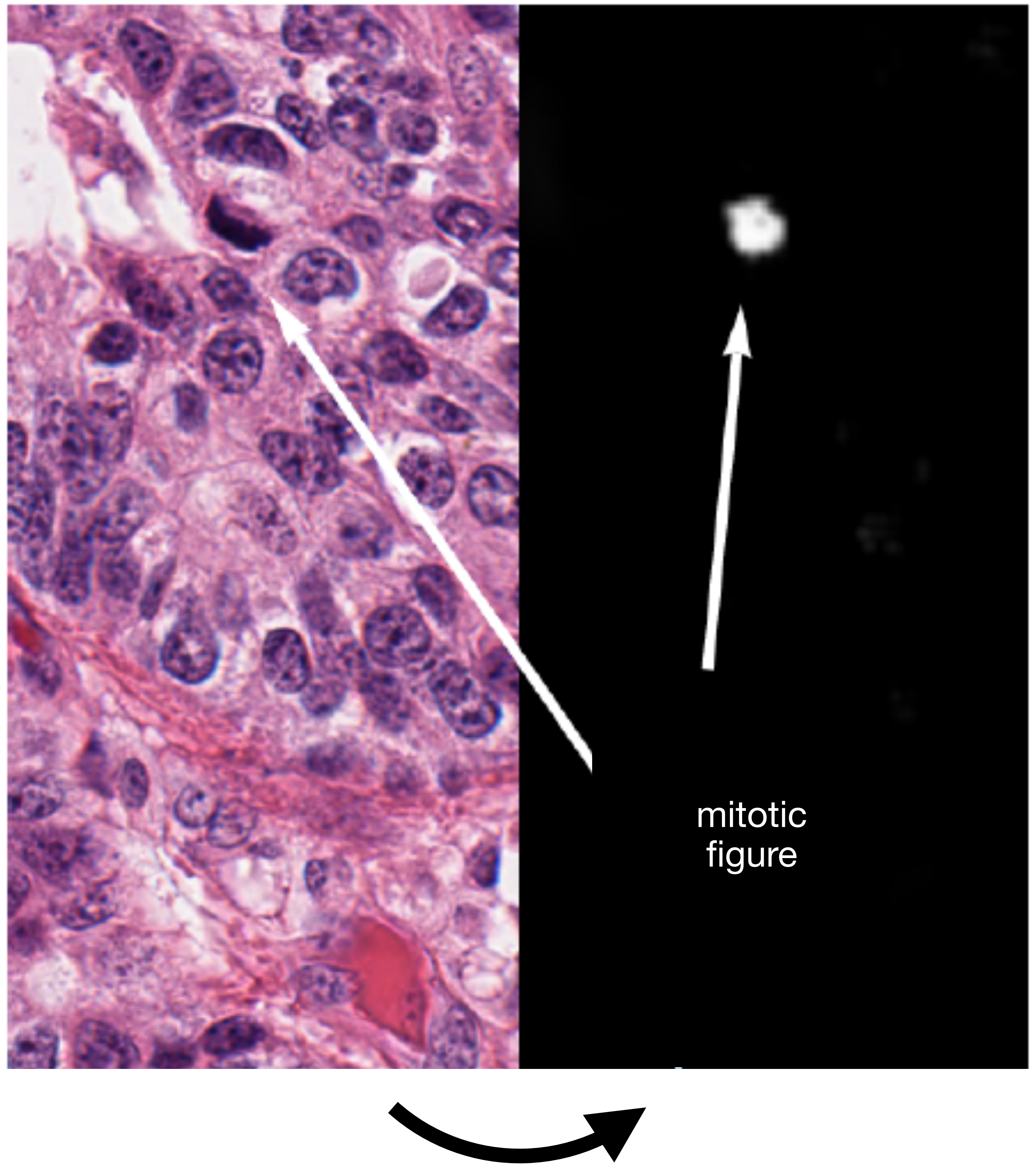
Neural Networks for Signal Data



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

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 3.2:

Let $\mathscr{K} : \mathbb{L}_2(X) \rightarrow \mathbb{L}_2(Y)$ 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: $[\mathscr{K}f](y) = \int_X k(g_y^{-1}x)f(x)\mathrm{d}x$
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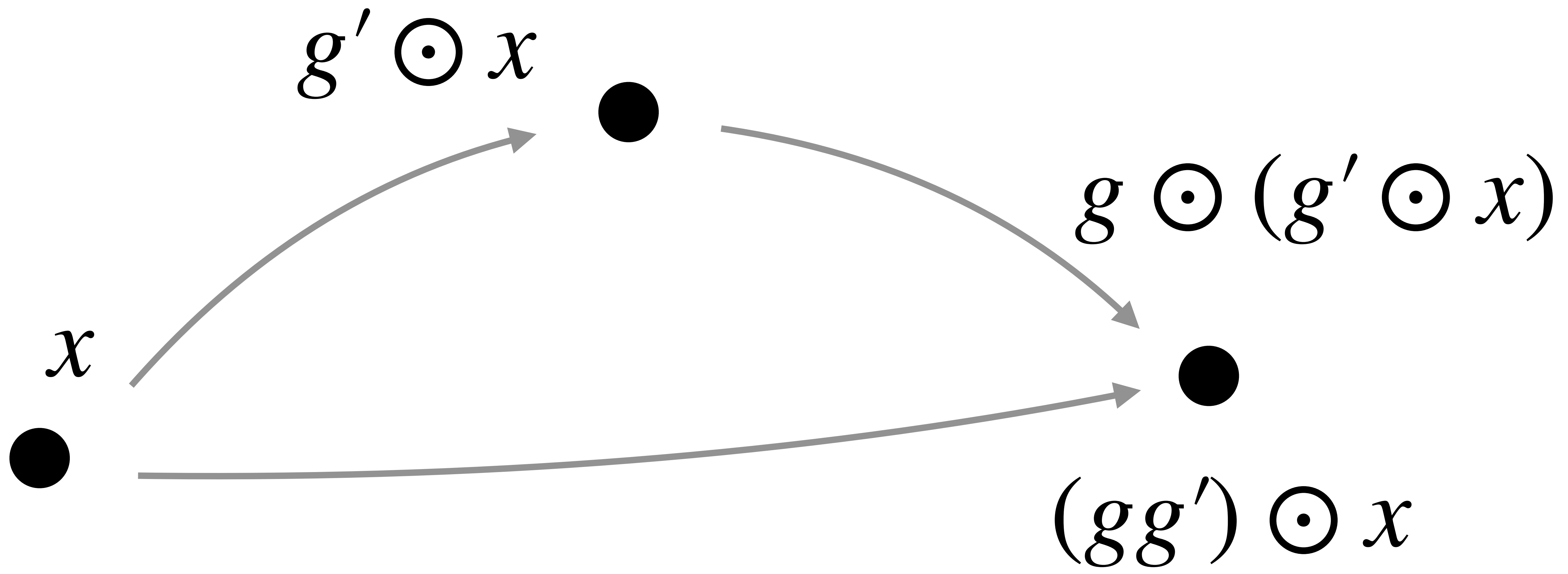
Group theory: Homogeneous spaces

Group action: An operator $\odot : G \times X \rightarrow X$ such that

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



Group theory: Homogeneous spaces

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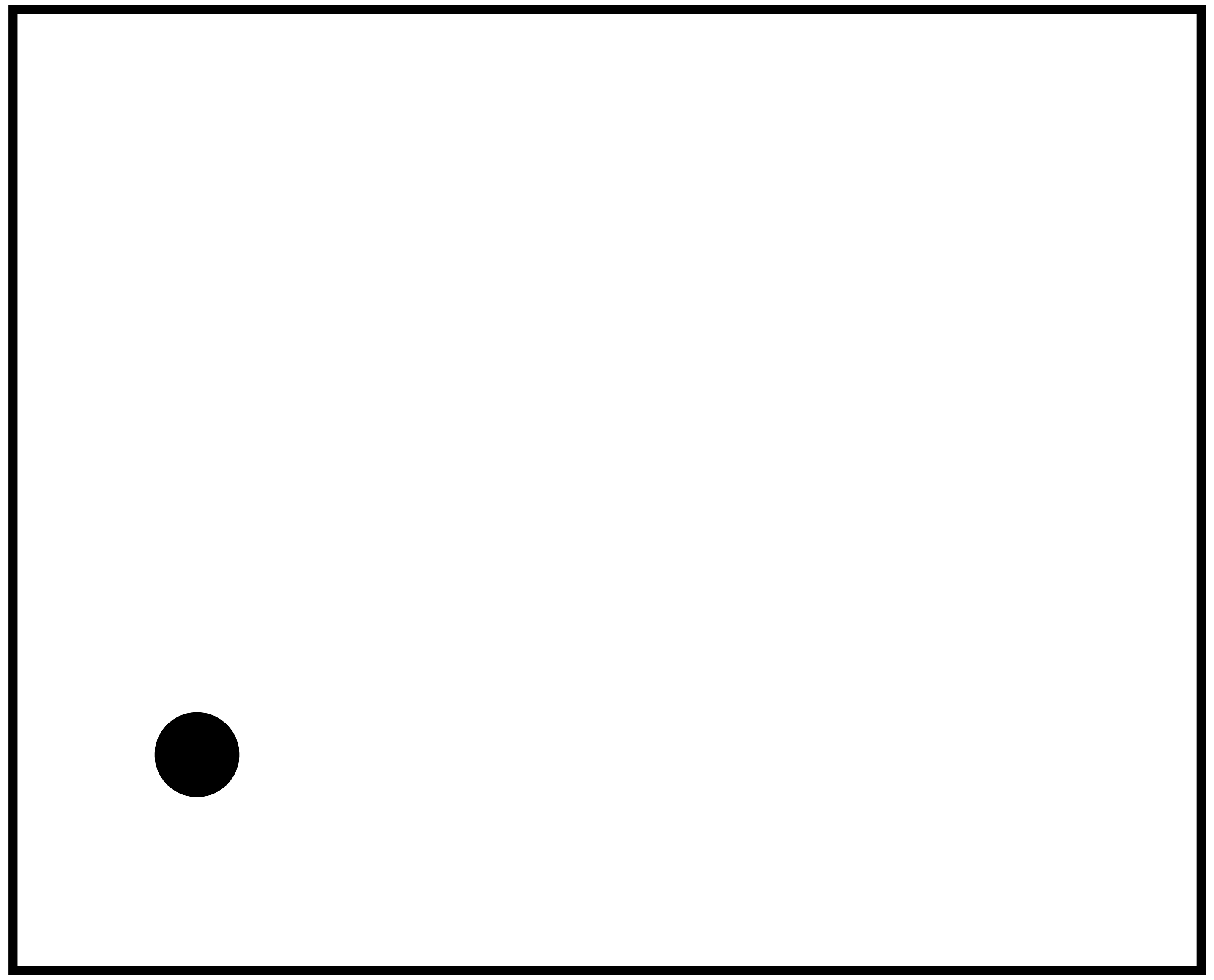
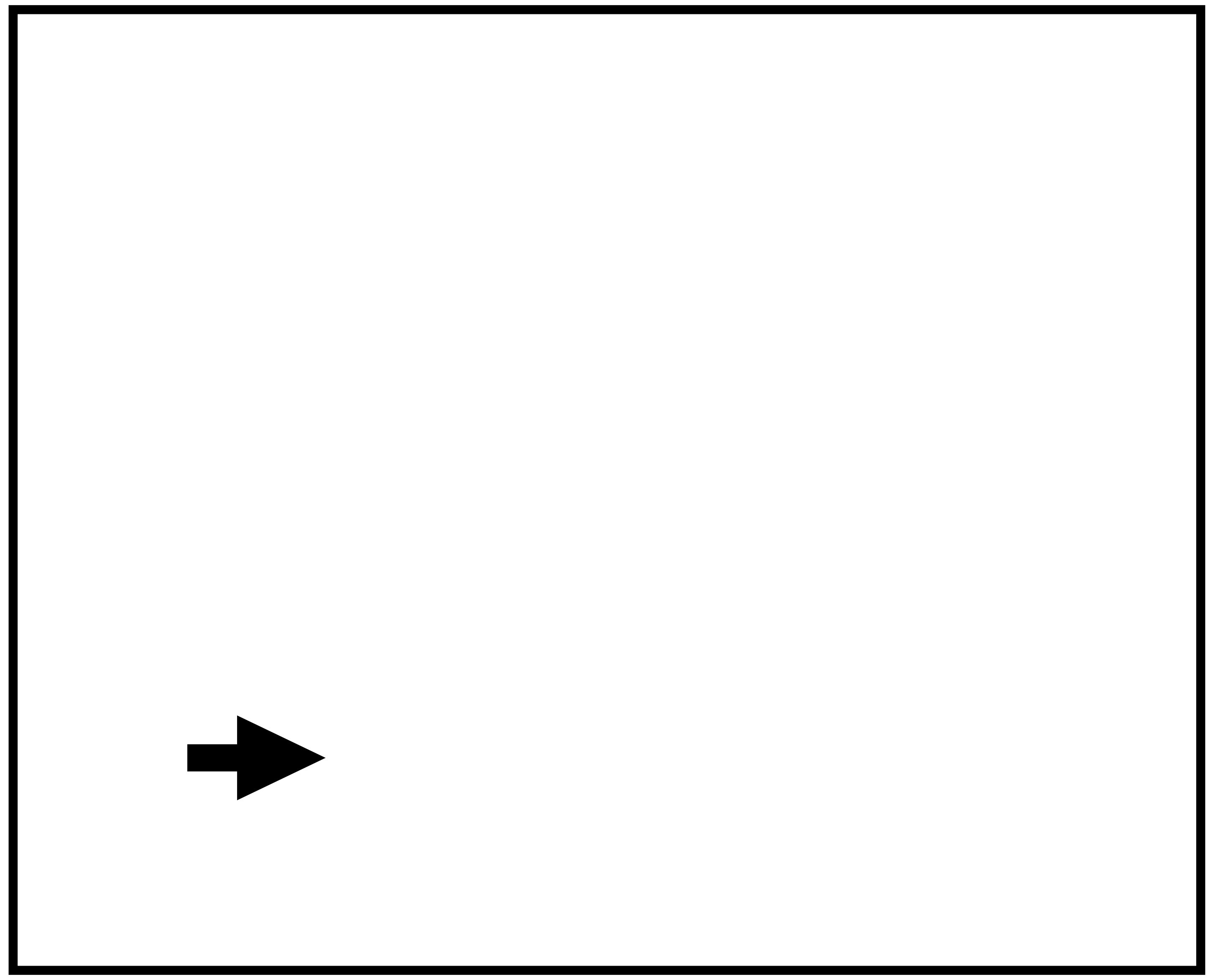
$$\forall_{x_0, x \in X} \exists_{g \in G} : x = g \odot x_0$$

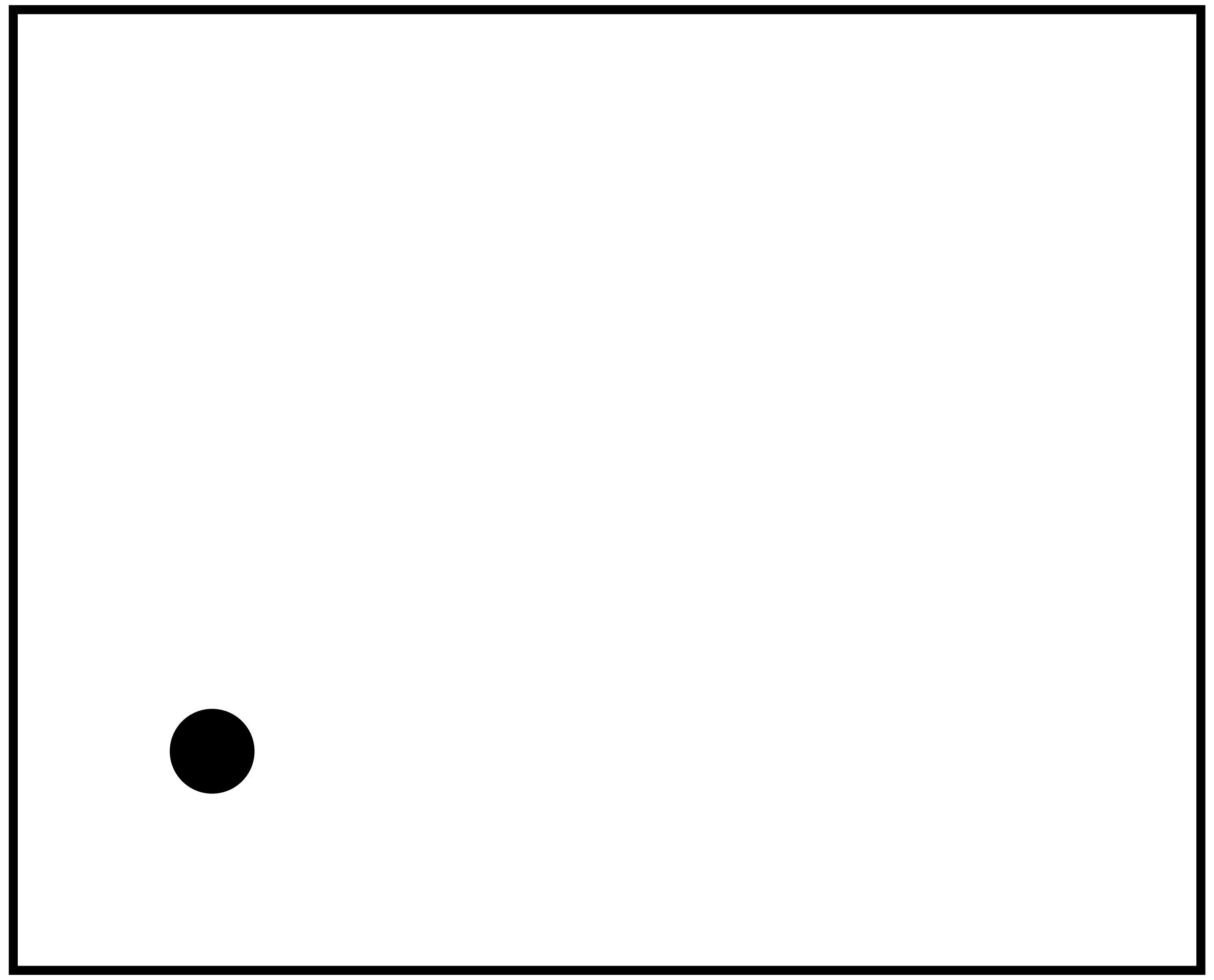
$(\mathbb{R}^2, +)$ acts transitively on $\mathbb{R}^2$

SE(2) acts transitively on $\mathbb{R}^2$

SO(2) does not …







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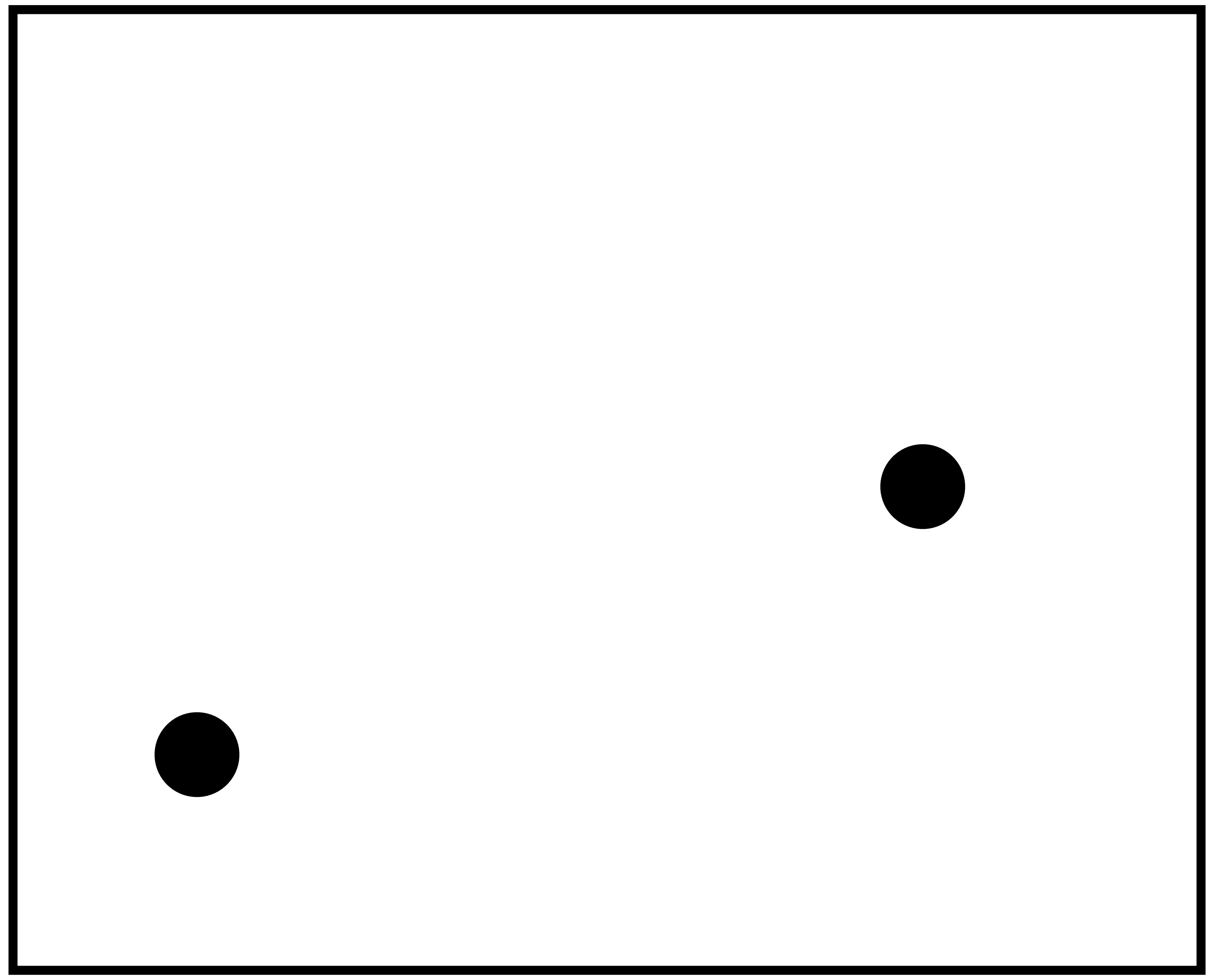

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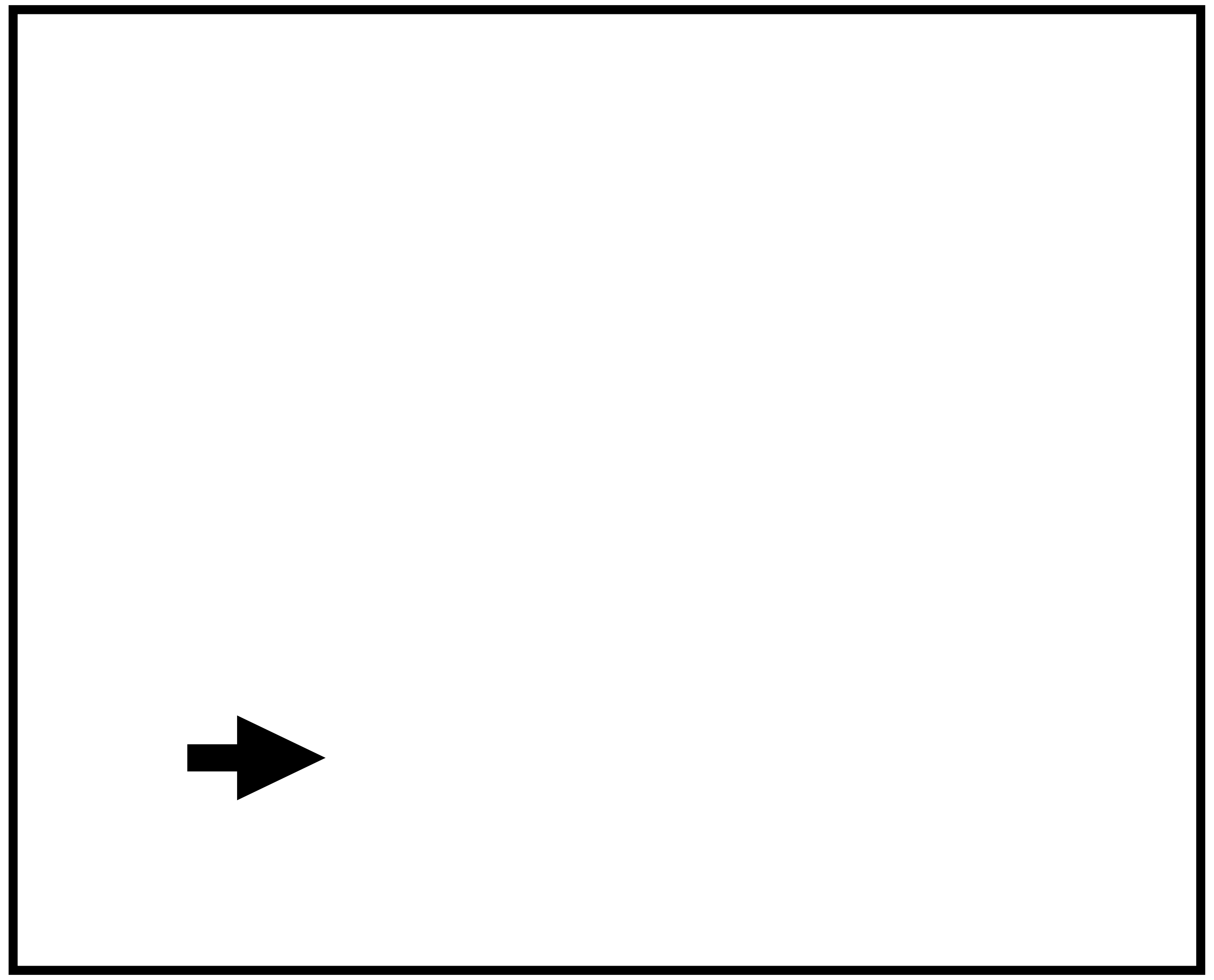

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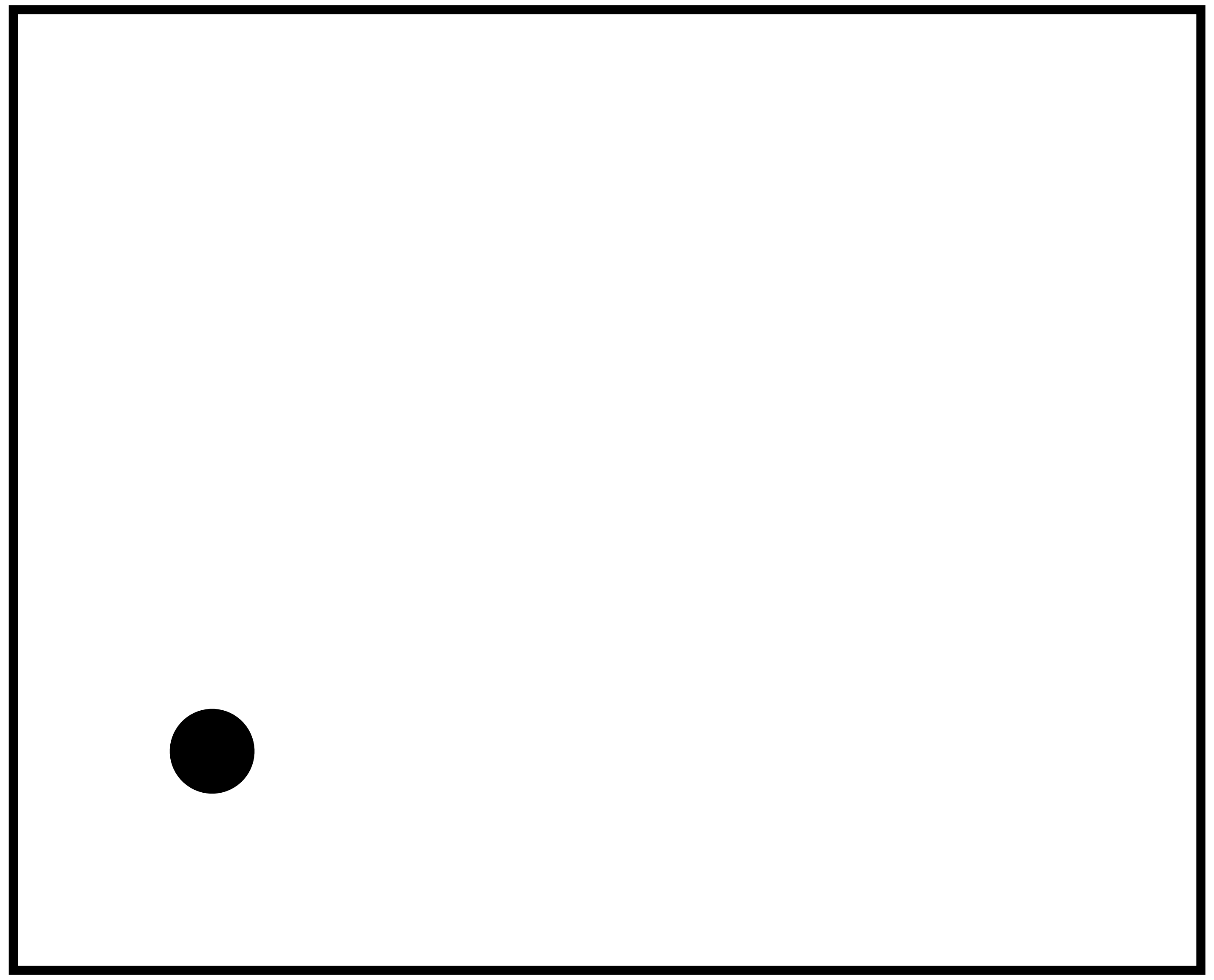

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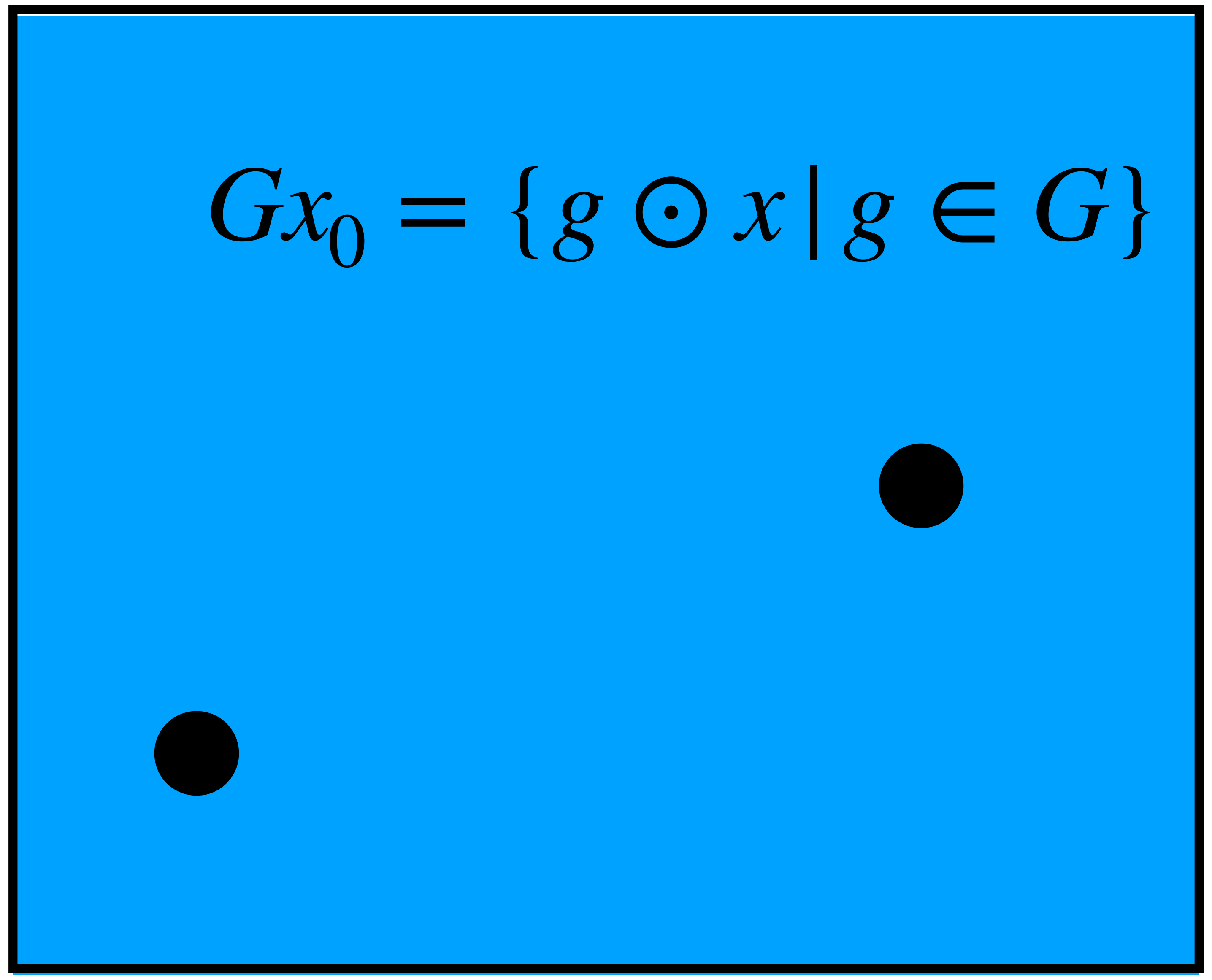

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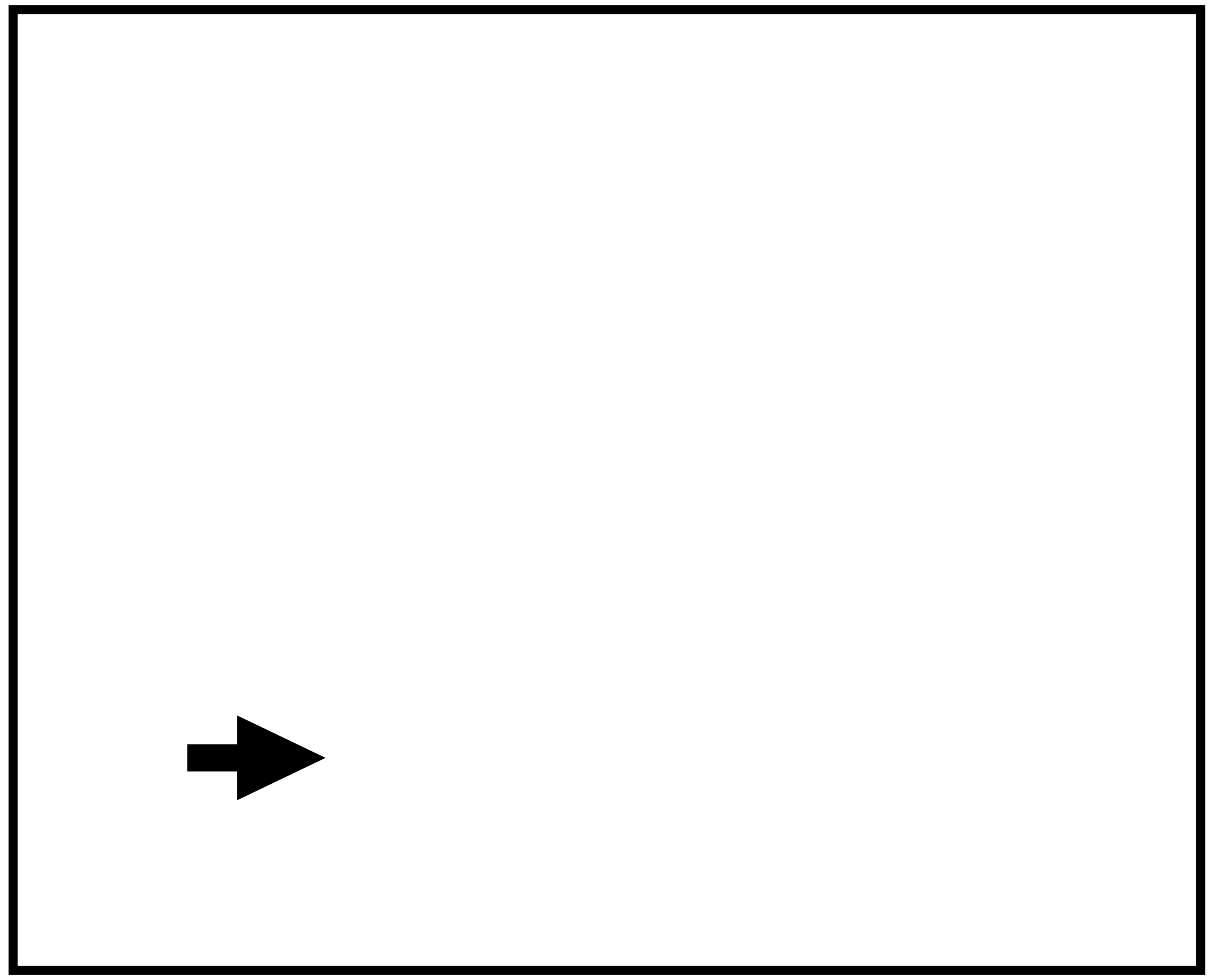

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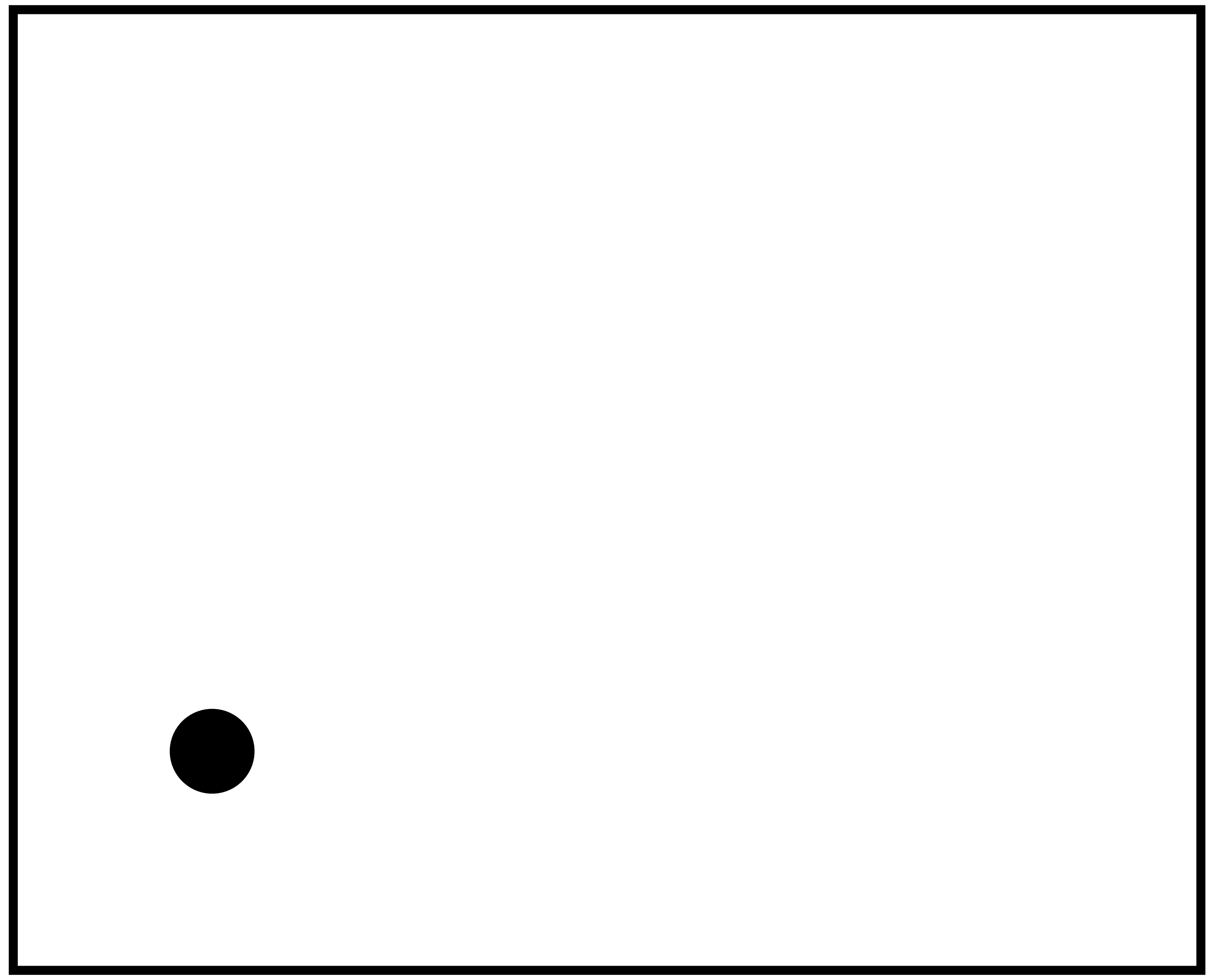

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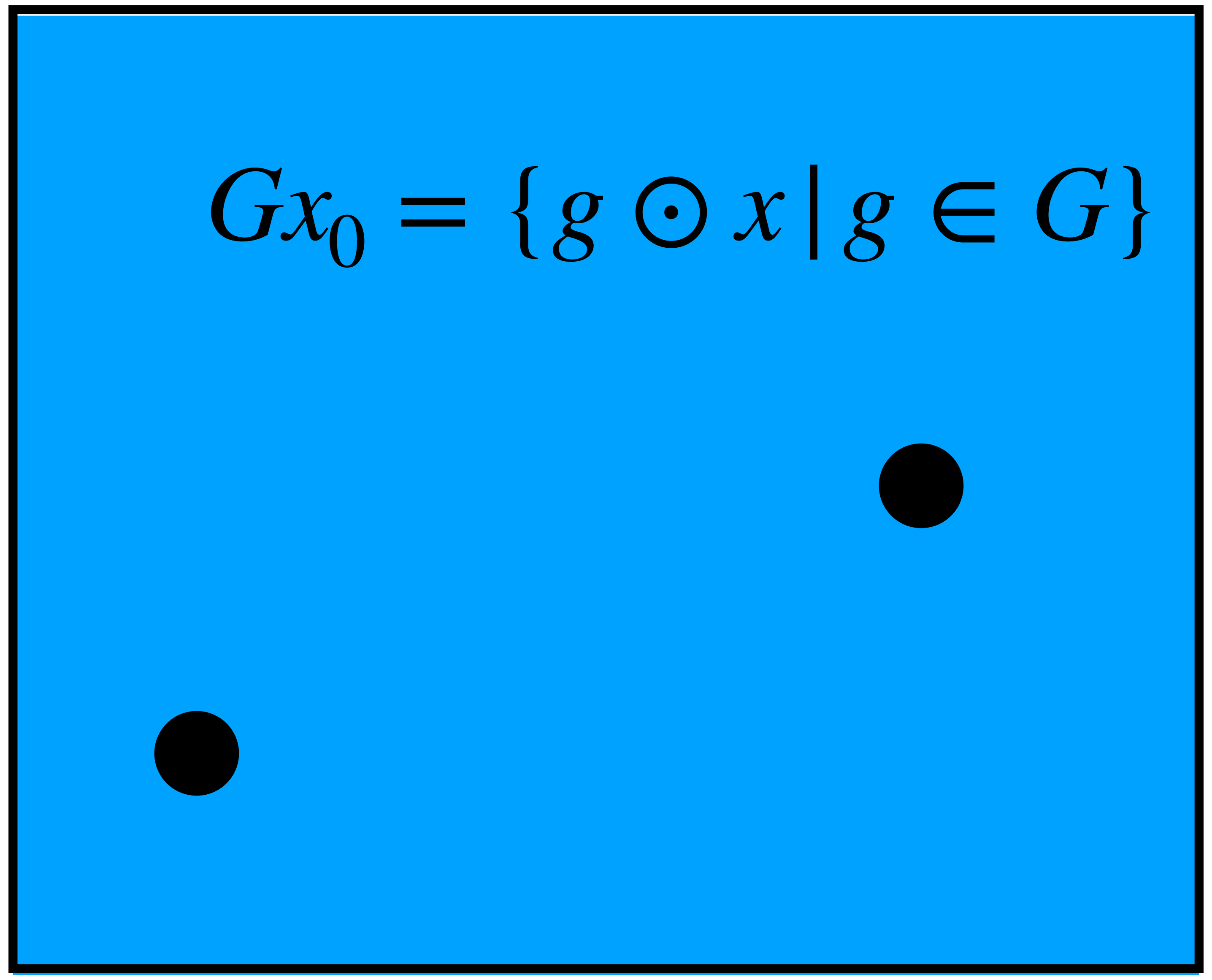

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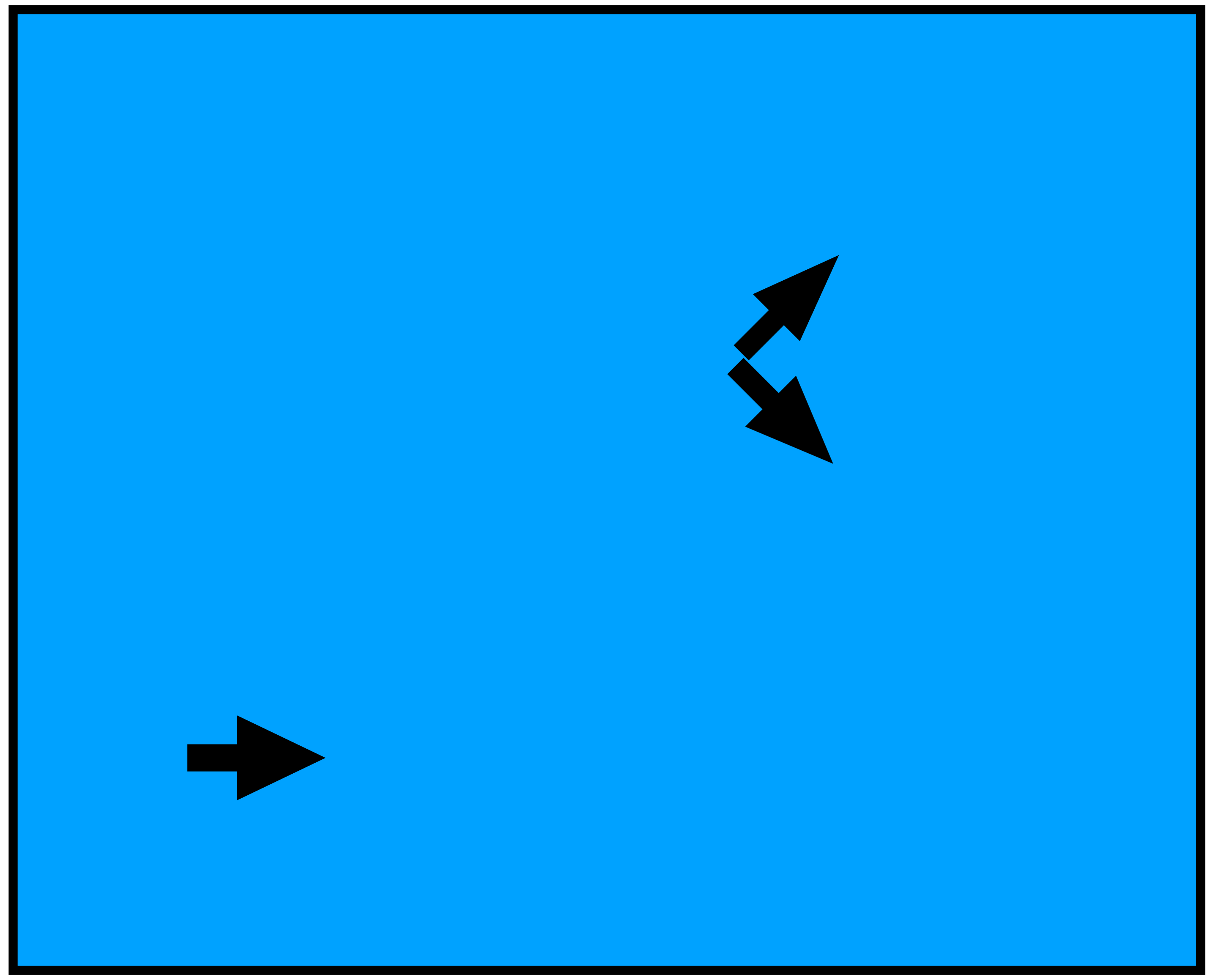

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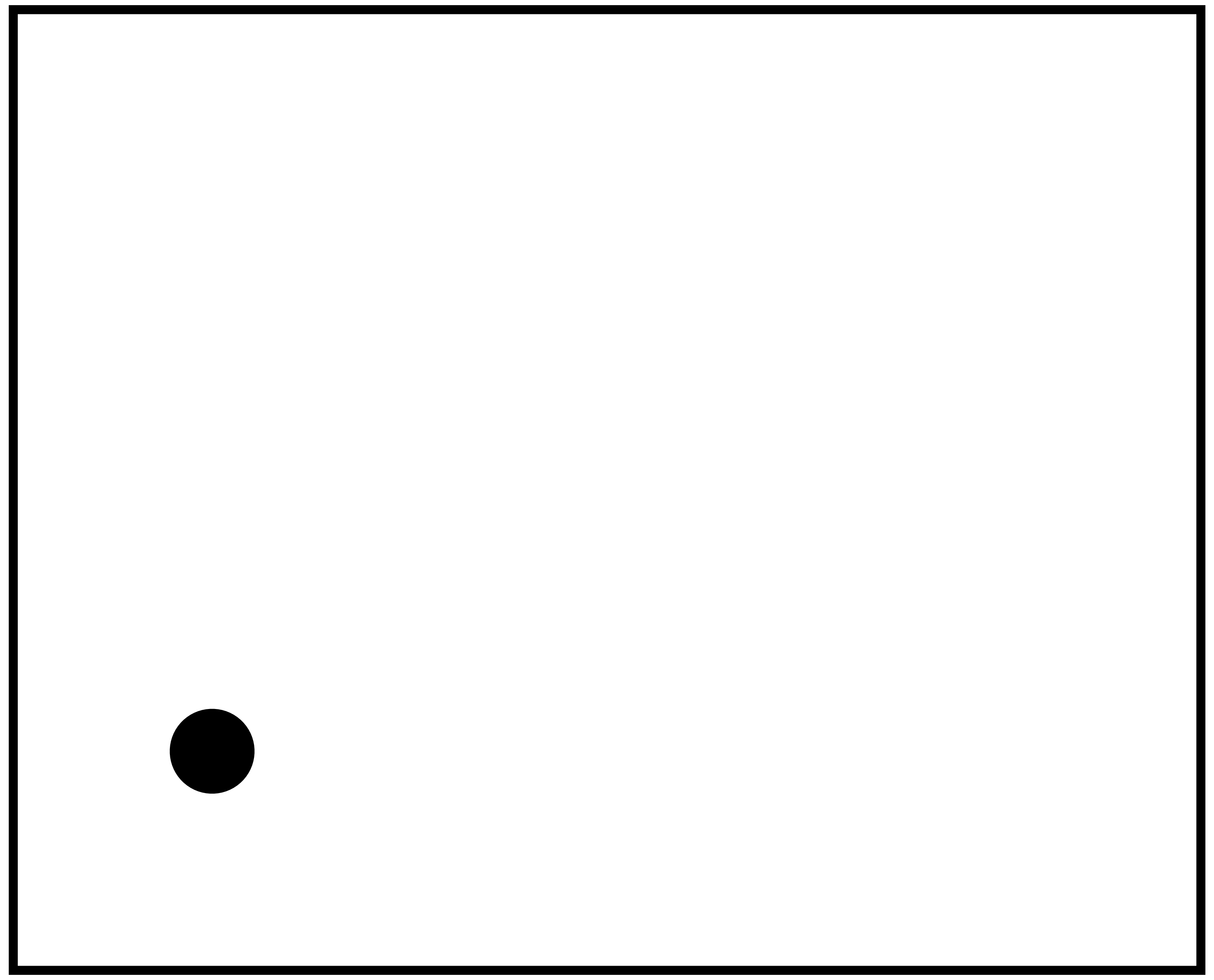

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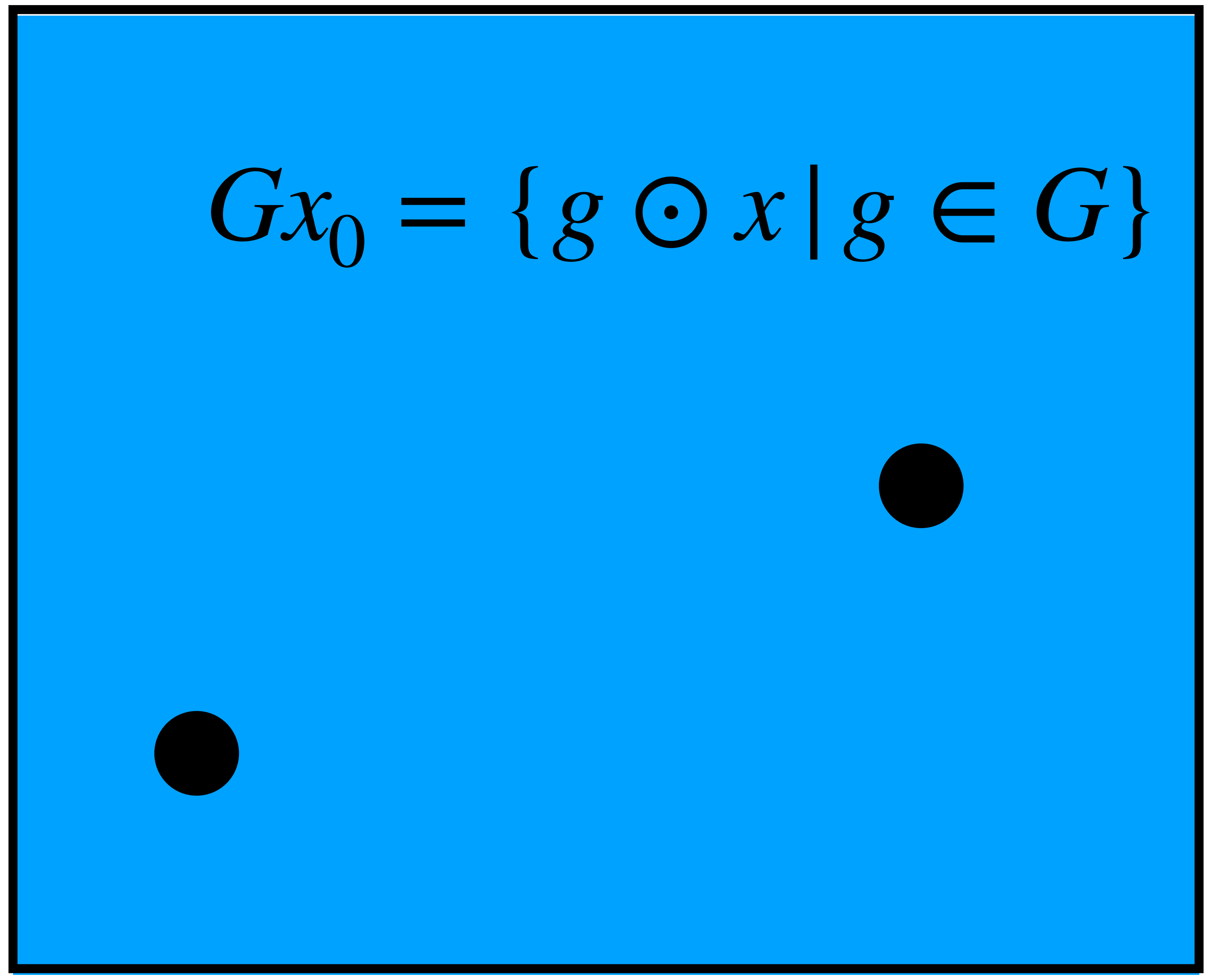

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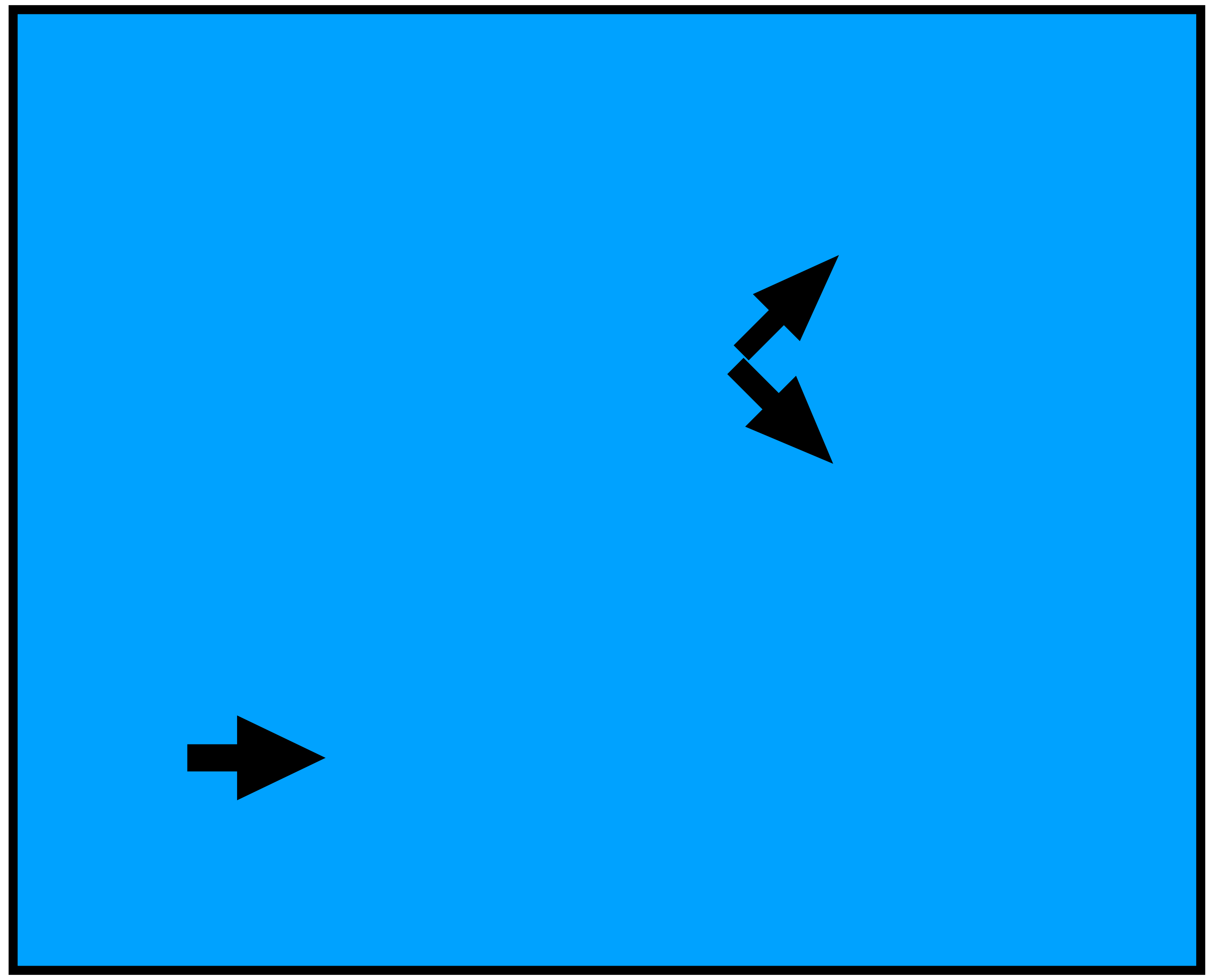

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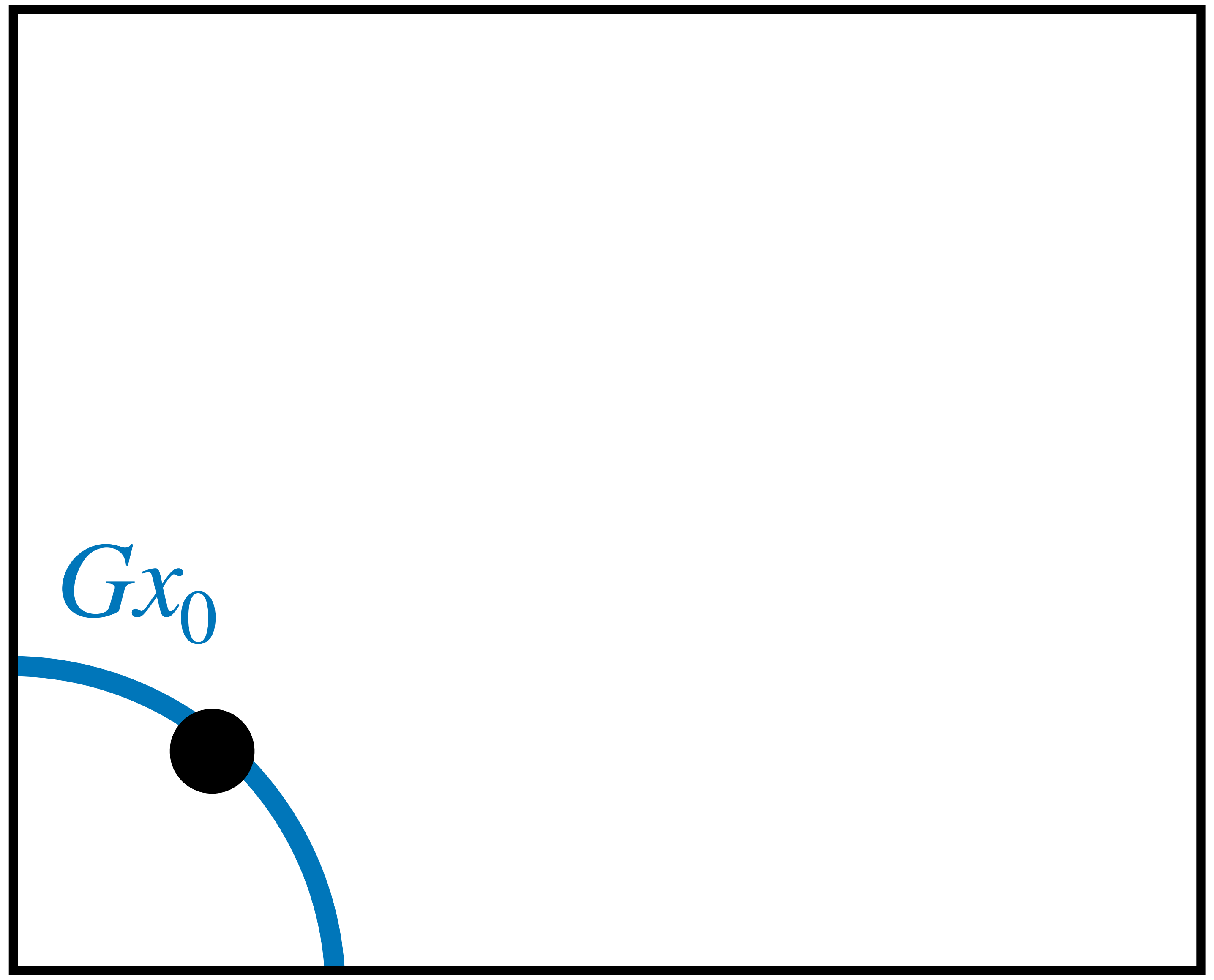

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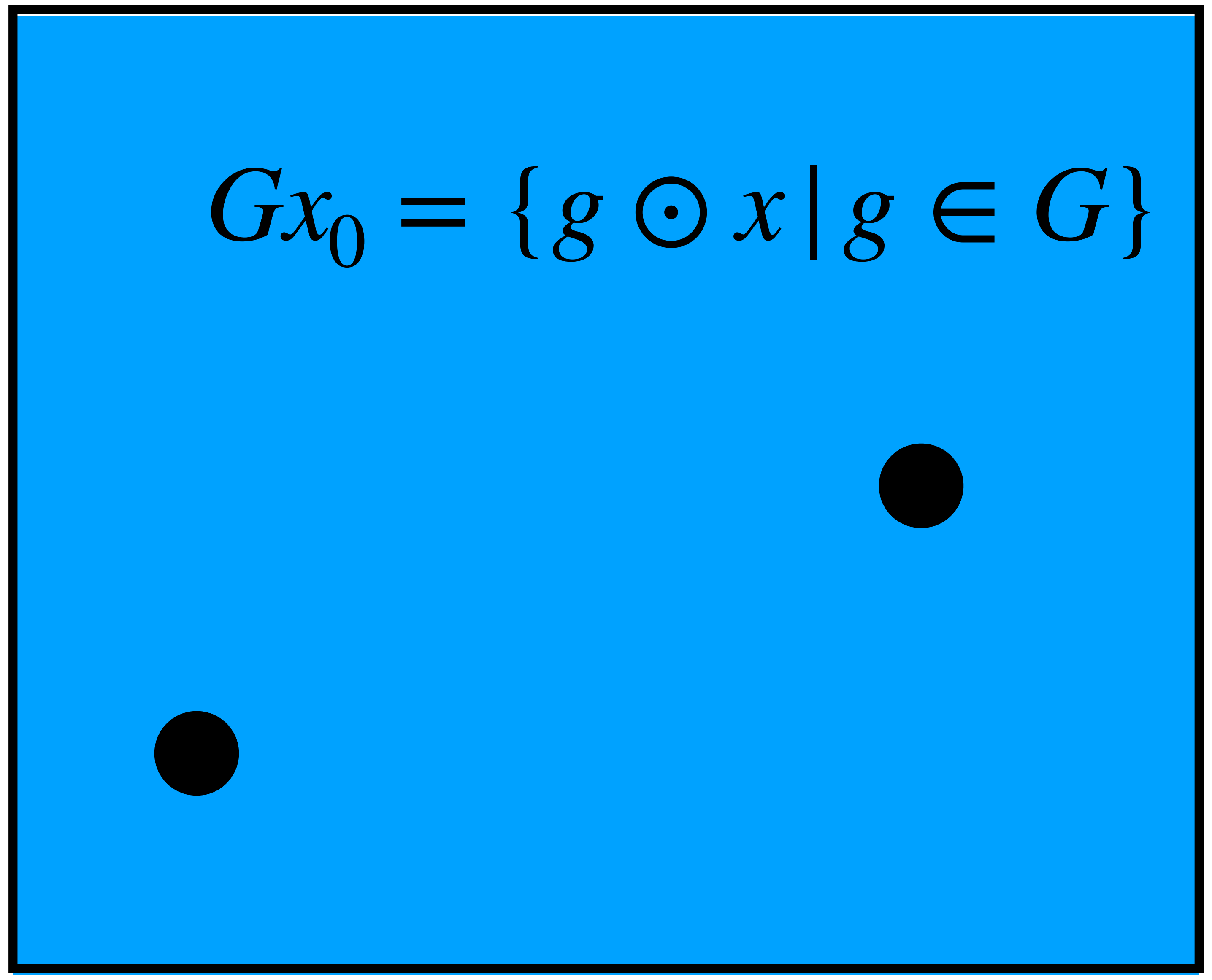

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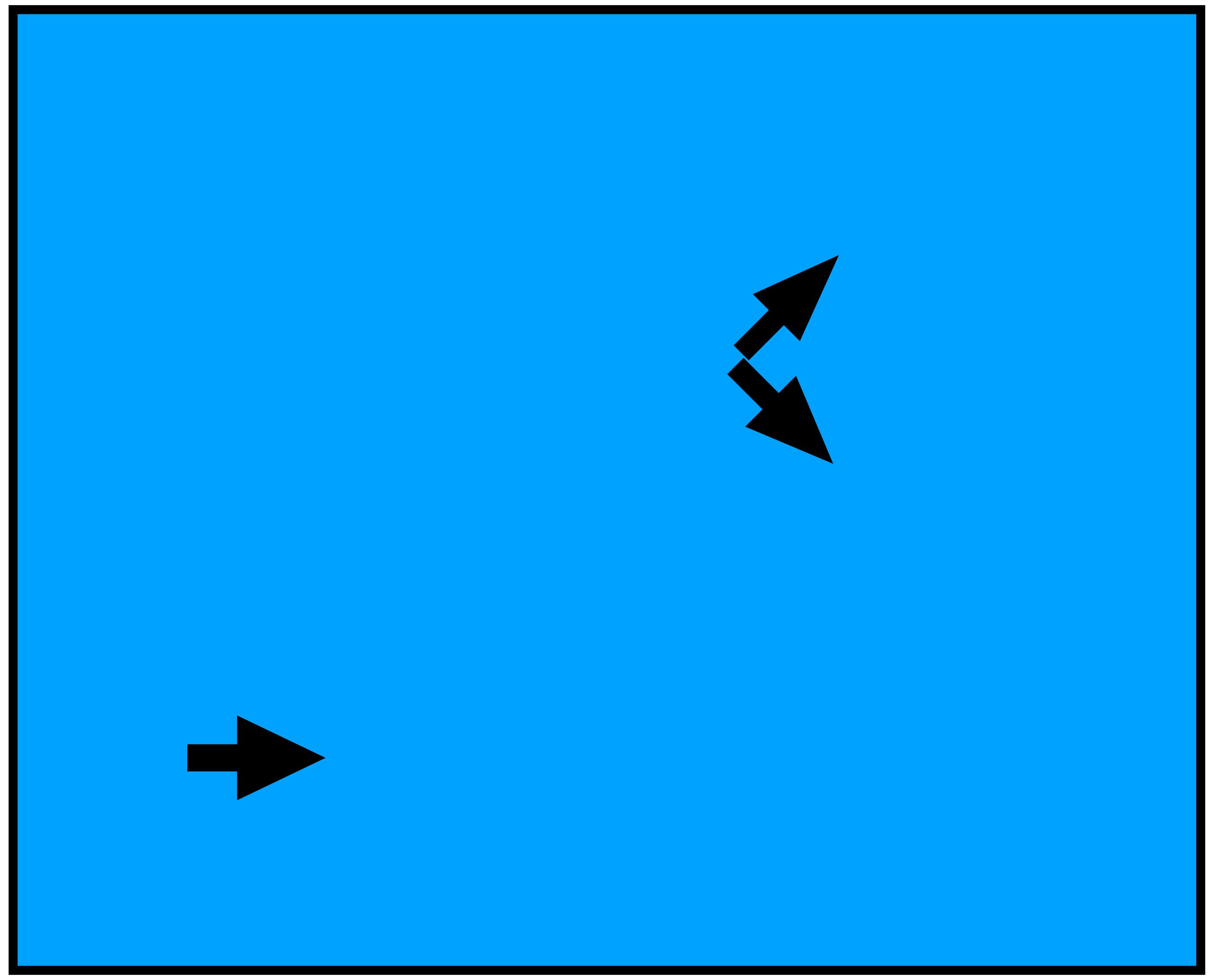

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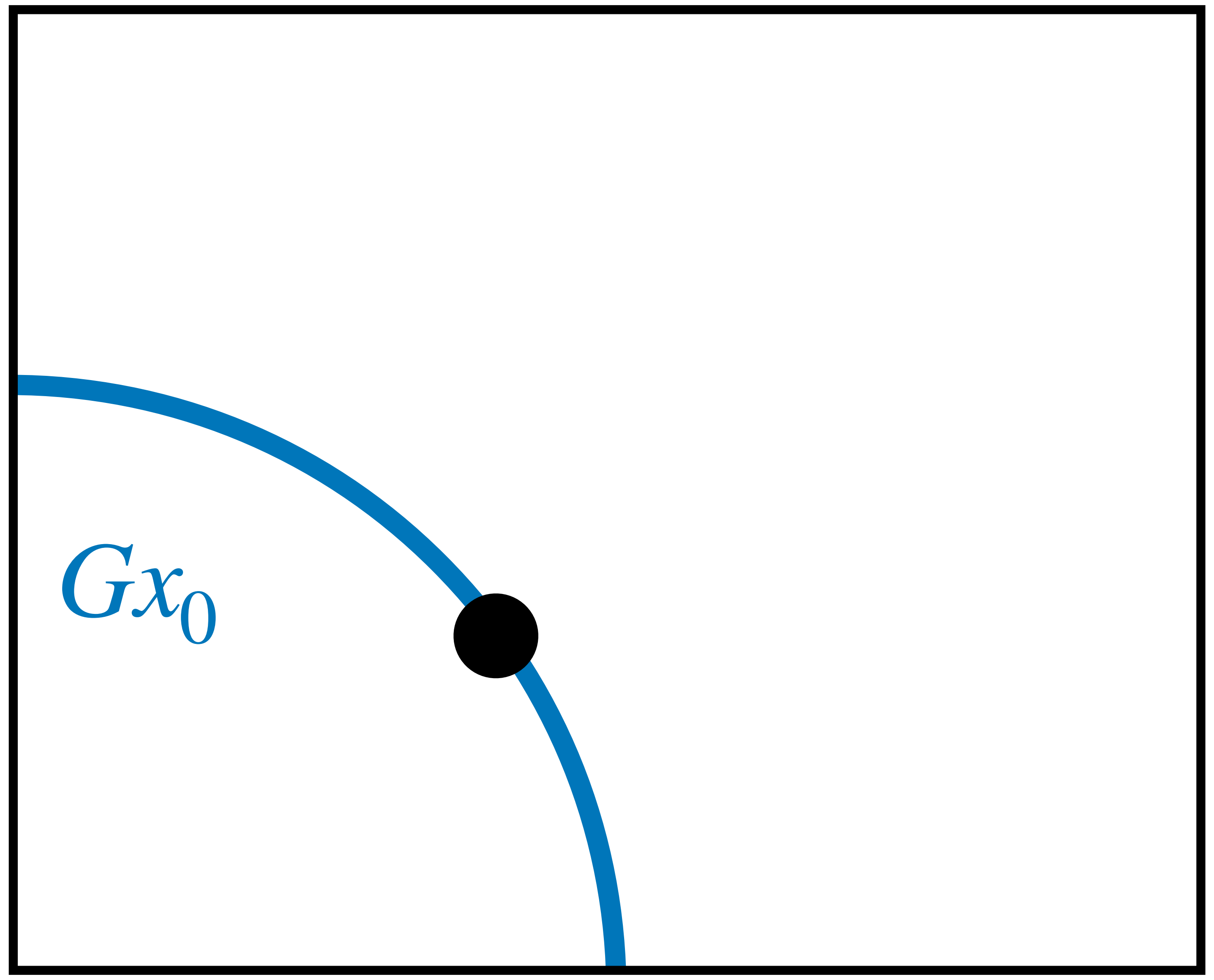

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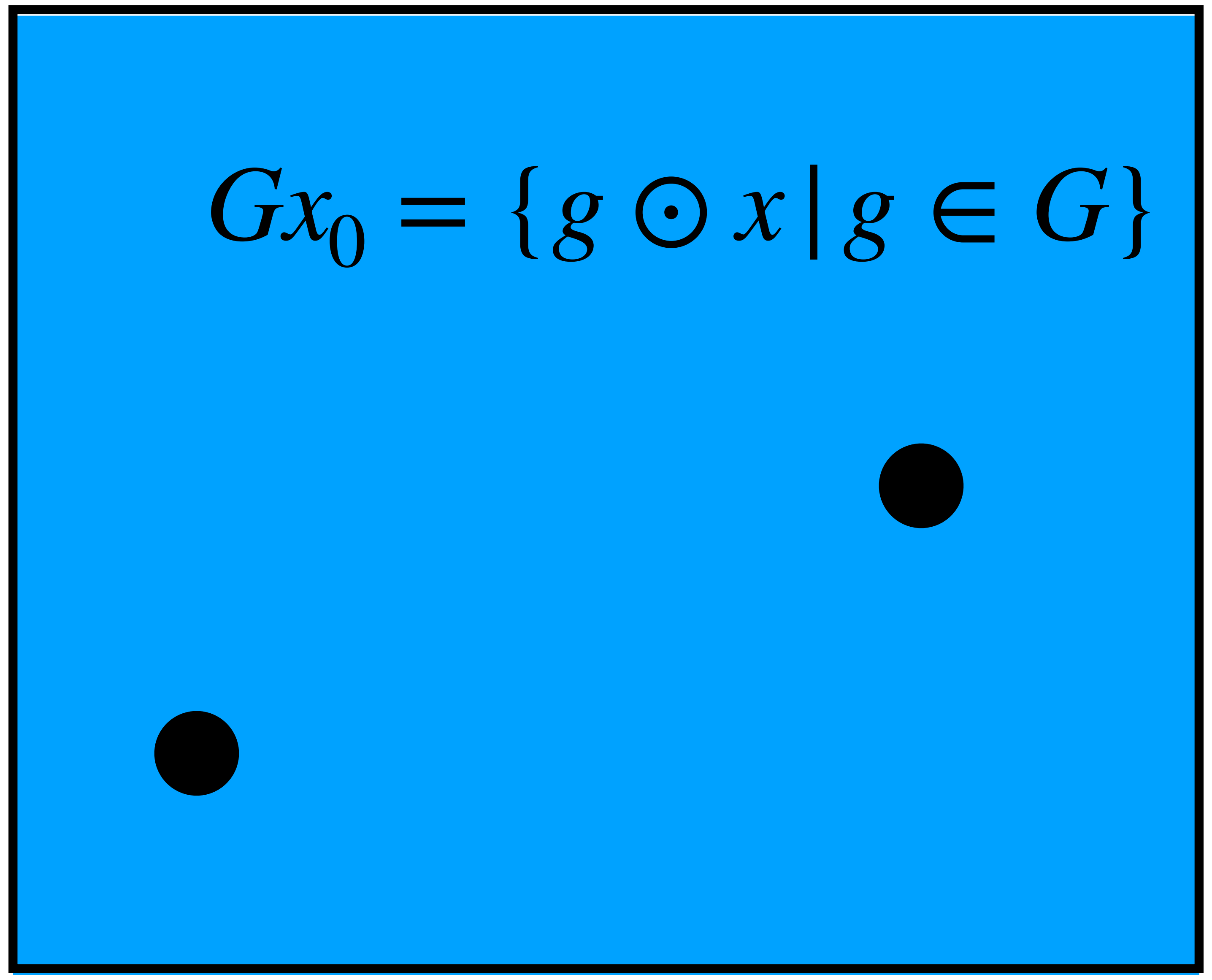

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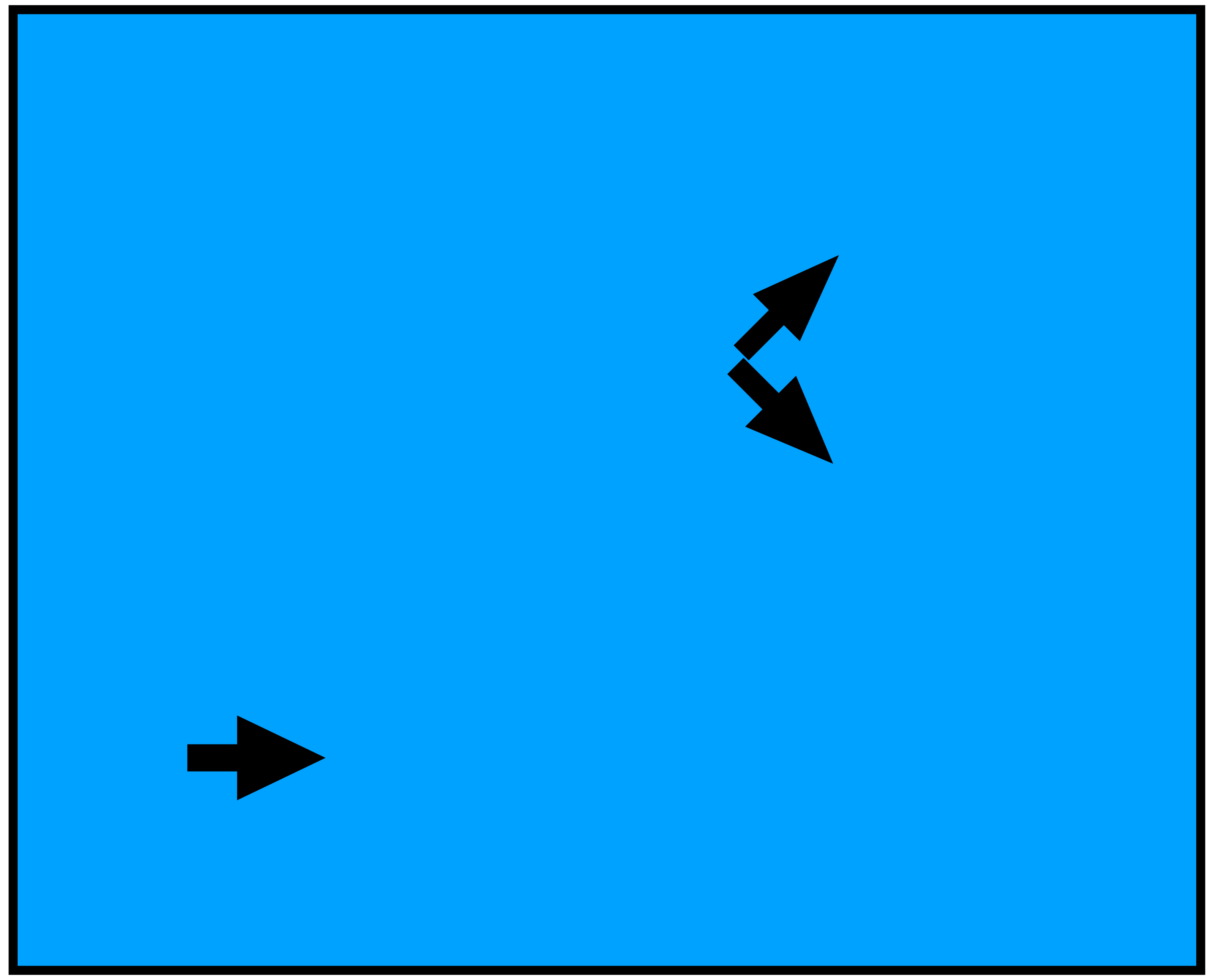

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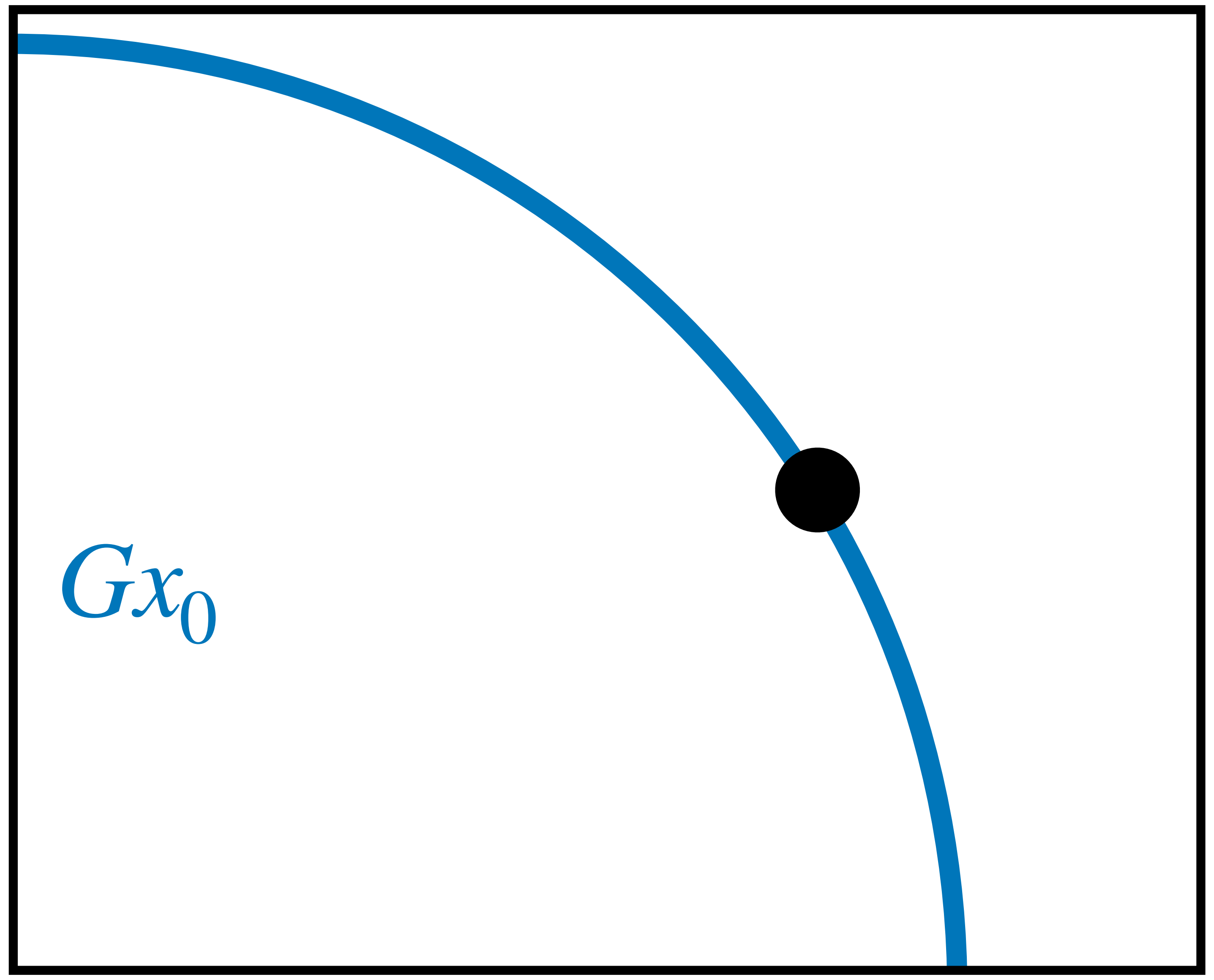

Group theory: Homogeneous spaces

Homogeneous space: A space on 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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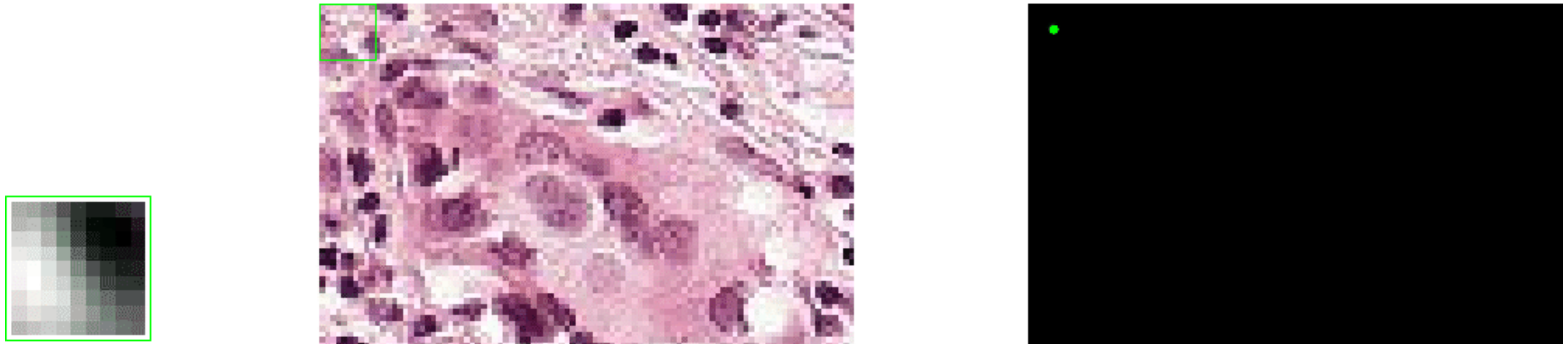
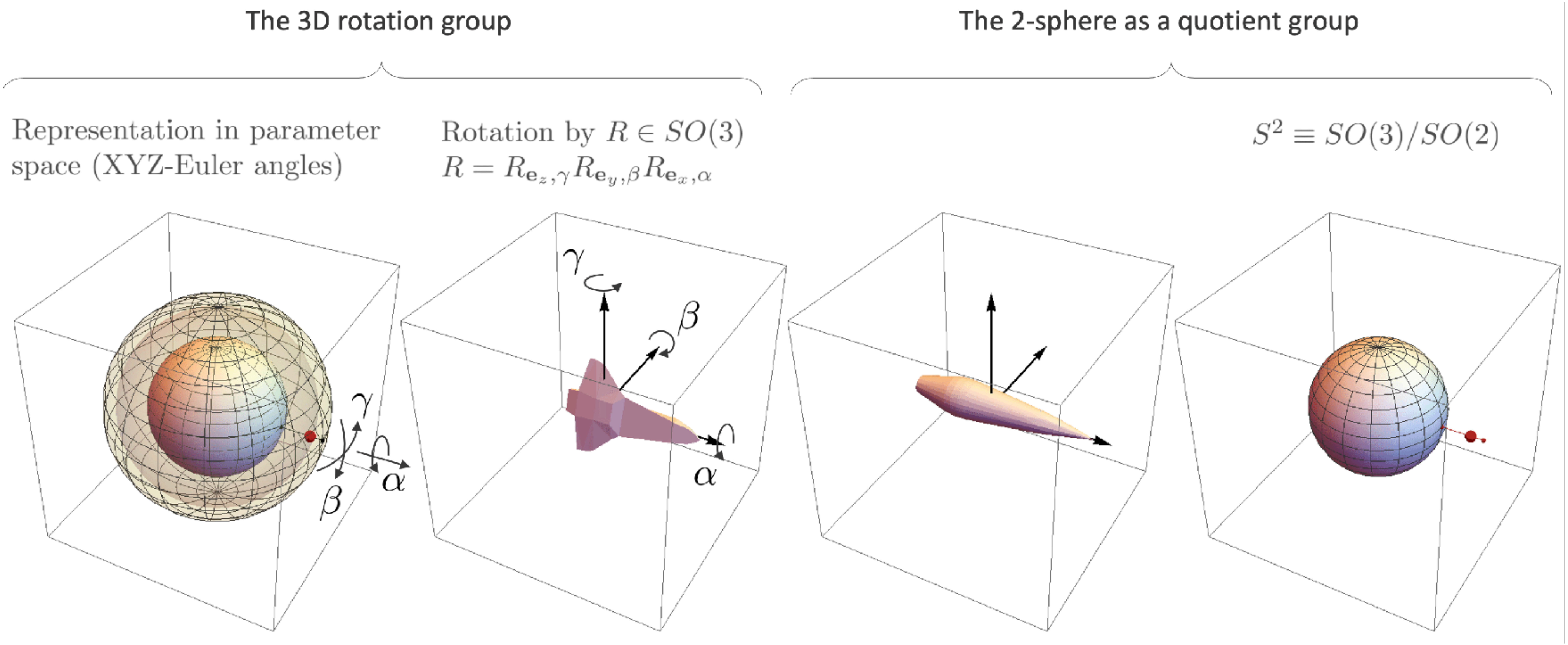


Group theory: Homogeneous spaces

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



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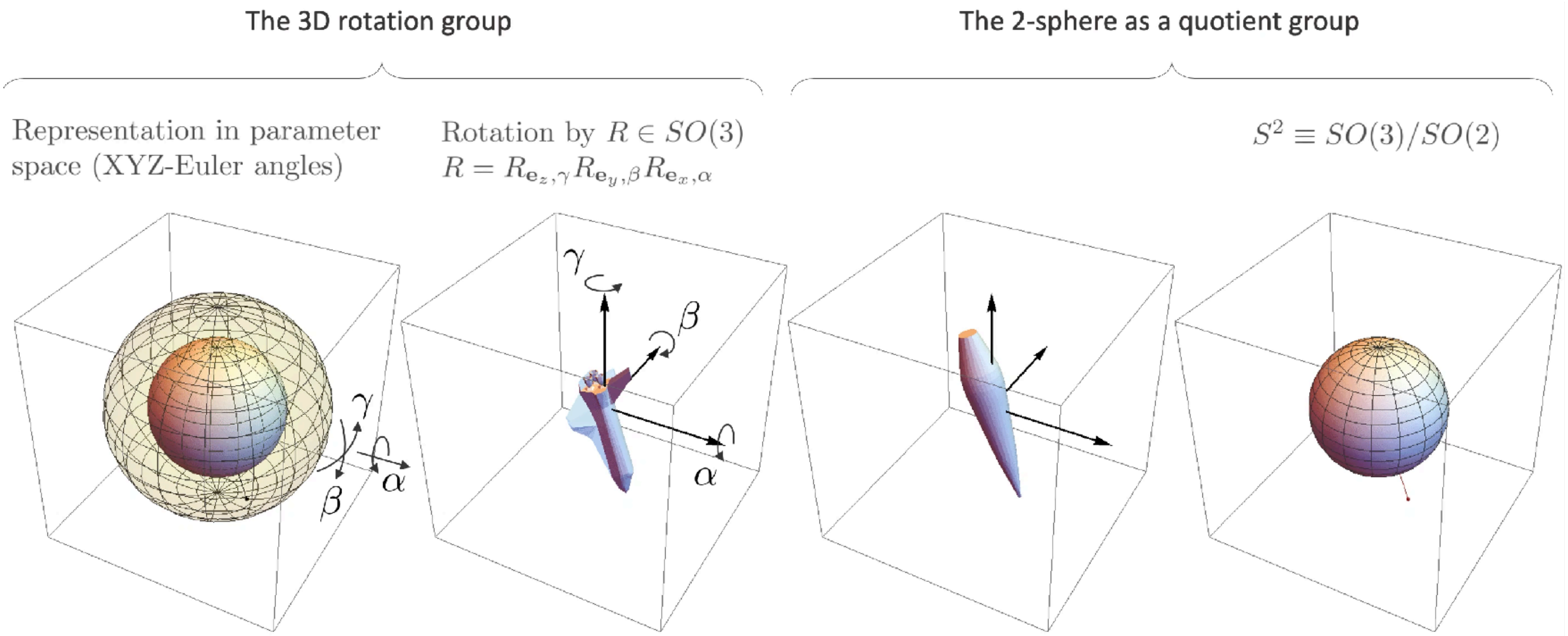
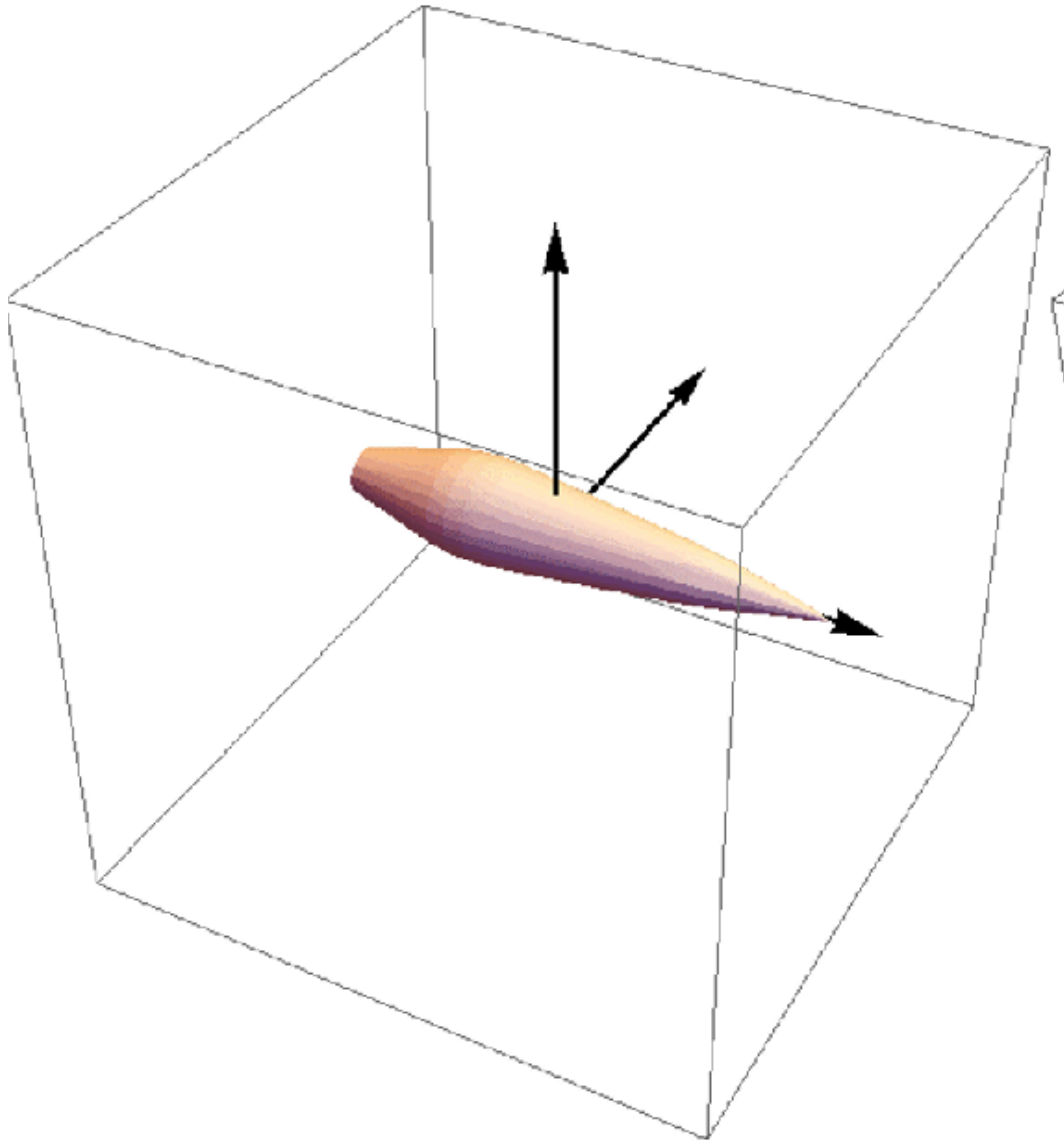
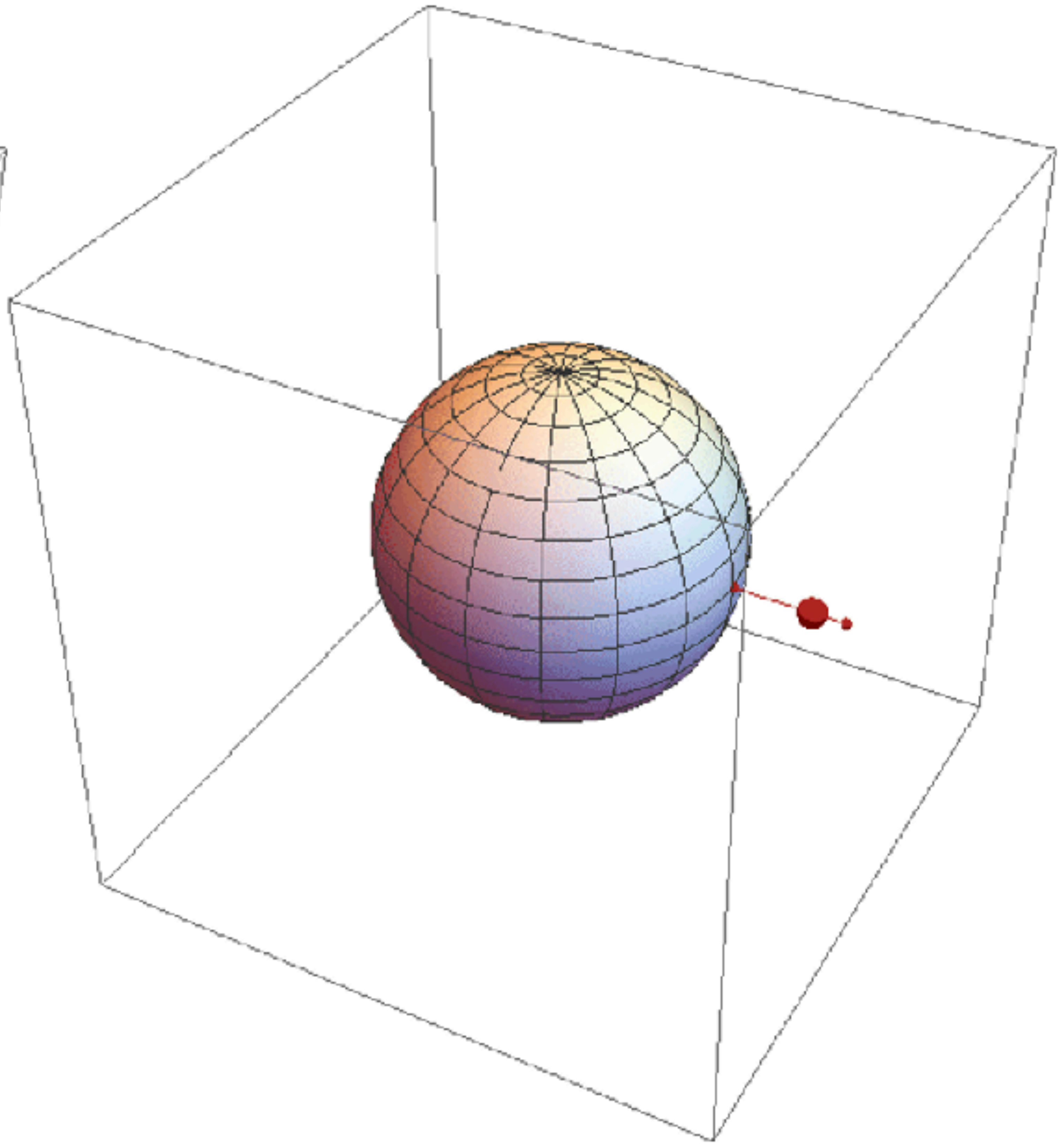
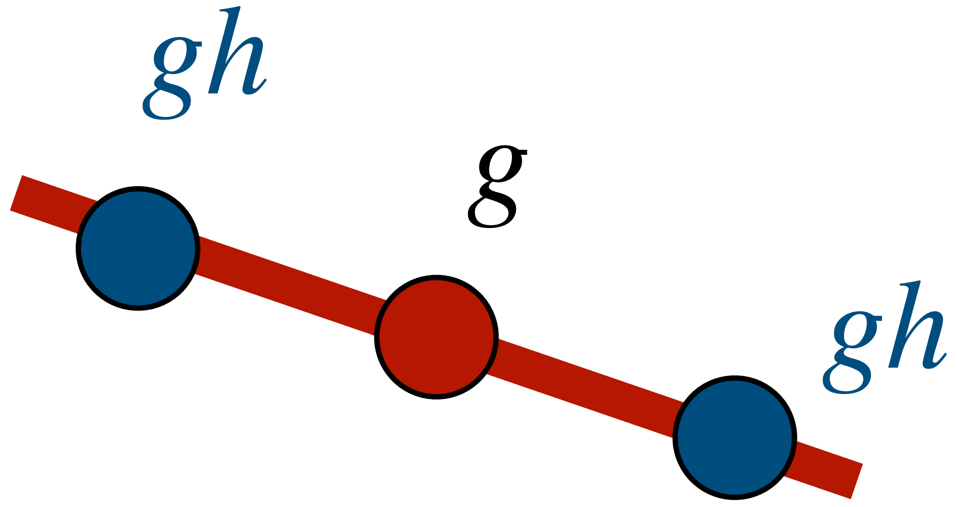


Group theory: Quotient spaces

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



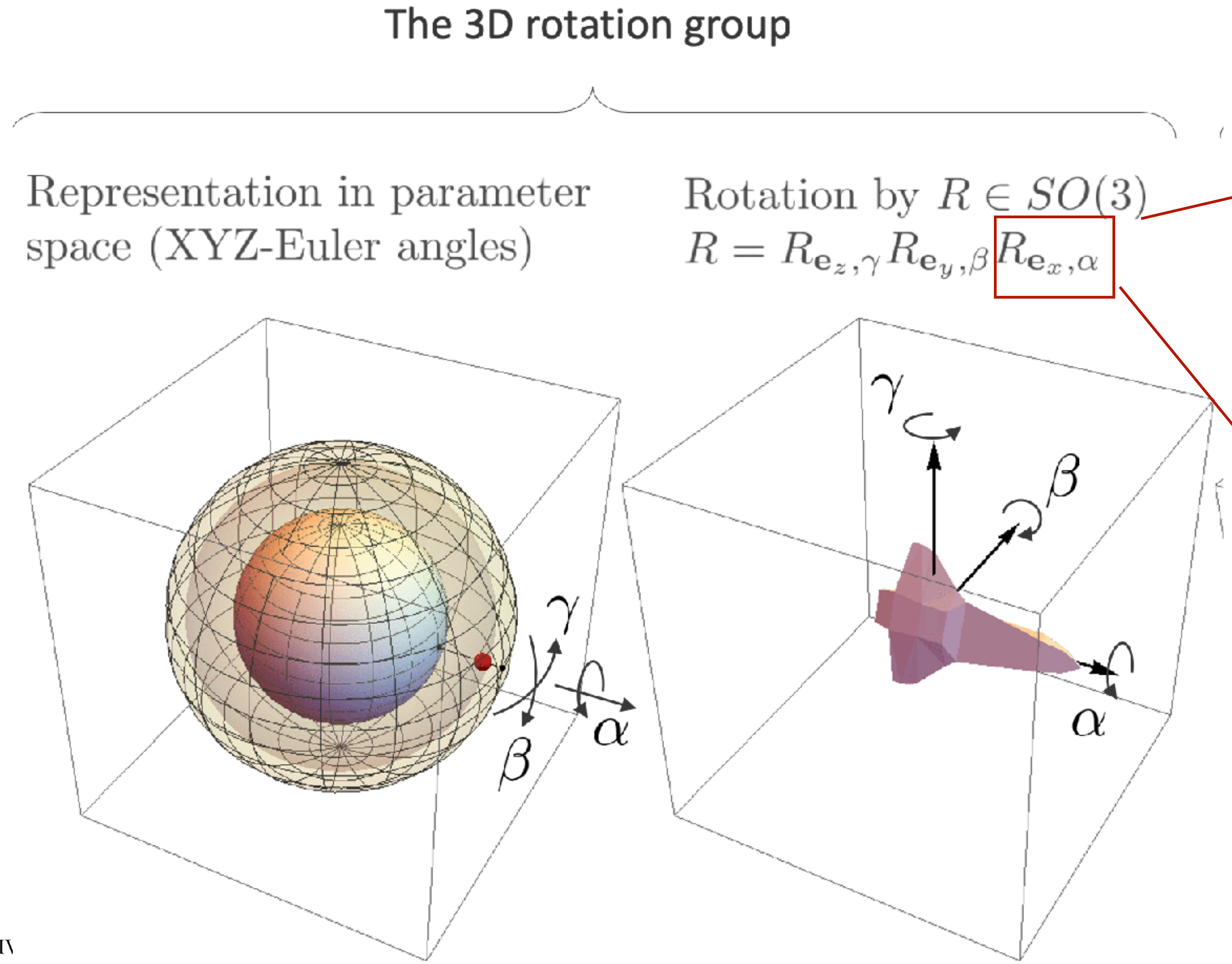




$$gH = \{gh \,|\, h \in H\}$$

Group theory: Stabilizer

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



So the sphere is a quotient space

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

with

$$H = \mathrm{Stab}_G(\mathbf{e}_x)$$

Group theory: Homogeneous space $\equiv$ Quotient space

Lemma 2.1: Any quotient space is a homogeneous space

Lemma 2.2: Any homogeneous space is a quotient space

Group theory: Quotient spaces

Lecture notes
Section 2.3

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

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

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.

Theorem 3.2:

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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.

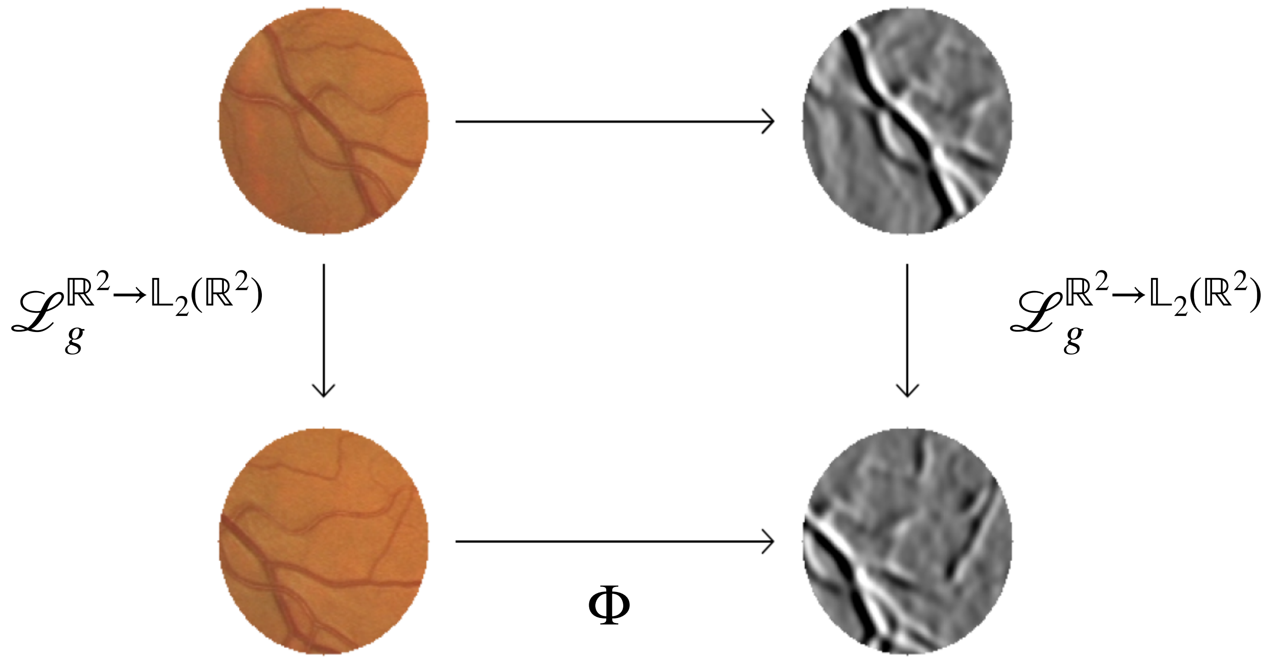
$(X = G, Y = \emptyset)$

Global pooling over G.

The case of $SE(2)$ equivariant layers

for signals on $\mathbb{R}^d \equiv SE(2)/SO(2)$

2D cross-correlation (translation equivariant) - $K : \mathbb{L}_2(\mathbb{R}^2) \to \mathbb{L}_2(\mathbb{R}^2)$



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

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

SE(2) equivariance iff

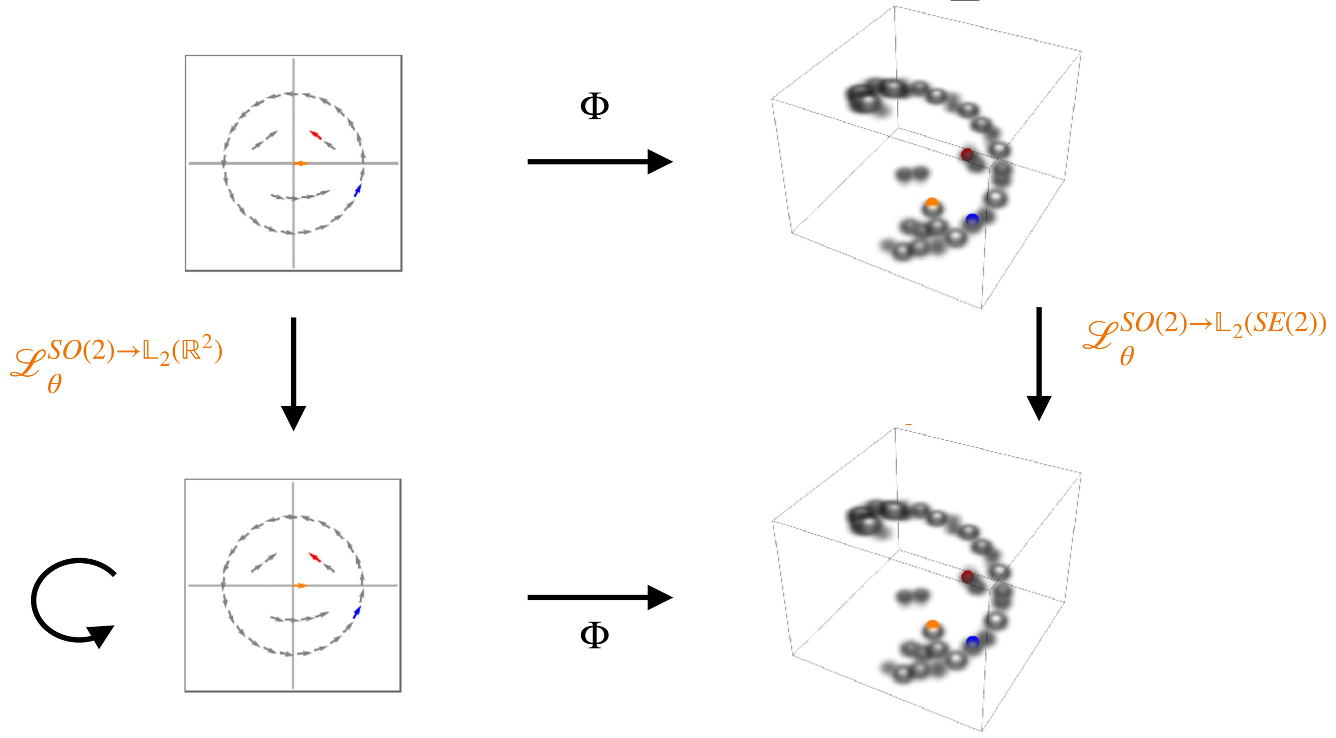
$$(\mathscr{L}_\theta^{SO(2) \to \mathbb{L}_2(\mathbb{R}^2)} k)(\mathbf{x}) = k(\mathbf{x})$$

$$\Leftrightarrow$$

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

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

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

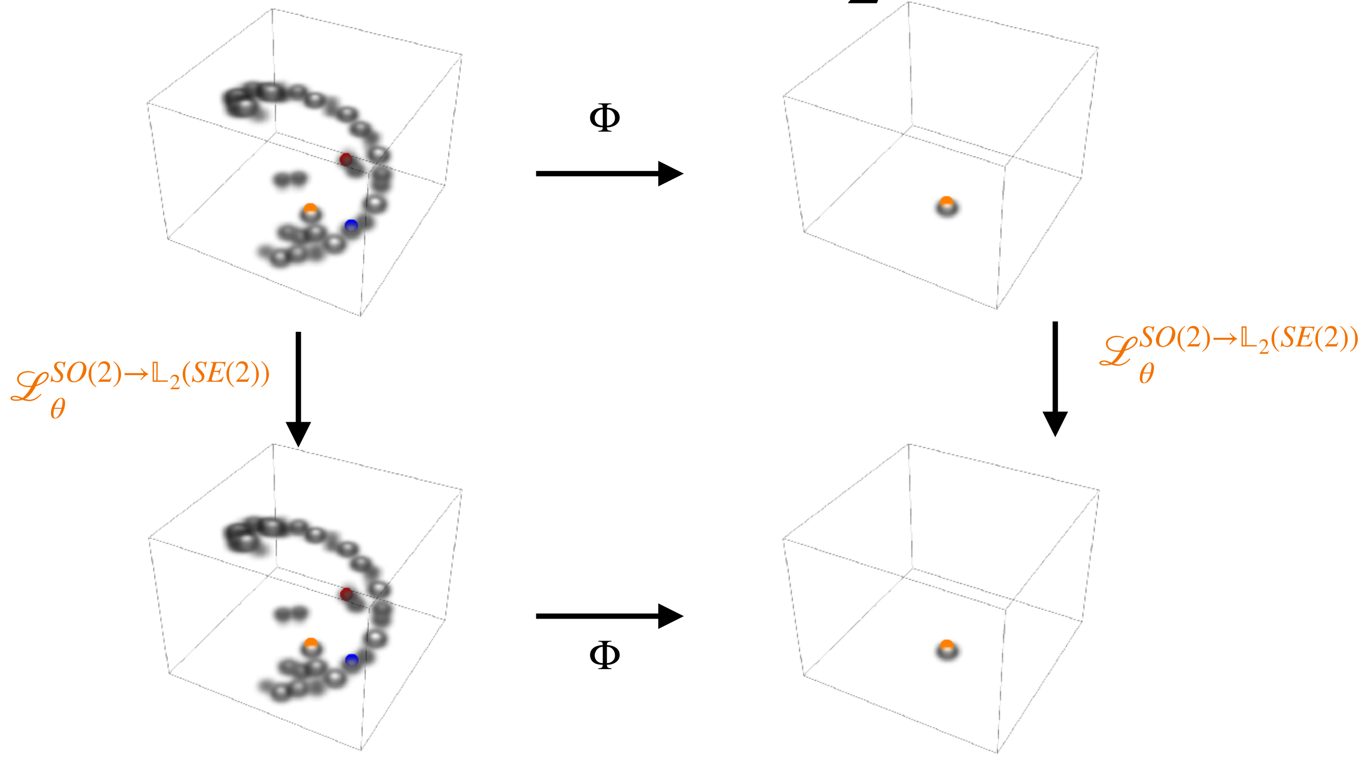


$$(k \tilde{\star} f)(\mathbf{x}) = (\mathscr{L}_g^{SE(2) \to \mathbb{L}_2(\mathbb{R}^2)} k \, , f)_{\mathbb{L}_2(\mathbb{R}^2)}$$

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

No constraints

SE(2) G-correlations - $K : \mathbb{L}_2(SE(2)) \to \mathbb{L}_2(SE(2))$



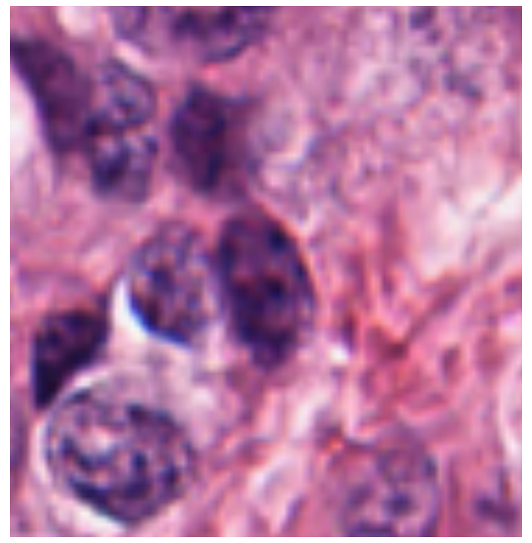
$$(k \tilde{\star} f)(\mathbf{x}) = (\mathscr{L}_g^{SE(2) \to \mathbb{L}_2(SE(2))} k \, , f)_{\mathbb{L}_2(SE(2)}$$

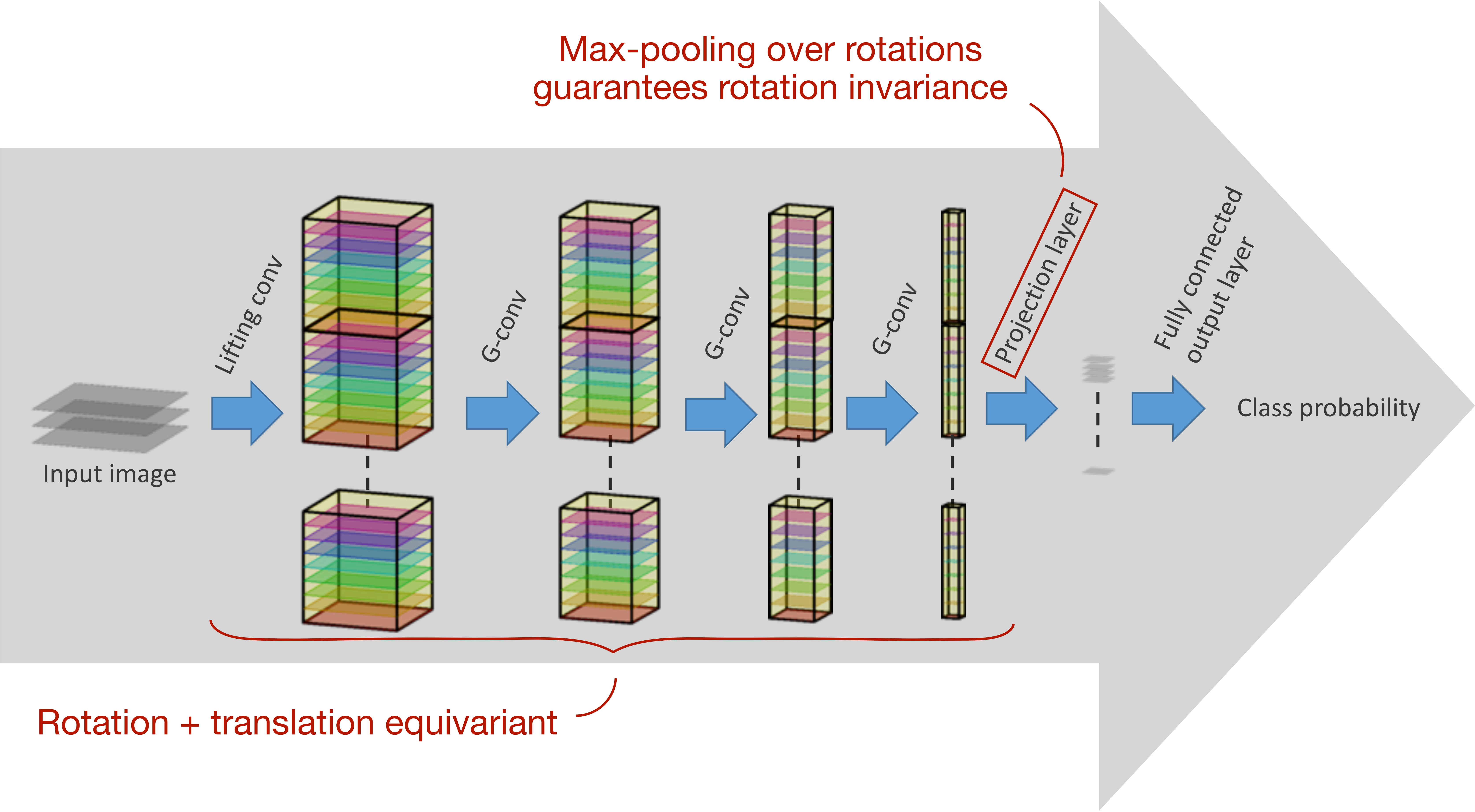
$$= \int_{\mathbb{R}^2} \int_{S^1} k(\mathbf{R}_\theta^{-1}(\mathbf{x}' - \mathbf{x}), \theta' - \theta \mod 2\pi) f(\mathbf{x}', \theta') d\mathbf{x}'$$

No constraints

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)

Content

Part I: Introduction to group convolutions

* Motivation
* Introduction to group theory
* Regular group convolutional neural networks
* Applications

Part II: General theory for group equivariant deep learning

* Group convolutions are all you need!
* Deeper into group theory: representation theory, homogeneous spaces
* Characterization of types of group equivariant layers

Part III: Steerable group convolutions

* Deep dive into group theory: irreducible representations, steerable operators and vector spaces
* Examples of steerable group convolutions: Spherical data and Volumetric data/3D point clouds

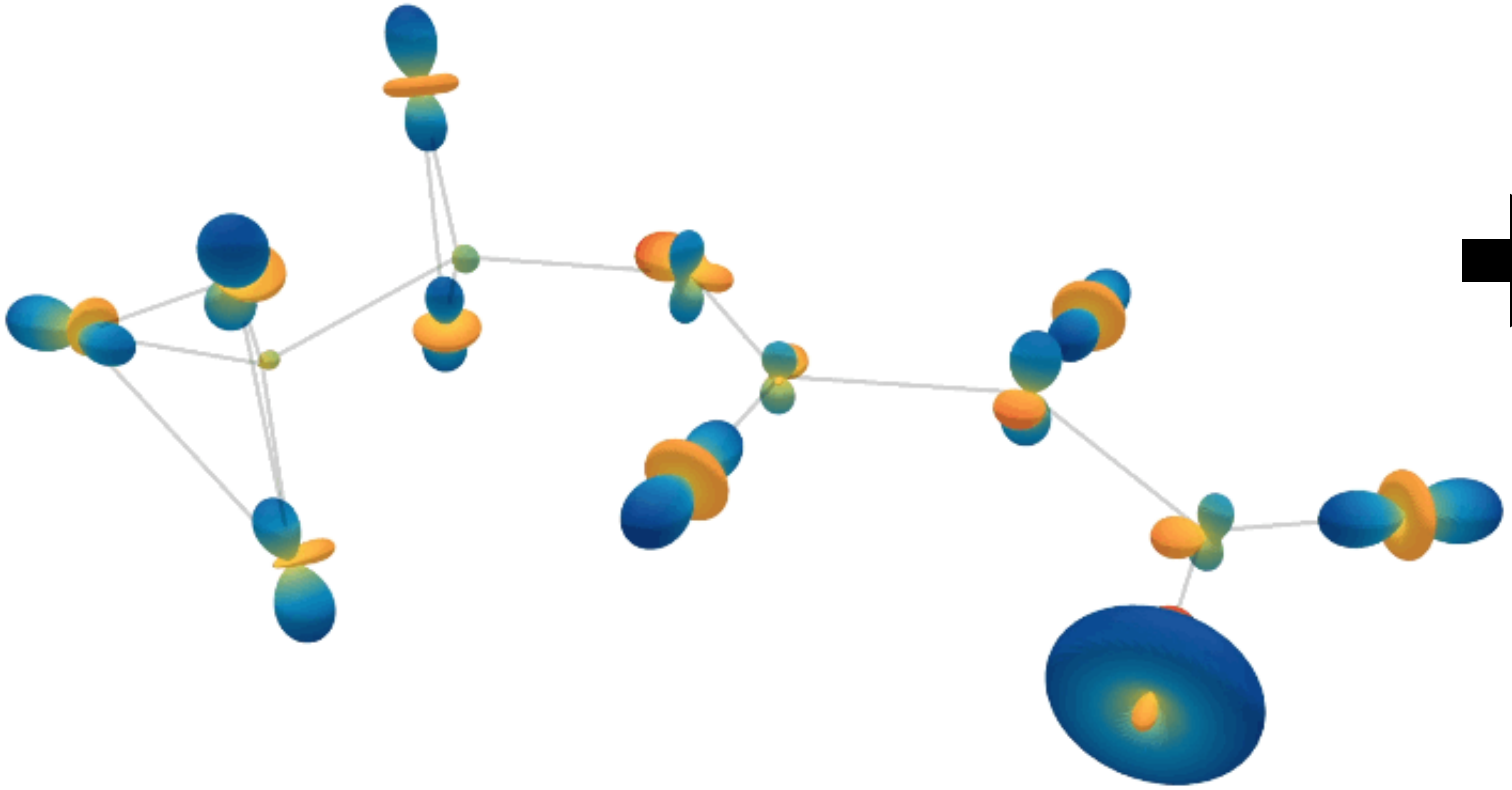
The need for steerable G-CNNs

Steerable methods are designed for groups that involve the action of $SO(d)$:

- Are based on a Fourier convolution theorem on $SO(d)$
- Avoids discretization of $SO(d)$:
    - Numerically more precise than regular group convolutions
    - Exact equivariance
    - Flexible to non-gridded data
- Provide a roadmap to local equivariance on arbitrary manifolds through Gauge theory

Steerable methods for computational chemistry

Brandstetter, Hesselink, van der Pol, Bekkers, Welling **Steerable Equivariant Message Passing on Molecular Graphs**



Molecular property prediction

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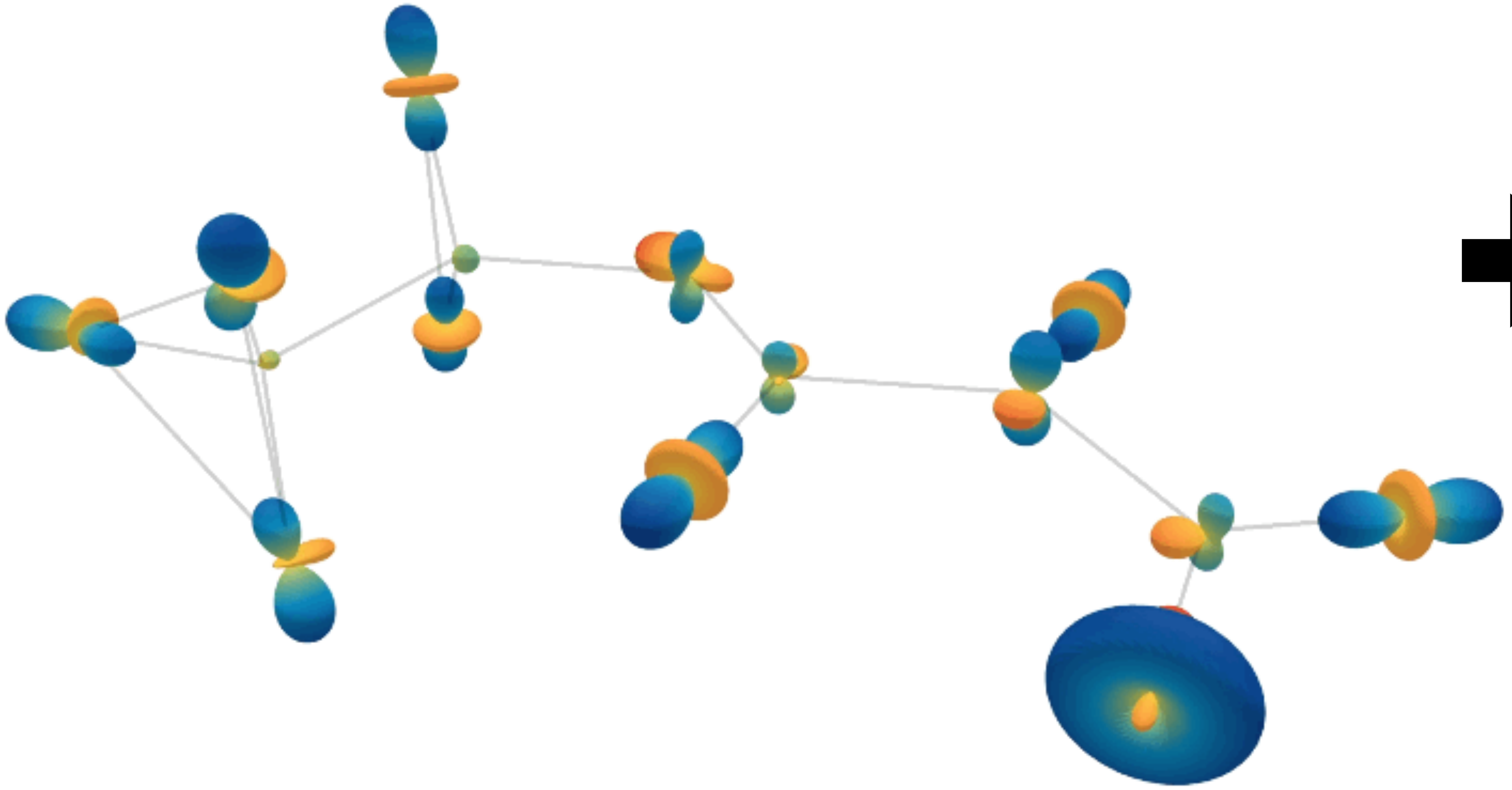

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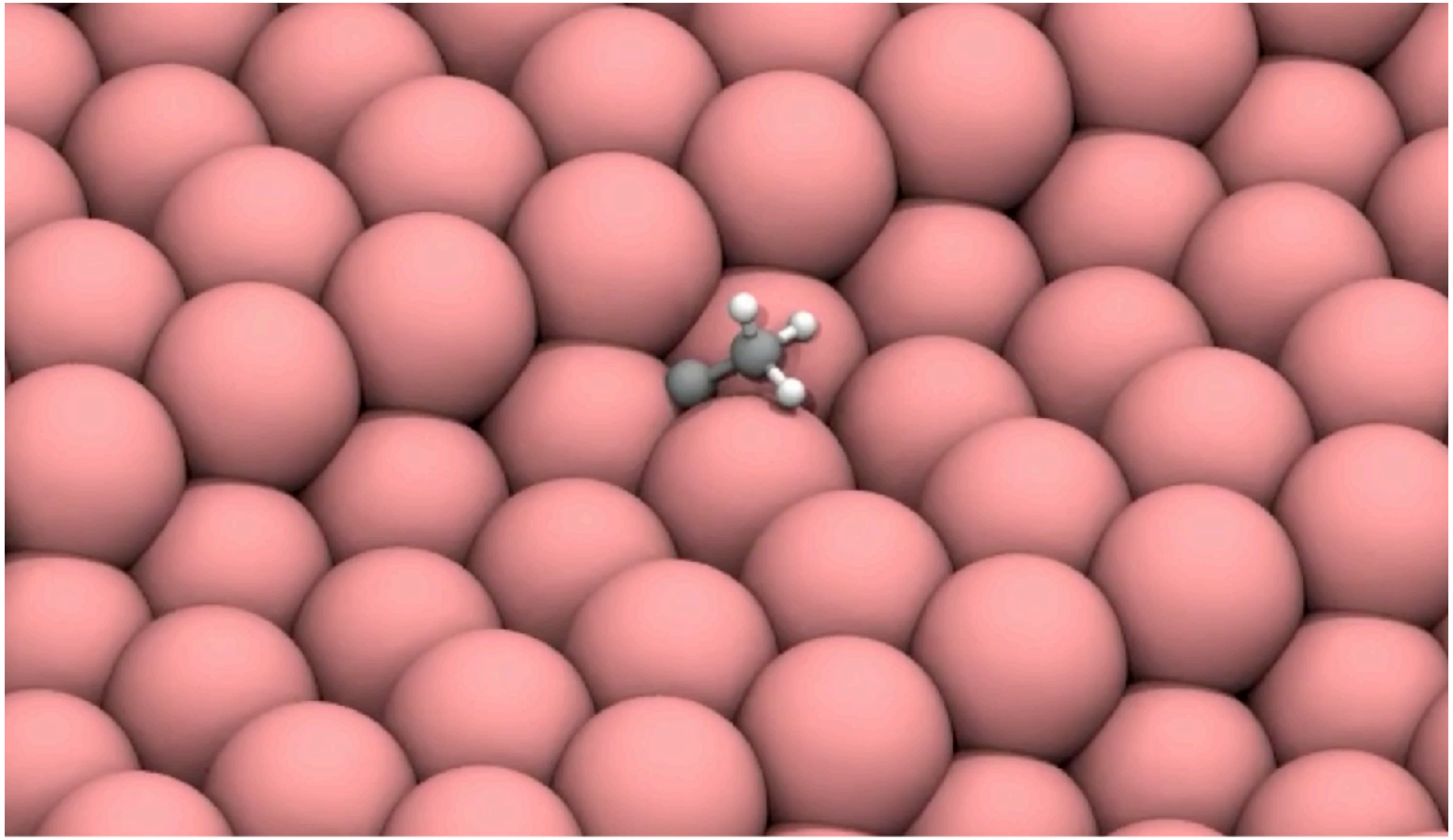

Video: Open Catalyst Project

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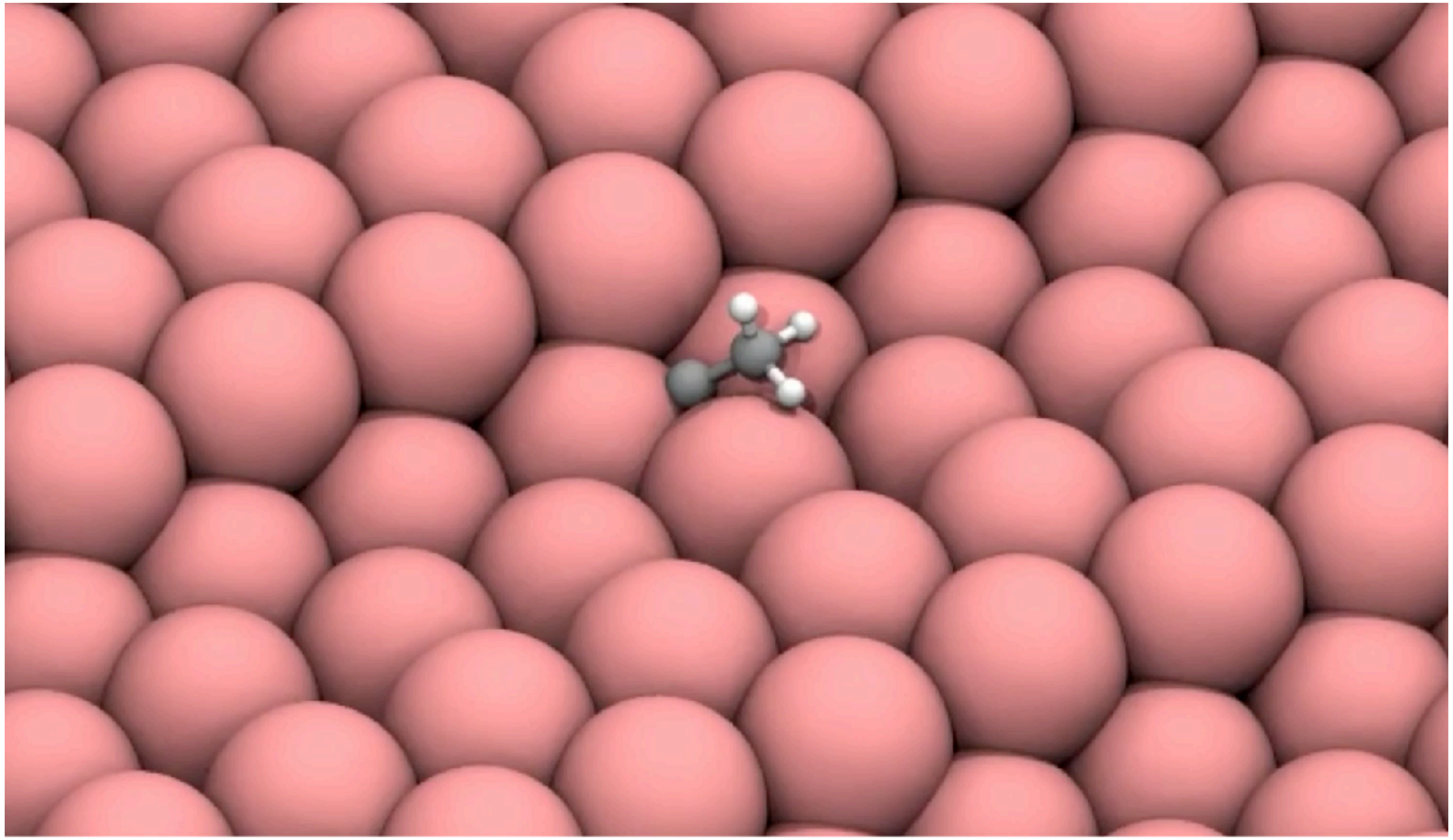

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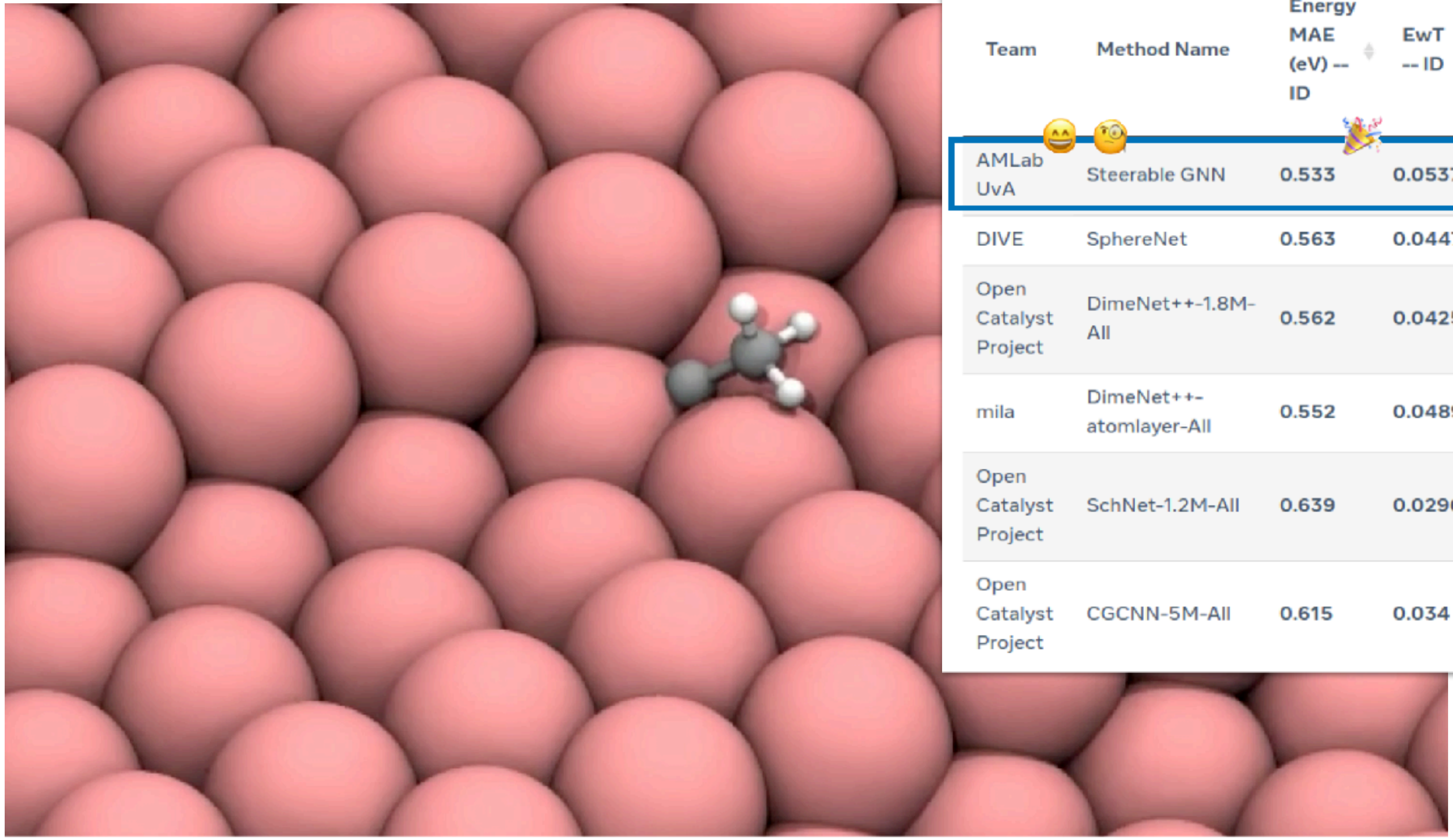

Team	Method Name	Energy MAE (eV) -- ID	EwT -- ID	Energy MAE (eV) -- OOD Ads	EwT -- OOD Ads	Energy MAE (eV) -- OOD Cat	EwT -- OOD Cat	Energy MAE (eV) -- OOD Both	EwT -- OOD Both	Submitted
AMLab UvA 😀	🧐 Steerable GNN	0.533 🎉	0.0537 🎉	0.692 🎉	0.0246	0.537 🎉	0.0492 🎉	0.679	0.0263 🎉	2021/06/12
DIVE	SphereNet	0.563	0.0447	0.703	0.0229	0.571	0.0409	0.638	0.0241	2021/03/31
Open Catalyst Project	DimeNet++-1.8M-All	0.562	0.0425	0.725	0.0207	0.576	0.041	0.661	0.0241	2021/02/16
mila	DimeNet++-atomlayer-All	0.552	0.0489	0.747	0.0259	0.557	0.0459	0.688	0.0233	2021/06/07
Open Catalyst Project	SchNet-1.2M-All	0.639	0.0296	0.734	0.0233	0.662	0.0294	0.704	0.0221	2021/02/17
Open Catalyst Project	CGCNN-5M-All	0.615	0.034	0.915	0.0193	0.622	0.031	0.851	0.02	2021/02/18

Video: Open Catalyst Project

Group theoretical background

Irreducible Representations (spherical harmonics, Wigner-D matrices)

Fourier transform on $SO(3)$

Convolution theorem

+ Clebsch-Gordan Tensor product

Steerable G-CNNs

Group theory: Irreducible Representations

Definition 4.1 (Equivalence of matrix representations). Any two matrix representations $\mathbf{D}(g)$ and $\mathbf{D}'(g)$ of a group G are *equivalent* if they relate via a similarity transform

$$\mathbf{D}'(g) = \mathbf{Q}^{-1}\mathbf{D}(g)\mathbf{Q} \ ,$$

in which $\mathbf{Q}$ carries out the change of basis.

Group theory: Irreducible Representations

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$$\mathbf{D}'(g) = \mathbf{Q}^{-1}\mathbf{D}(g)\mathbf{Q} ,$$

in which $\mathbf{Q}$ carries out the change of basis.

Definition 4.2 (Reducible/irreducible matrix representation). A matrix representation is called reducible if it can be written as

$$\mathbf{D}(g) = \mathbf{Q}^{-1}(\mathbf{D}_1(g) \oplus \mathbf{D}_2(g))\mathbf{Q} = \mathbf{Q}^{-1}\begin{pmatrix} \mathbf{D}_1(g) & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_2(g) \end{pmatrix}\mathbf{Q} ,$$

in which $\mathbf{Q}$ carries out a change of basis. If the matrices $\mathbf{D}_1$ and $\mathbf{D}_2$ are not reducible they are called irreducible representations (irreps).

Group theory: Wigner-D Matrices

Wigner-D matrices are the irreducible matrix representations of $SO(3)$

Every representation $\mathbf{D}(g)$ of $SO(3)$ is block diagonalizable to a representation with Wigner-D matrices along the diagonal:

$$\mathbf{D}(g) = \mathbf{Q}^{-1}(\mathbf{D}^{(l_1)}(g) \oplus \mathbf{D}^{(l_2)}(g) \oplus \dots)\mathbf{Q} = \mathbf{Q}^{-1} \begin{pmatrix} \mathbf{D}^{(l_1)}(g) & & \\ & \mathbf{D}^{(l_2)}(g) & \\ & & \ddots \end{pmatrix} \mathbf{Q}$$

Group theory: Steerable vector space

Definition 4.3 (Wigner-D matrix)**.** The Wigner-D matrices of type-l are the irreducible $(2l+1)$ matrix representations of $SO(3)$. A Wigner-D matrix of type l as a function of $g \in G$ will be denoted with $\mathbf{D}^{(l)}(g)$.

Wigner-D matrices generalize the notion of a rotation matrix for the rotation of $(2l+1)$-dimensional vectors

Group theory: Steerable vector space

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Definition 4.4 (Wigner-D functions). The $(2l+1) \times (2l+1)$ components of the type-l Wigner-D matrices will be referred to as the type-l Wigner-D functions. The Wigner-D functions are denoted with $D^{(l)}_{mn}$ with m and n row and column index respectively.

Group theory: Steerable vector space

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Definition 4.4 (Wigner-D functions). The $(2l+1) \times (2l+1)$ components of the type-l Wigner-D matrices will be referred to as the type-l Wigner-D functions. The Wigner-D functions are denoted with $D_{mn}^{(l)}$ with m and n row and column index respectively.

Definition 4.5 (Steerable vector spaces and steerable vectors). The $(2l+1)$-dimensional vector space on which a Wigner-D matrix of order l acts will be called *a type l steerable vector space* and is denoted with V_l. A $(2l+1)$-dimensional vector $\mathbf{v} \in V_l$ will be called a type-l vector.

Group theory: Spherical Harmonics

- Functions on the sphere
- Solutions to Laplace's equation on S^2
- The S^2 equivalent of the circular harmonics (1D Fourier basis)
- Form orthonormal basis for $\mathbb{L}_2(S^2)$
- Are Wigner-D functions:

$$Y_m^{(l)} = \mathbf{D}_{m0}^{(l)}$$

Spherical harmonics $Y_m^{(l)} : S^2 \to \mathbb{R}$

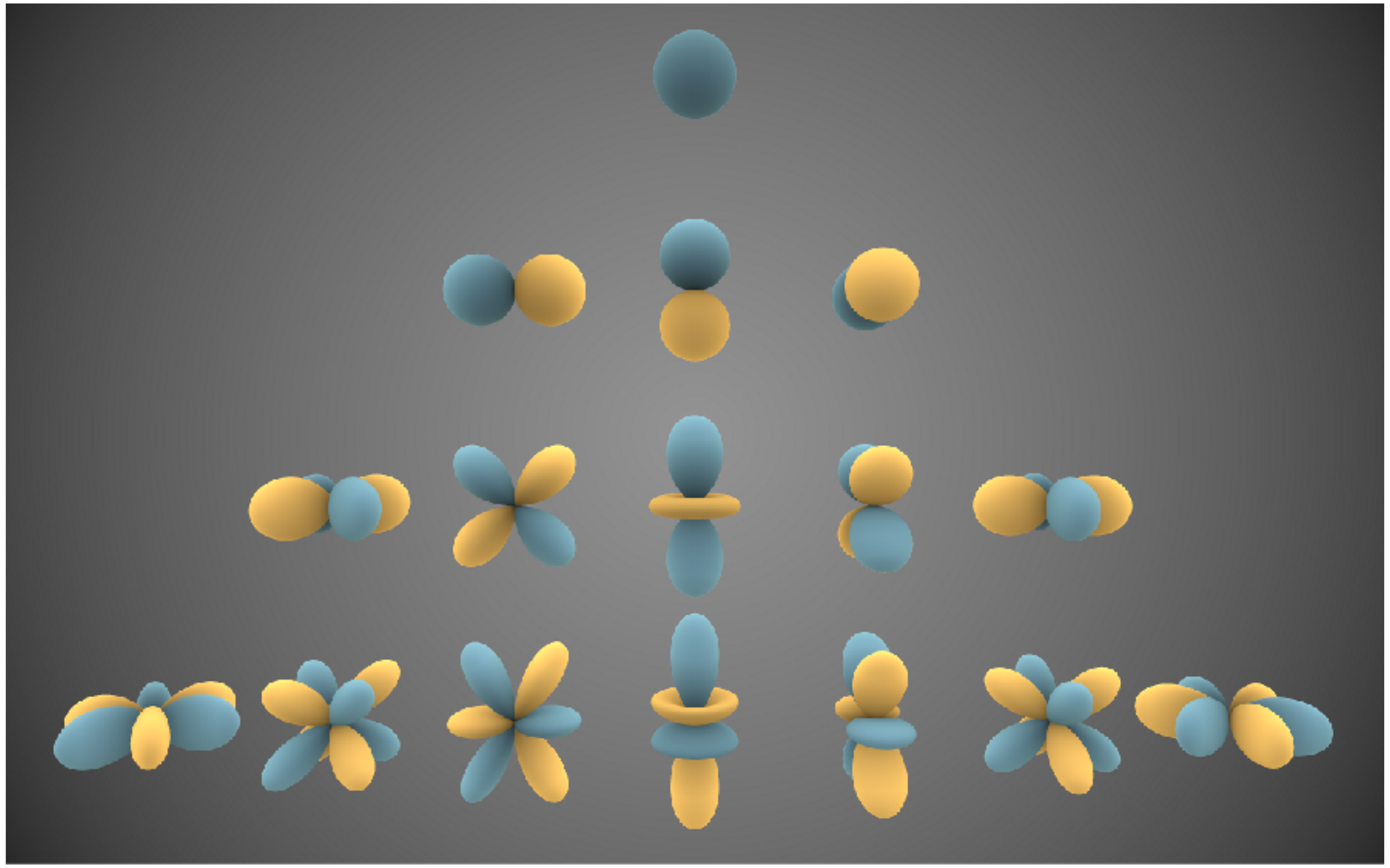
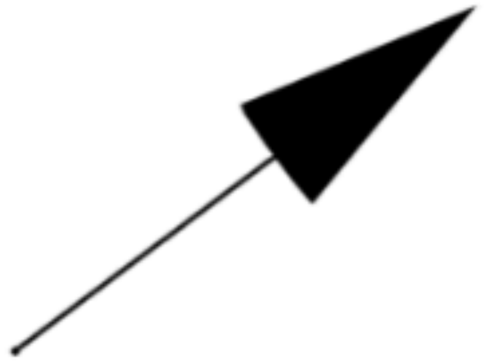


Image: wikipedia

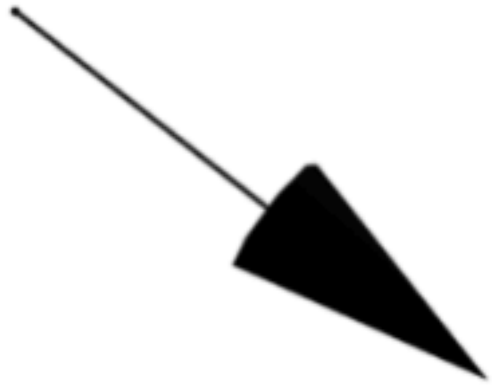
Group theory: Spherical Harmonics Form Steerable Vectors

$\mathbf{x} \qquad \tilde{\mathbf{h}}^{(l)} = Y^{(l)}(\mathbf{x}) \qquad Y_m^{(l)}(\cdot) \qquad \sum h_m^l Y_m^{(l)}(\cdot)$



$$[h_0^0] \quad \begin{bmatrix} h_0^1 \\ h_1^1 \\ h_2^1 \end{bmatrix} \quad \begin{bmatrix} h_0^2 \\ h_1^2 \\ h_2^2 \\ h_3^2 \\ h_4^2 \end{bmatrix}$$

$\mathbf{R}\mathbf{x} \qquad \tilde{\mathbf{h}}^{(l)} = \mathbf{D}^l(g) Y^{(l)}(\mathbf{x}) \qquad Y_m^{(l)}(\cdot) \qquad \sum h_m^l Y_m^{(l)}(\cdot)$



$$\mathbf{D}^0(g)[h_0^0] \quad \mathbf{D}^1(g)\begin{bmatrix} h_0^1 \\ h_1^1 \\ h_2^1 \end{bmatrix} \quad \mathbf{D}^2(g)\begin{bmatrix} h_0^2 \\ h_1^2 \\ h_2^2 \\ h_3^2 \\ h_4^2 \end{bmatrix}$$

Group theory: Fourier Transform on S^2

Definition 4.6 (Spherical Fourier transform). Let $f \in \mathbb{L}_2(S^2)$ be a spherical signal and let $\hat{f}(l) \in \mathbb{R}^{2l+1}$ denote the vector of Fourier coefficients of order l. We may refer to l as the frequency index. The forward and inverse Fourier transform are respectively given by

$$\hat{f}(l) = \int_{S^2} f(\mathbf{n}) \underline{Y}^{(l)}(\mathbf{n}) d\mathbf{n} \tag{64}$$

$$f(\mathbf{n}) = \sum_{l \geq 0} \hat{f}(l)^T \underline{Y}^{(l)}(\mathbf{n}), \tag{65}$$

with $\underline{Y}^{(l)} = (Y_{-l}^{(l)}, \ldots, Y_l^{(l)})^T \in \mathbb{L}_2(S^2)^{2l+1}$ the vector of spherical harmonics.

Group theory: Fourier Transform on $SO(3)$

Definition 4.7 ($SO(3)$ Fourier transform). Let $f \in \mathbb{L}_2(SO(3))$ be a spherical signal and let $\hat{f}(l) \in \mathbb{R}^{2l+1 \times 2l+1}$ denote the matrix of Fourier coefficients of order l. The number l may be referred to as frequency index. The forward and inverse Fourier transform are respectively given by

$$\hat{f}(l) = \int_{SO(3)} f(g) \mathbf{D}^{(l)}(g) \mathrm{d}g \ , \tag{68}$$

$$f(g) = \sum_{l \geq 0} \mathrm{Tr}(\hat{f}(l) \mathbf{D}^{(l)}(g^{-1})) \ . \tag{69}$$

$$\sum_{l \geq 0} \sum_{m=-l}^{l} \hat{f}_{mn}^{(l)} D_{mn}^{(l)}(g^{-1})$$

Group theory: $SO(3)$ Fourier Theorems

Lemma 4.1 (Shift property)**.** Let $\mathcal{L}_g$ denote the left-regular representation of $SO(3)$ on $\mathbb{L}_2(SO(3))$ and $\hat{f}$ denote the $SO(3)$ Fourier transform $SO(3)$ (Definition 4.7). The $SO(3)$ Fourier transform is equivariant via

$$\widehat{\mathcal{L}_g f}(l) = \mathbf{D}^{(l)}(g)\hat{f}(l)\,. \tag{70}$$

Group theory: $SO(3)$ Fourier Theorems

Lemma 4.1 (Shift property). Let $\mathcal{L}_g$ denote the left-regular representation of $SO(3)$ on $\mathbb{L}_2(SO(3))$ and $\hat{f}$ denote the $SO(3)$ Fourier transform $SO(3)$ (Definition 4.7). The $SO(3)$ Fourier transform is equivariant via

$$\widehat{\mathcal{L}_g f}(l) = \mathbf{D}^{(l)}(g)\hat{f}(l)\,. \tag{70}$$

Theorem 4.1 (Convolution theorem on $SO(3)$). Let $k, f \in \mathbb{L}_2(SO(3))$ and let $\hat{k}(l), \hat{f}(l)$ denote their matrix valued Fourier coefficients. Then the Fourier transform of a (group) correlation of a k with f is given by

$$\widehat{k \star f}(l) = \hat{f}(l)\hat{k}(l)^T\,. \tag{71}$$

Group theory: Clebsch-Gordan Tensor Product

General tensor product between two vectors:

Group theory: Clebsch-Gordan Tensor Product

General tensor product between two vectors:

$$\mathbf{h}_1 \otimes \mathbf{h}_2 = \mathbf{h}_1 \mathbf{h}_2^T = \begin{pmatrix} h_1 h_1 & h_1 h_2 & \cdots \\ h_2 h_1 & h_2 h_2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Group theory: Clebsch-Gordan Tensor Product

We want the tensor product to be equivariant via

$$\mathbf{D}(g)(\tilde{\mathbf{h}}_1 \otimes \tilde{\mathbf{h}}_2) = (\mathbf{D}^{(l_1)}(g)\tilde{\mathbf{h}}_1) \otimes (\mathbf{D}^{(l_2)}(g)\tilde{\mathbf{h}}_2)$$

for some $\mathbf{D}(g)$

Group theory: Clebsch-Gordan Tensor Product

The tensor product between two steerable vectors results again in a steerable vector:

$$\begin{aligned}\text{vec}\left((\mathbf{D}^{(l_1)}(g)\tilde{\mathbf{h}}_1)(\mathbf{D}^{(l_2)}(g)\tilde{\mathbf{h}}_2)^T \right) &= \text{vec}\left(\mathbf{D}^{(l_1)}(g)\tilde{\mathbf{h}}_1\tilde{\mathbf{h}}_2^T\mathbf{D}^{(l_2)T}(g) \right) \\ &= \boxed{\left(\mathbf{D}^{(l_2)}(g) \otimes \mathbf{D}^{(l_1)}(g)\right)} \text{vec}\left(\tilde{\mathbf{h}}_1\tilde{\mathbf{h}}_2^T \right)\end{aligned}$$

The resulting representation is reducible.

The CG-product $\otimes_{cg}$ is defined in such a way that the output is directly obtained in direct sum of steerable vector spaces

$\tilde{\mathbf{h}}_1 \otimes_{cg} \tilde{\mathbf{h}}_2 \in V_0 \oplus V_1 \oplus \ldots$

Group theory: Clebsch-Gordan Tensor Product

Definition 4.8 (Clebsch-Gordan tensor product). Let $\tilde{\mathbf{h}}^{(l)} \in V_l = \mathbb{R}^{2l+1}$ denote a steerable vector of type l and $h^{(l)}_m$ its components with $m = -l, -l+1, \ldots, l$. Then the Clebsch-Gordan tensor product is defined is a tensor product such tat the m-th component of the type l sub-vector of the output of the tensor product between two steerable vectors of type l_1 and l_2 is given by

$$(\tilde{\mathbf{h}}^{(l_1)} \otimes_{cg} \tilde{\mathbf{h}}^{(l_2)})^{(l)}_m = \sum_{m_1=-l_1}^{l_1} \sum_{m_2=-l_2}^{l_2} C^{(l,m)}_{(l_1,m_1)(l_2,m_2)} h^{(l_1)}_{m_1} h^{(l_2)}_{m_2} \,, \tag{73}$$

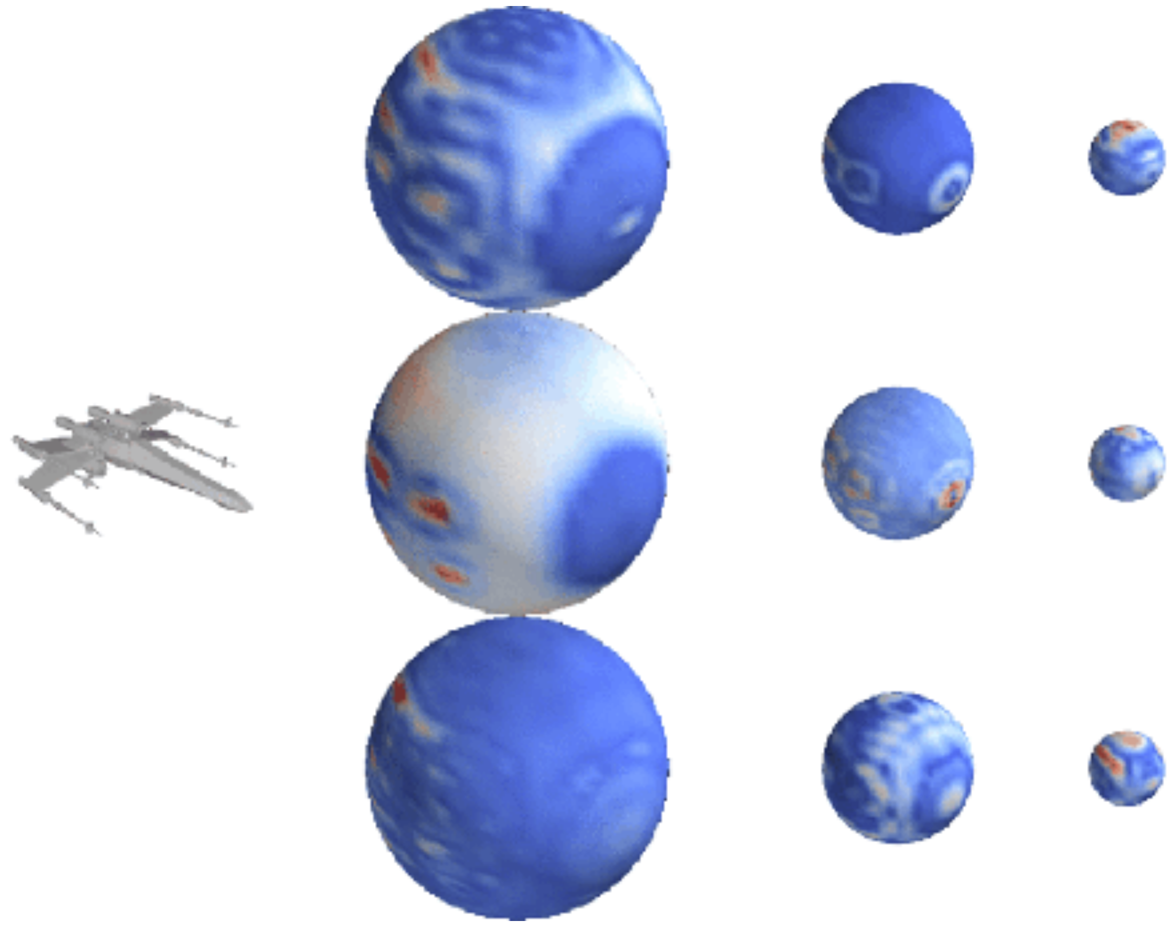
in which $C^{(l,m)}_{(l_1,m_1)(l_2,m_2)}$ are the Clebsch-Gordan coefficients. The l-th output vector $(\tilde{\mathbf{h}}^{(l_1)} \otimes_{cg} \tilde{\mathbf{h}}^{(l_2)})^{(l)} \in \mathbb{R}^{2l+1}$ is a type-l steerable vector.

Steerable Neural Networks

Steerable Neural Networks

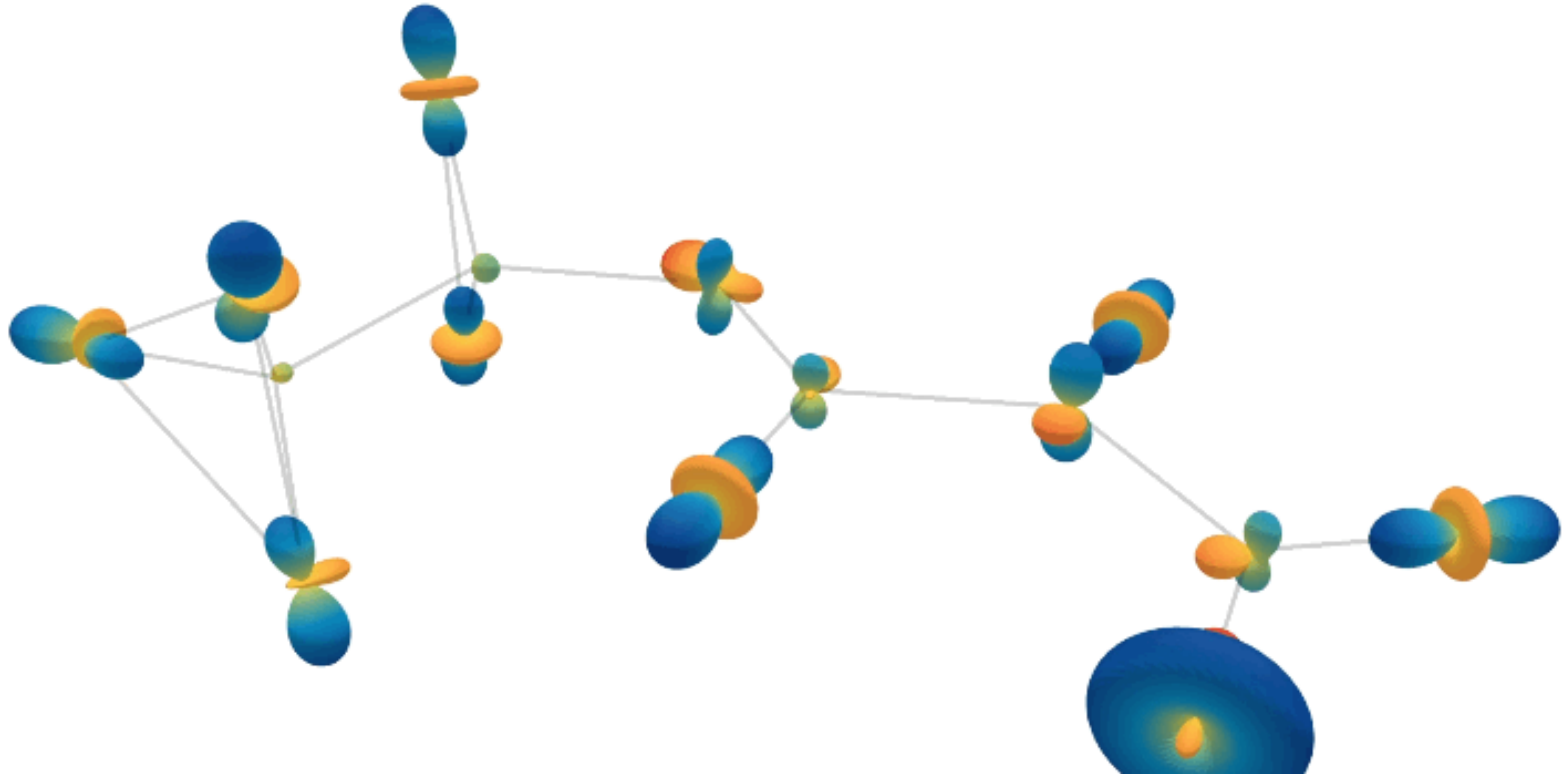
Method 1: Convolutions in the Fourier domain $(SO(3)$ gconvs)

Lecture notes Section 5.1



Method 2: Clebsch-Gordan tensor product $(SE(3)$ gconvs)

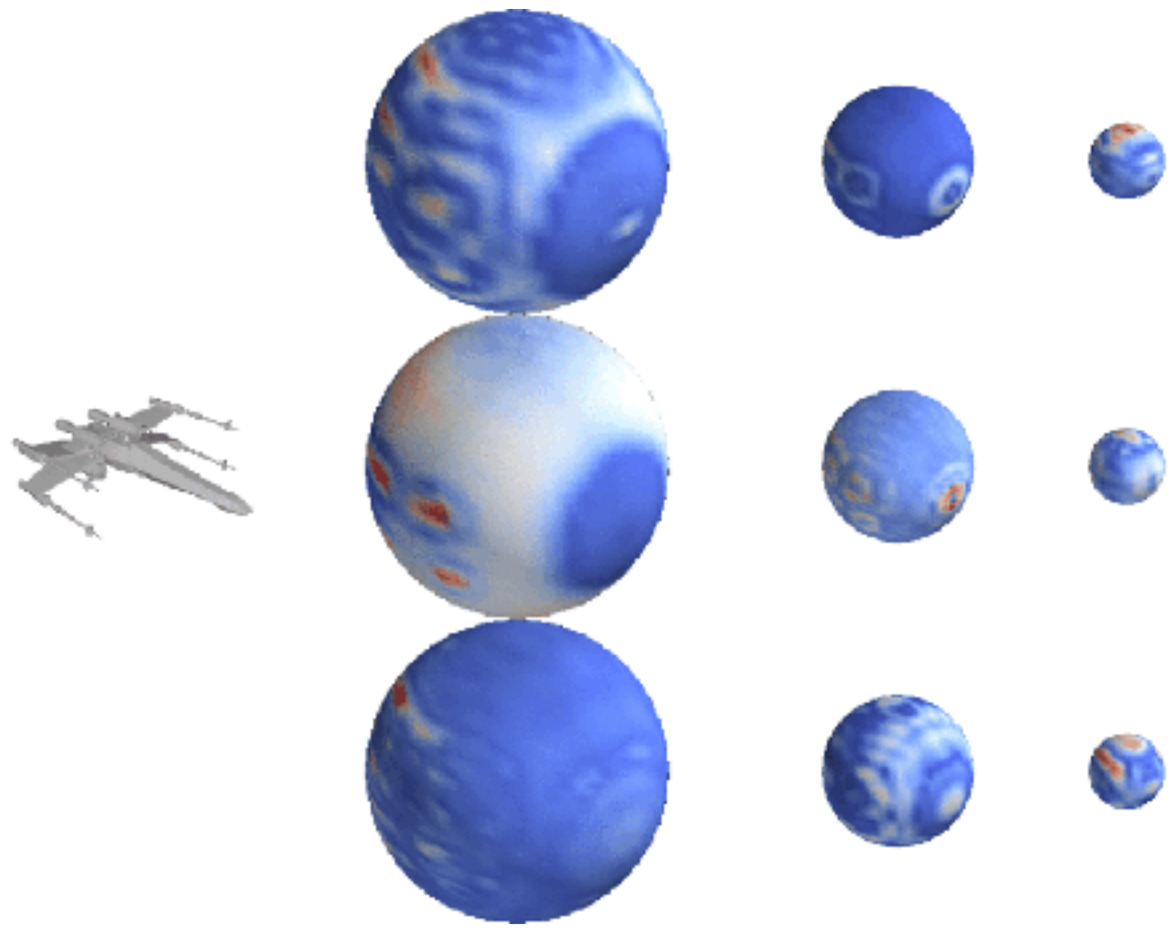
Lecture notes Section 5.2



Steerable Neural Networks

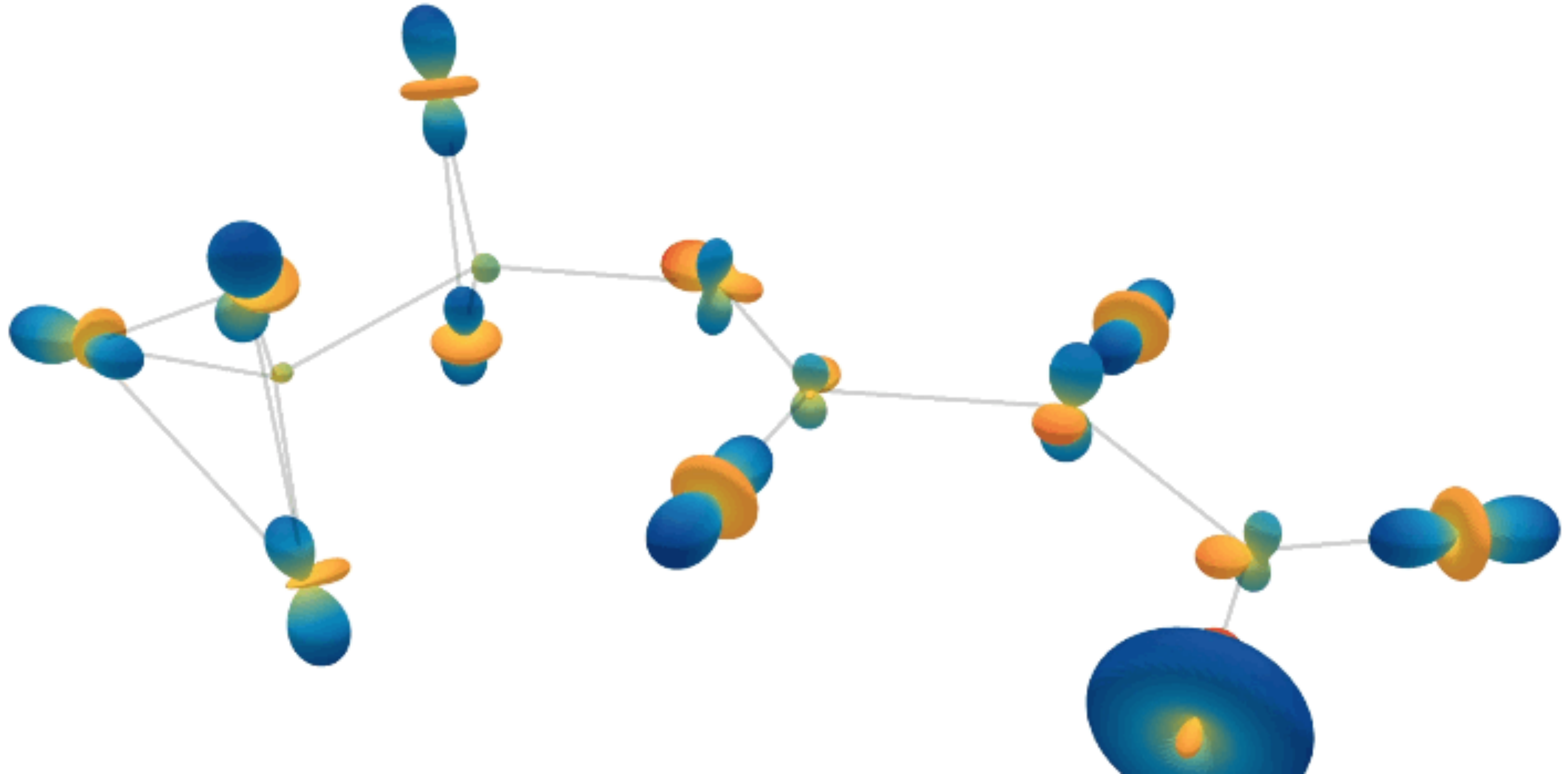
Method 1: Convolutions in the Fourier domain $(SO(3)$ gconvs)

Lecture notes Section 5.1



Method 2: Clebsch-Gordan tensor product $(SE(3)$ gconvs)

Lecture notes Section 5.2



Steerable Neural Networks

Method 1: Convolutions in the Fourier domain $(SO(3)$ gconvs)

Lecture notes Section 5.1

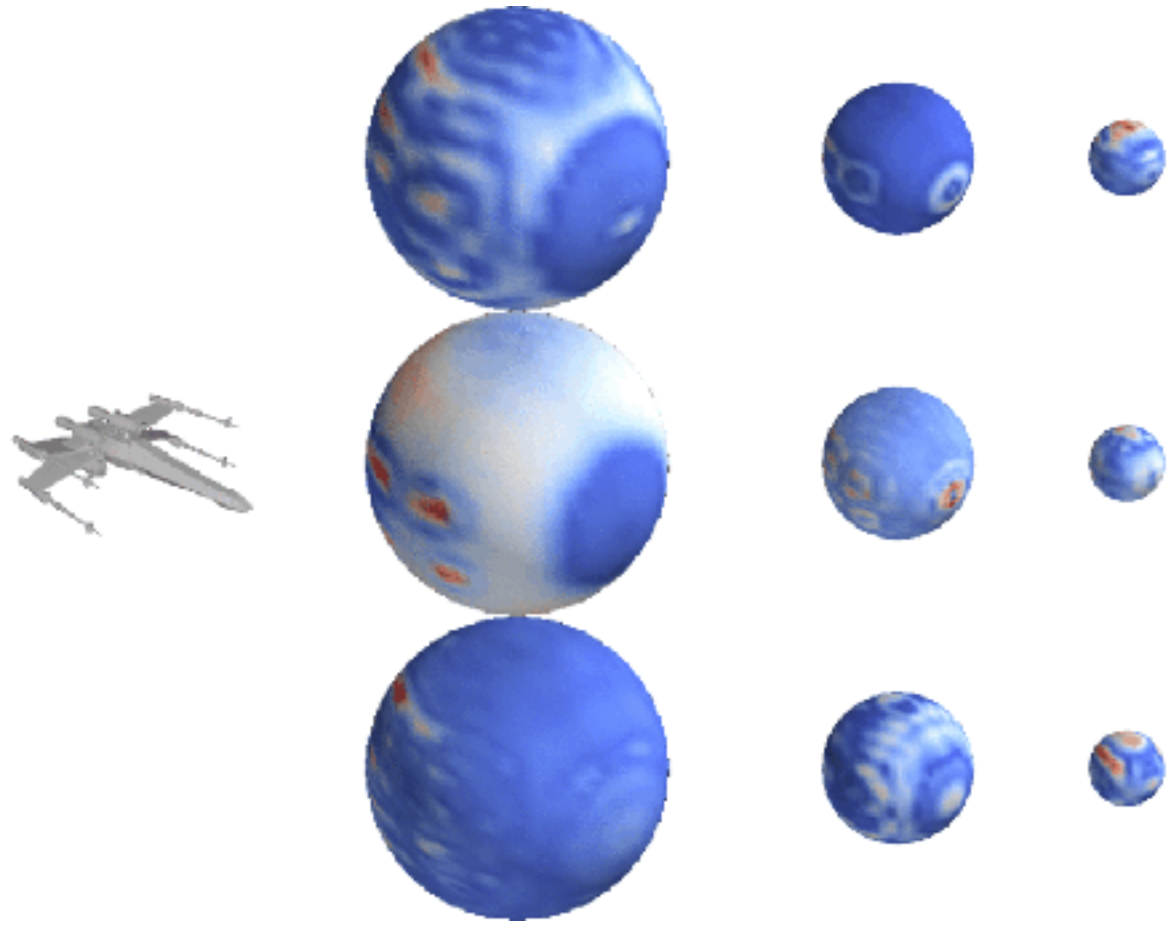


Figure from: https://github.com/daniilidis-group/spherical-cnn
Esteves, C., Allen-Blanchette, C., Makadia, A., & Daniilidis, K. Learning SO(3) Equivariant Representations with Spherical CNNs. European Conference on Computer Vision, ECCV 2018

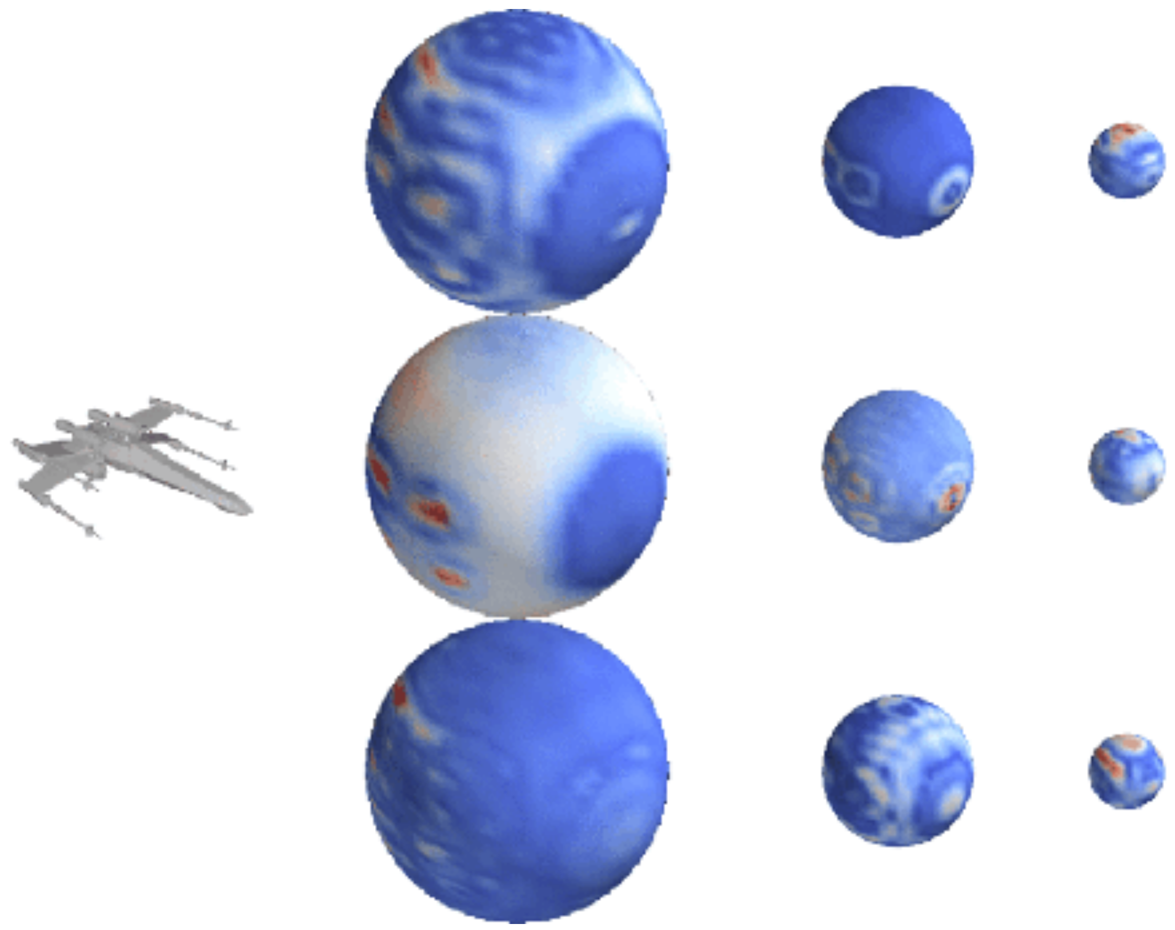
Method 2: Clebsch-Gordan tensor product $(SE(3)$ gconvs)

Lecture notes Section 5.2

Steerable Neural Networks

Method 1: Convolutions in the Fourier domain ($SO(3)$ gconvs)

Lecture notes Section 5.1



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Method 2: Clebsch-Gordan tensor product ($SE(3)$ gconvs)

Lecture notes Section 5.2

Spherical group convolutions in the Fourier domain

Spherical CNNs are build via convolutions in the Fourier domain

$$\widehat{k \star f}(l) = \hat{f}(l)\hat{k}^T(l)$$

In vectorized form this is simply a matrix vector multiplication

$$\mathrm{vec}(\widehat{k \star f})(l) = (\hat{w}(l) \otimes I)\,\mathrm{vec}(\hat{f}(l))$$

Spherical group convolutions in the Fourier domain

Spherical CNNs are build via convolutions in the Fourier domain

$$\widehat{k \star f}(l) = \hat{f}(l)\hat{k}^T(l)$$

Let us make it explicit and consider signals with only frequency $l = 1$.
Such signals are represented with 3-dimensional vectors.

$$\mathrm{vec}(\hat{f}) = \begin{pmatrix} \hat{f}_{:,-1} \\ \hat{f}_{:,0} \\ \hat{f}_{:,+1} \end{pmatrix}$$

Spherical group convolutions in the Fourier domain

Spherical CNNs are build via convolutions in the Fourier domain

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Let us make it explicit and consider signals with only frequency $l = 1$.
Such signals are represented with 3-dimensional vectors.

$$\mathrm{vec}(\hat{f}) = \begin{pmatrix} \color{red}{\hat{f}_{:,-1}} \\ \hat{f}_{:,0} \\ \color{red}{\hat{f}_{:,+1}} \end{pmatrix}$$

For S^2 signals: red=zero

Spherical group convolutions in the Fourier domain

Spherical CNNs are build via convolutions in the Fourier domain

$$\widehat{k \star f}(l) = \hat{f}(l)\hat{k}^T(l)$$

Let us make it explicit and consider signals with only frequency $l = 1$. Then

$$\begin{pmatrix} \widehat{k \star f}_{:,-1} \\ \widehat{k \star f}_{:,0} \\ \widehat{k \star f}_{:,+1} \end{pmatrix} = \begin{pmatrix} w_{-1,-1}I & w_{-1,0}I & w_{-1,1}I \\ w_{0,-1}I & w_{0,0}I & w_{0,1}I \\ w_{1,-1}I & w_{1,0}I & w_{1,1}I \end{pmatrix} \begin{pmatrix} \hat{f}_{:,-1} \\ \hat{f}_{:,0} \\ \hat{f}_{:,+1} \end{pmatrix}$$

Only three weights: the kernel is also a spherical harmonic!

Spherical group convolutions in the Fourier domain

Spherical CNNs are build via convolutions in the Fourier domain

$$\widehat{k \star f}(l) = \hat{f}(l)\hat{k}^T(l)$$

Let us make it explicit and consider signals with only frequency $l = 1$. Then

$$\begin{pmatrix} \widehat{k \star f}_{:,-1} \\ \widehat{k \star f}_{:,0} \\ \widehat{k \star f}_{:,+1} \end{pmatrix} = \begin{pmatrix} w_{-1,-1}I & w_{-1,0}I & w_{-1,1}I \\ w_{0,-1}I & w_{0,0}I & w_{0,1}I \\ w_{1,-1}I & w_{1,0}I & w_{1,1}I \end{pmatrix} \begin{pmatrix} \hat{f}_{:,-1} \\ \hat{f}_{:,0} \\ \hat{f}_{:,+1} \end{pmatrix}$$

If we want the output to be a SH, only 1 weight can be non-zero!

Spherical group convolutions in the Fourier domain

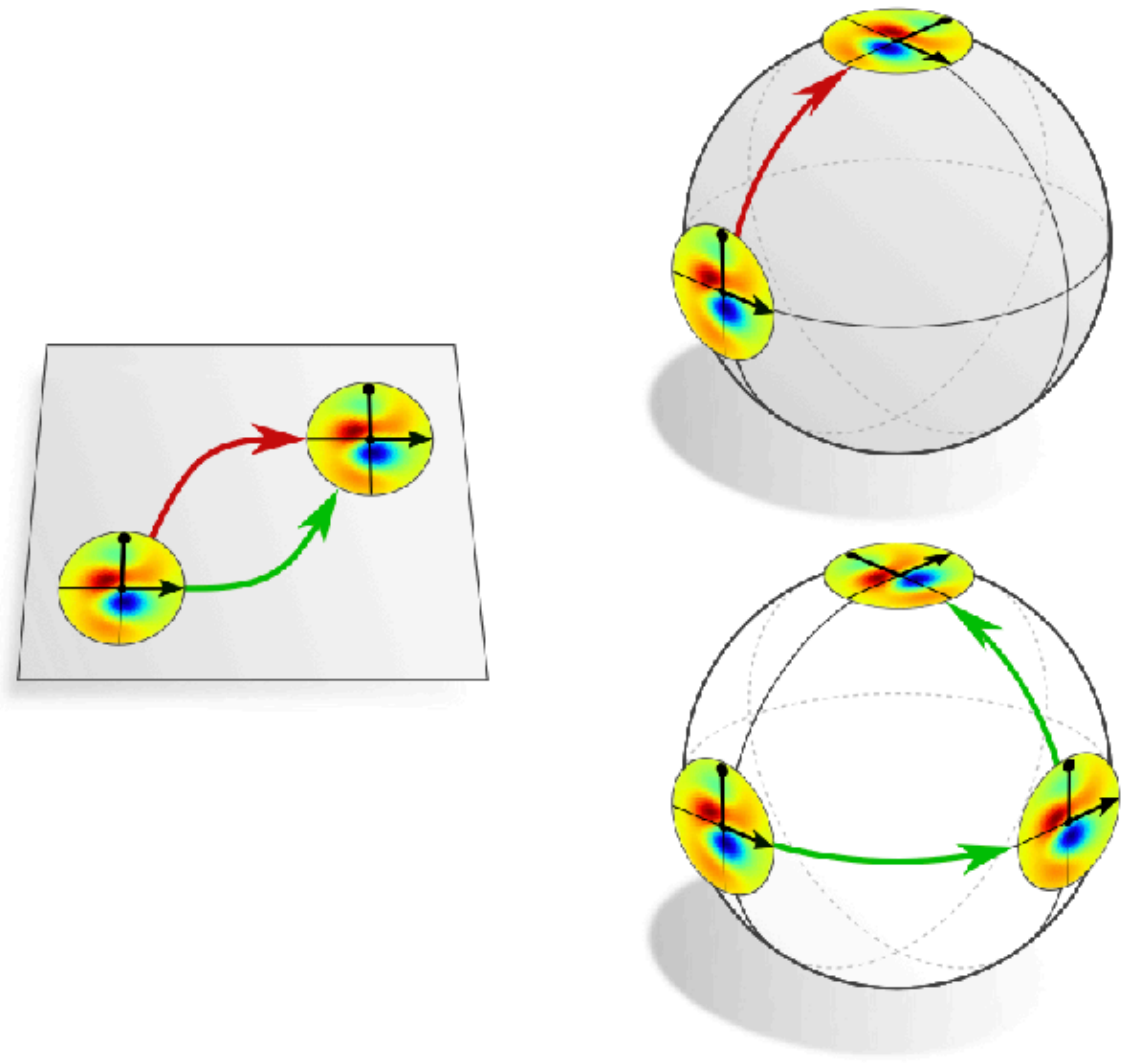


Figure from COORDINATE INDEPENDENT CONVOLUTIONAL NETWORKS, Weiler, Forré, Verlinde, Welling

Lemma 5.1. Consider the cases of $SO(3)$ equivariant linear layers for signals on $X = S^2 \equiv SO(3)/SO(2)$ or $X = SO(3)$. Such convolutions can be performed via the Fourier transform on $SO(3)$

$$\widehat{k \star f}(l) = \hat{f}(l)\hat{w}^T(l)\,,$$

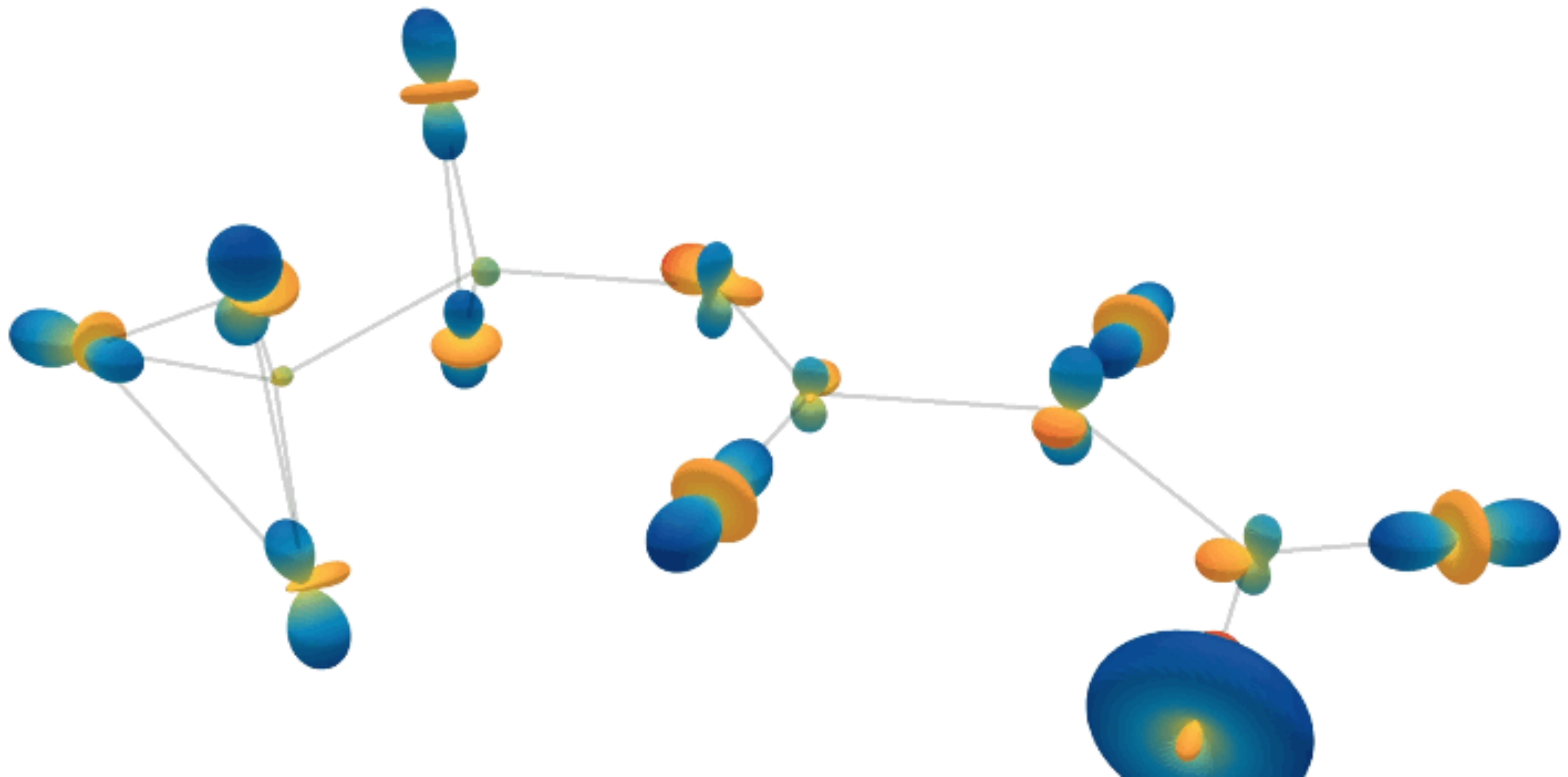
with $\hat{w}(l) \in \mathbb{R}^{2l+1 \times 2l_1}$ the learnable parameters of the convolution kernel. The following can be said about the parametrization of the kernels through $\hat{w}$.

- **Isotropic S^2 kernel convolutions** ($X = Y = S^2$) For isotropic kernel convolutions the kernel is parametrized by a single weight per frequency l. Namely the only possibly non-zero component is $\hat{w}_{00}(l)$ and all others have to be 0. This means that the kernels represent signals on the sphere S^2 that are symmetry around the $\mathbf{n}_x$ axis, as required by Theorem 3.2.
- **Lifting convolutions** ($X = S^2$, $Y = SO(3)$) For lifting convolutions the kernel is parametrized by $(2l+1)$ learnable weights per frequency l. The only possible non-zero weights are $\hat{w}_{:,0}$, i.e., the central column $(n = 0)$ of $\hat{w}(l)$. This means that the convolution kernels are unconstrained signals on the sphere S^2.
- **Group convolution** ($X = Y = SO(3)$) Group convolutions are parametrized by $(2l+1) \times (2l+1)$ learnable weights per frequency l. The kernels represent unconstrained functions on $SO(3)$.

Steerable Neural Networks

Method 2: Clebsch-Gordan tensor product ($SE(3)$ gconvs)

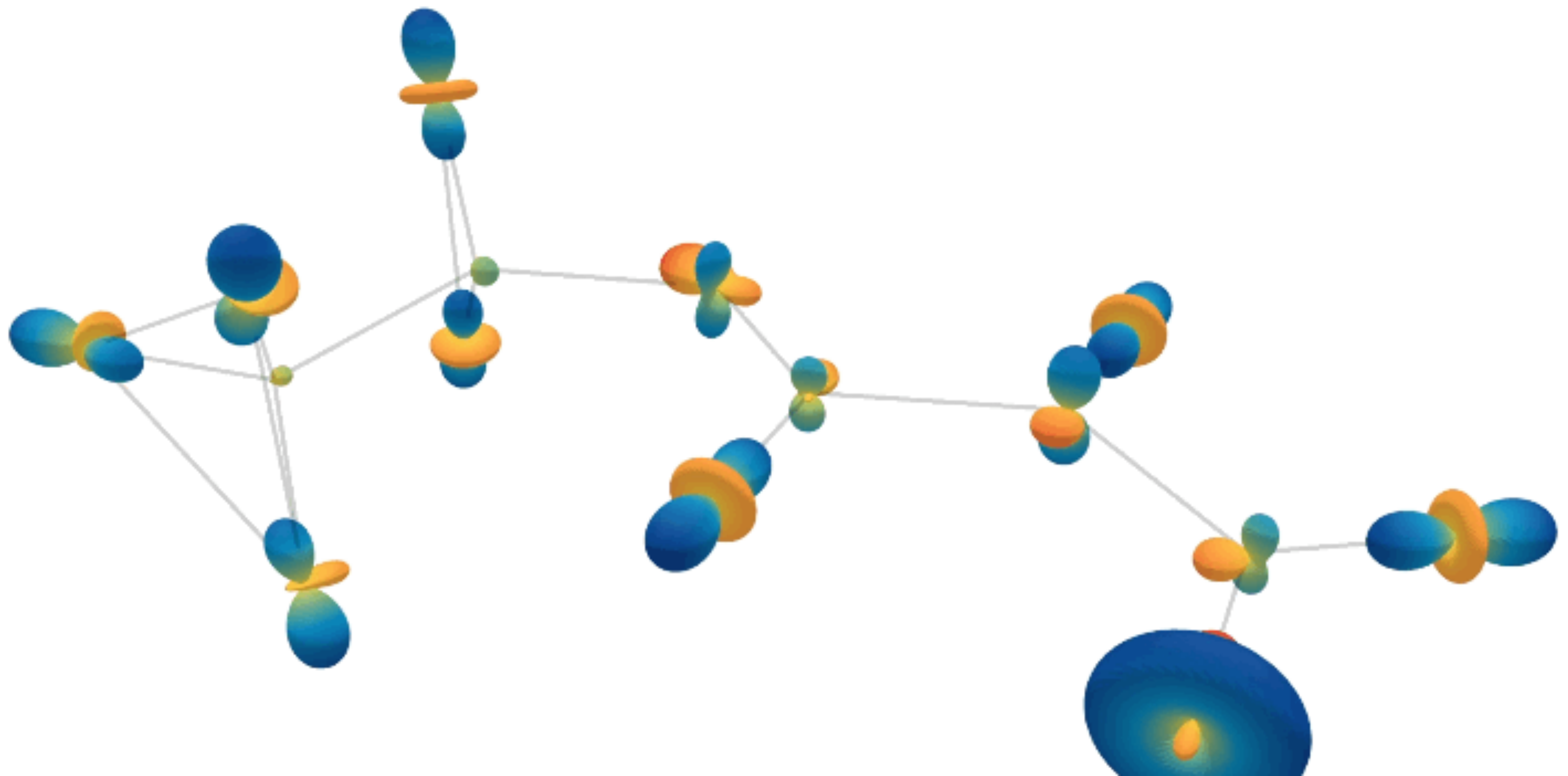
Lecture notes Section 5.2



Steerable Neural Networks

Method 2: Clebsch-Gordan tensor product $(SE(3)$ gconvs)

Lecture notes Section 5.2



Steerable Neural Networks

Steerable group convolutions

$$\tilde{\mathbf{f}}'(\mathbf{x}) = \int_{\mathbb{R}^3} \tilde{\mathbf{f}}(\mathbf{x}) \otimes_{cg}^{w(\|\mathbf{x}\|)} \underline{Y}^{(l)}\left(\frac{\mathbf{x}'-\mathbf{x}}{\|\mathbf{x}'-\mathbf{x}\|}\right) \mathrm{d}\mathbf{x}'$$

$\Leftrightarrow$

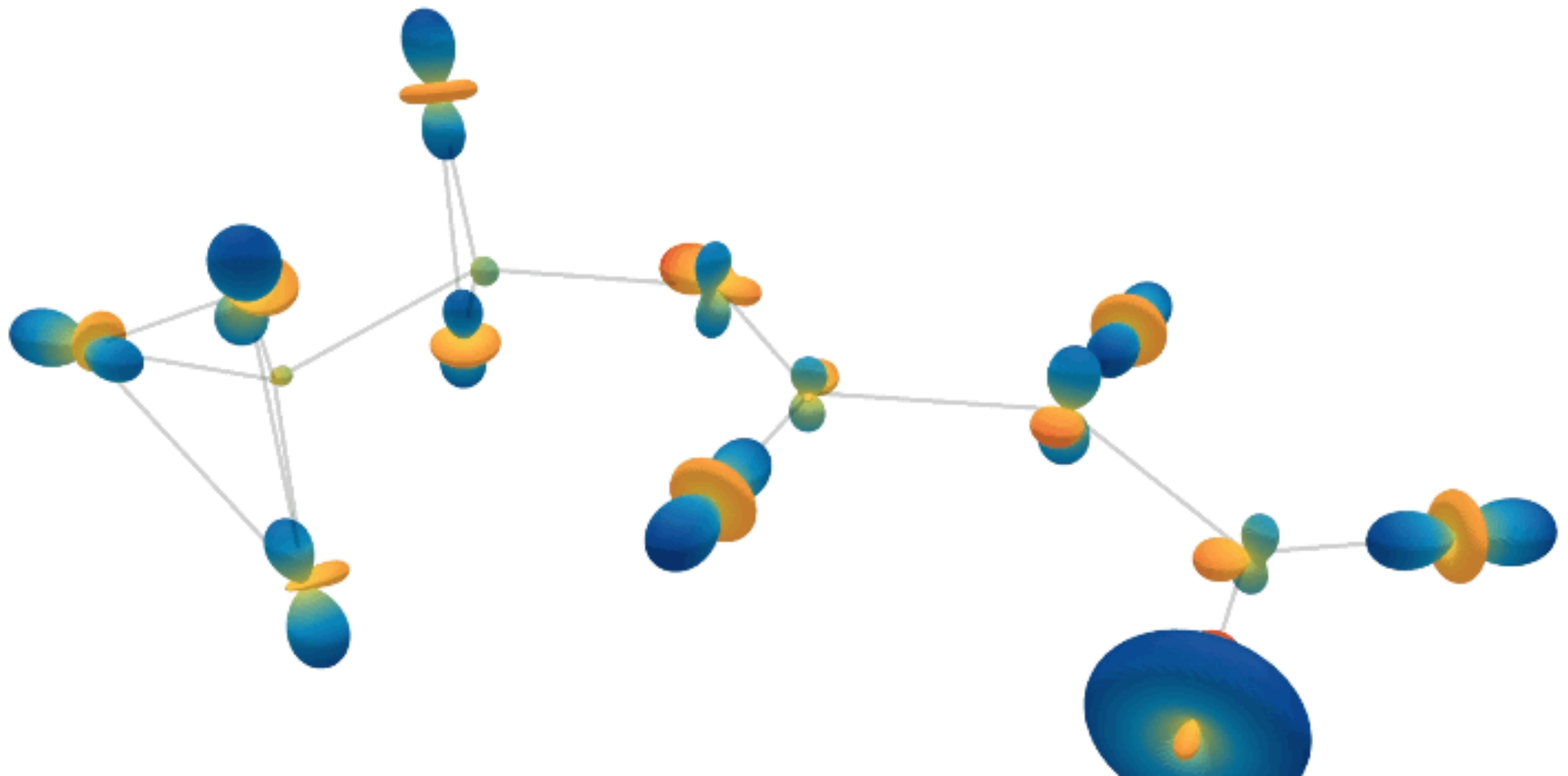
Regular group convolutions

$$f'(\mathbf{x},\mathbf{R}) = \iint_{\mathbb{R}^3 \times SO(3)} k(\mathbf{R}^{-1}(\mathbf{x}'-\mathbf{x}), \mathbf{R}^{-1}\mathbf{R}'))f(\mathbf{x}',\mathbf{R}')))\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{R}'$$

with $$k(\mathbf{x}) = \sum_{l}^{L} \sum_{m=-l}^{l} \tilde{\mathbf{w}}_m^{(l)}(\|\mathbf{x}\|) Y_m^{(l)}\left(\frac{\mathbf{x}}{\|\mathbf{x}\|}\right)$$

Method 2: Clebsch-Gordan tensor product $\qquad$ ($SE(3)$ gconvs)

Lecture notes Section 5.2



Steerable Neural Networks

Steerable group convolutions

$$\tilde{\mathbf{f}}'(\mathbf{x}) = \int_{\mathbb{R}^3} \tilde{\mathbf{f}}(\mathbf{x}) \otimes_{cg}^{w(\|\mathbf{x}\|)} \underline{Y}^{(l)} \left(\frac{\mathbf{x}'-\mathbf{x}}{\|\mathbf{x}'-\mathbf{x}\|} \right) d\mathbf{x}'$$

$\Leftrightarrow$

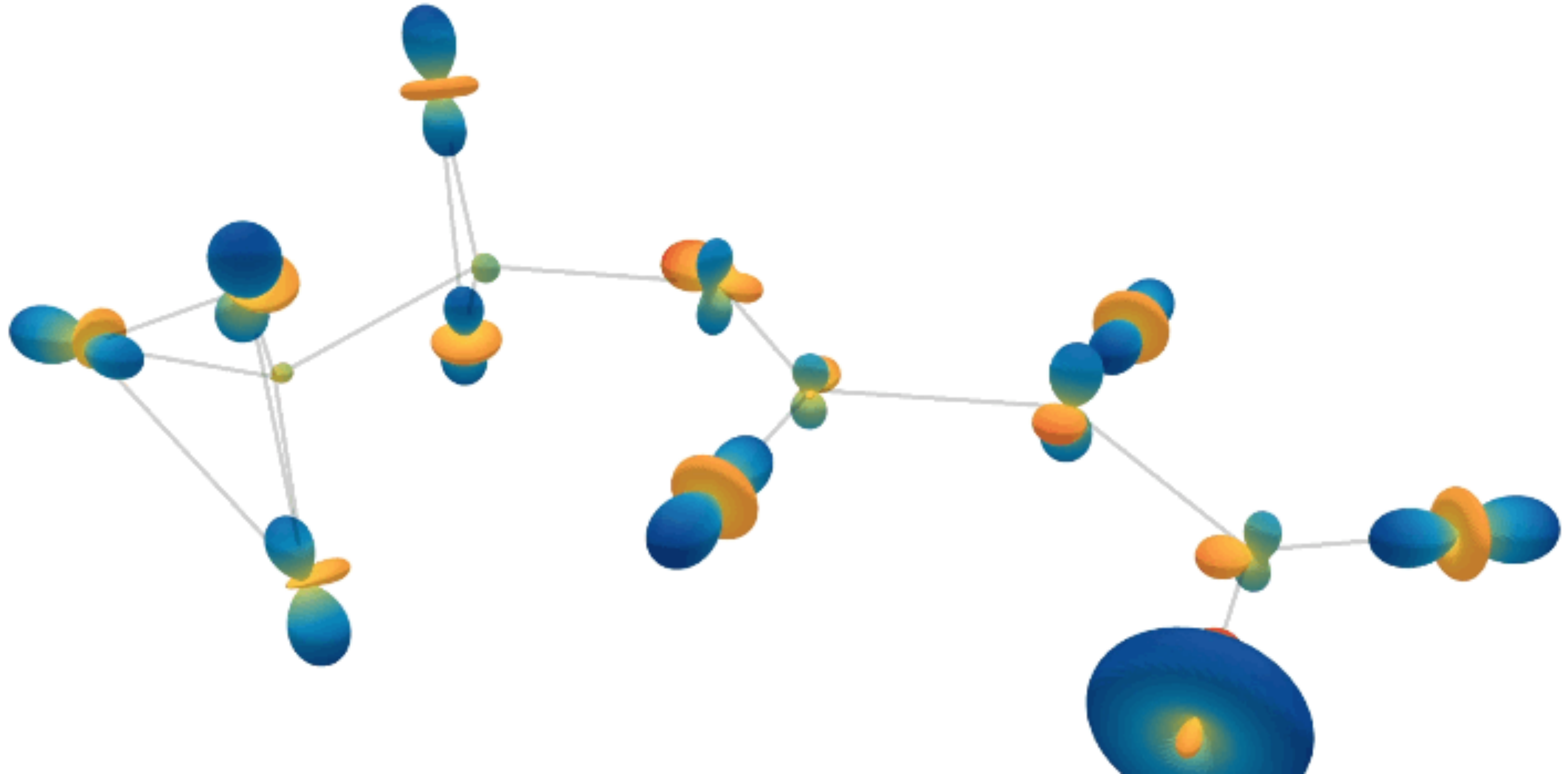
Regular group convolutions

$$f'(\mathbf{x}, \mathbf{R}) = \iint_{\mathbb{R}^3 \times SO(3)} k(\mathbf{R}^{-1}(\mathbf{x}'-\mathbf{x}), \mathbf{R}^{-1}\mathbf{R}')) f(\mathbf{x}', \mathbf{R}'))) d\mathbf{x}' d\mathbf{R}'$$

with $$k(\mathbf{x}) = \sum_{l}^{L} \sum_{m=-l}^{l} \tilde{\mathbf{w}}_m^{(l)}(\|\mathbf{x}\|) Y_m^{(l)} \left(\frac{\mathbf{x}}{\|\mathbf{x}\|} \right)$$

Method 2: Clebsch-Gordan tensor product ($SE(3)$ gconvs)

Lecture notes Section 5.2



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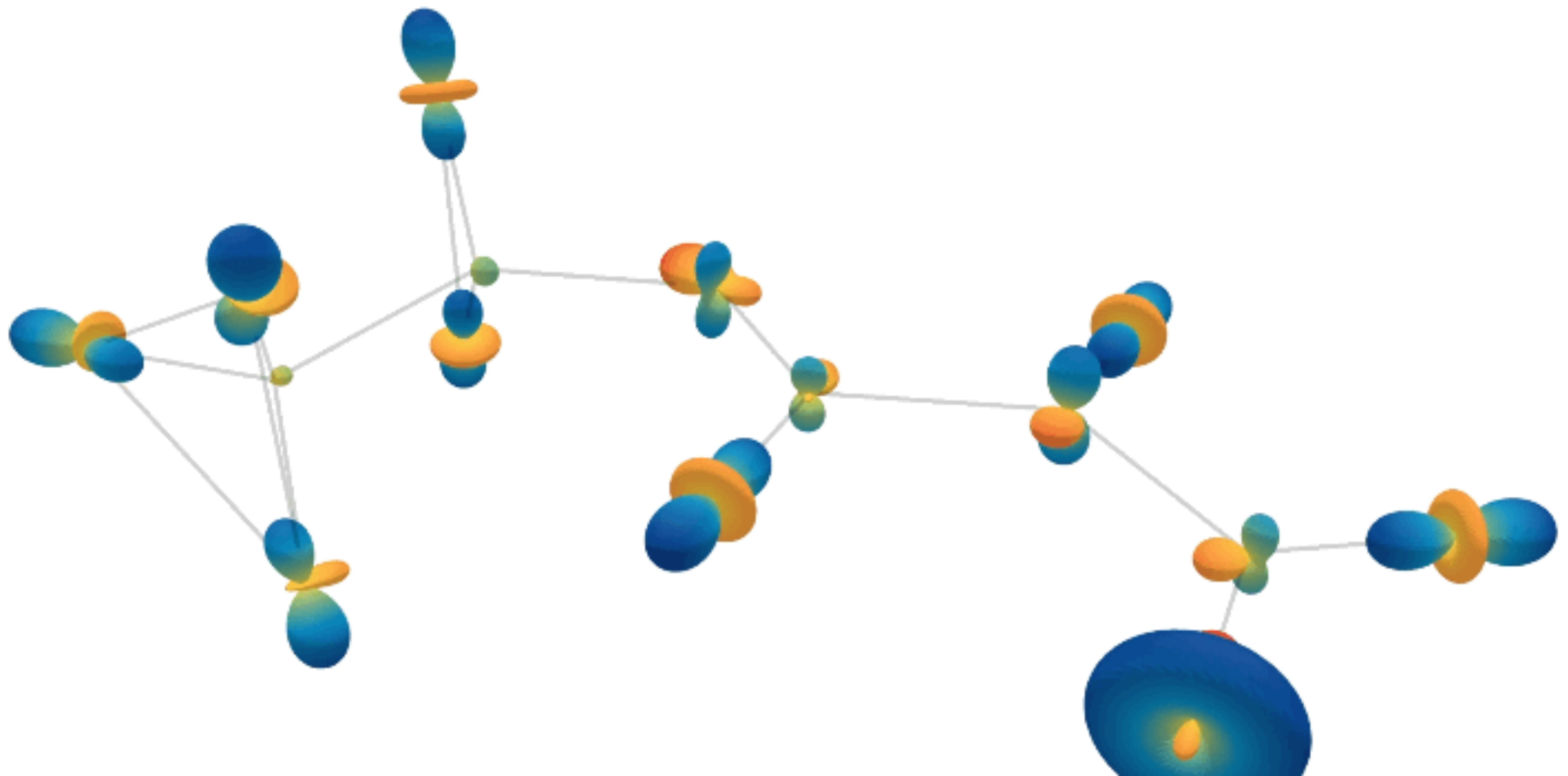
Lecture notes Section 5.2



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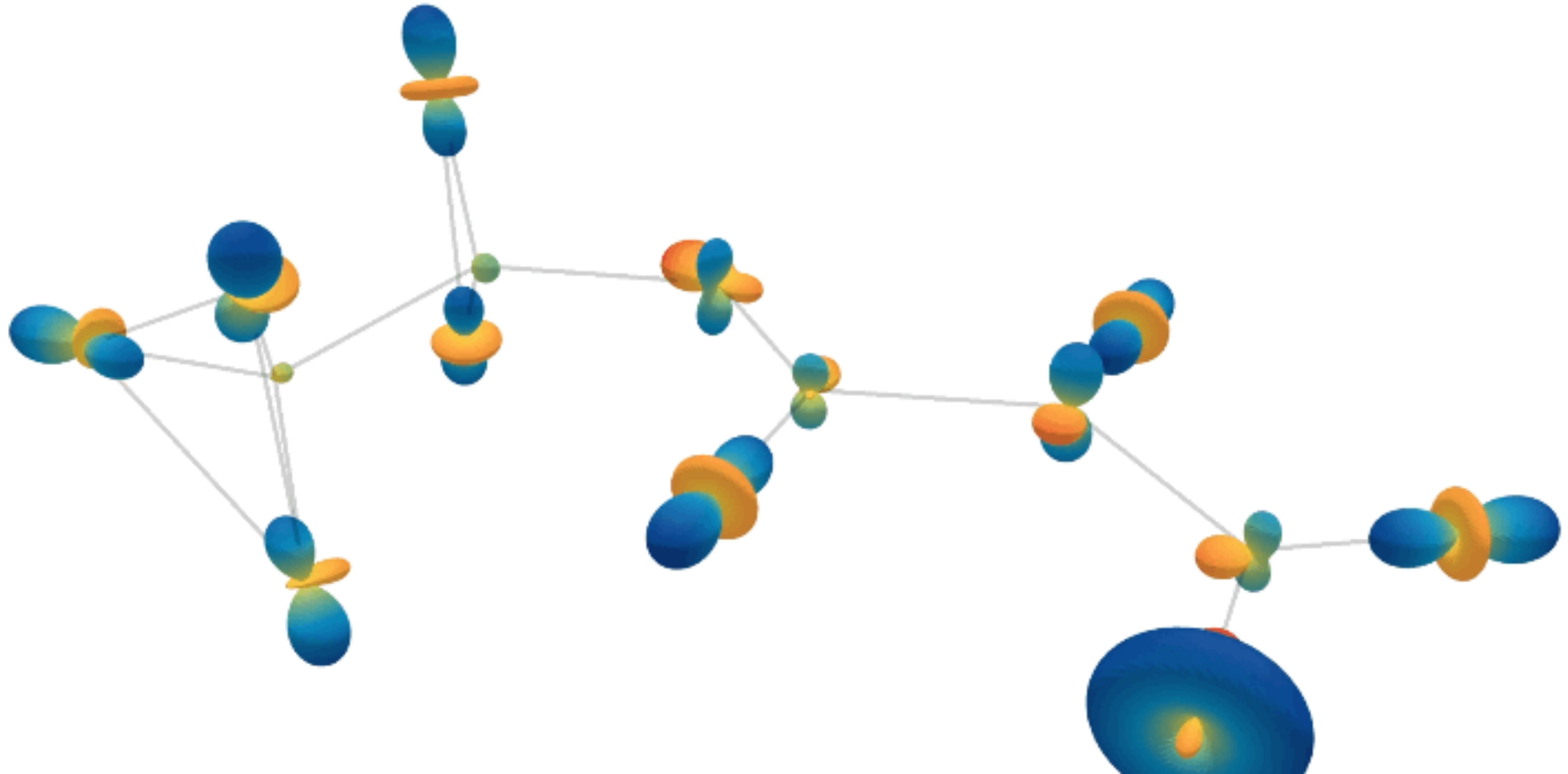
($SE(3)$ gconvs)

Lecture notes Section 5.2



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Angular part of k

$\Leftrightarrow$

Regular group convolutions

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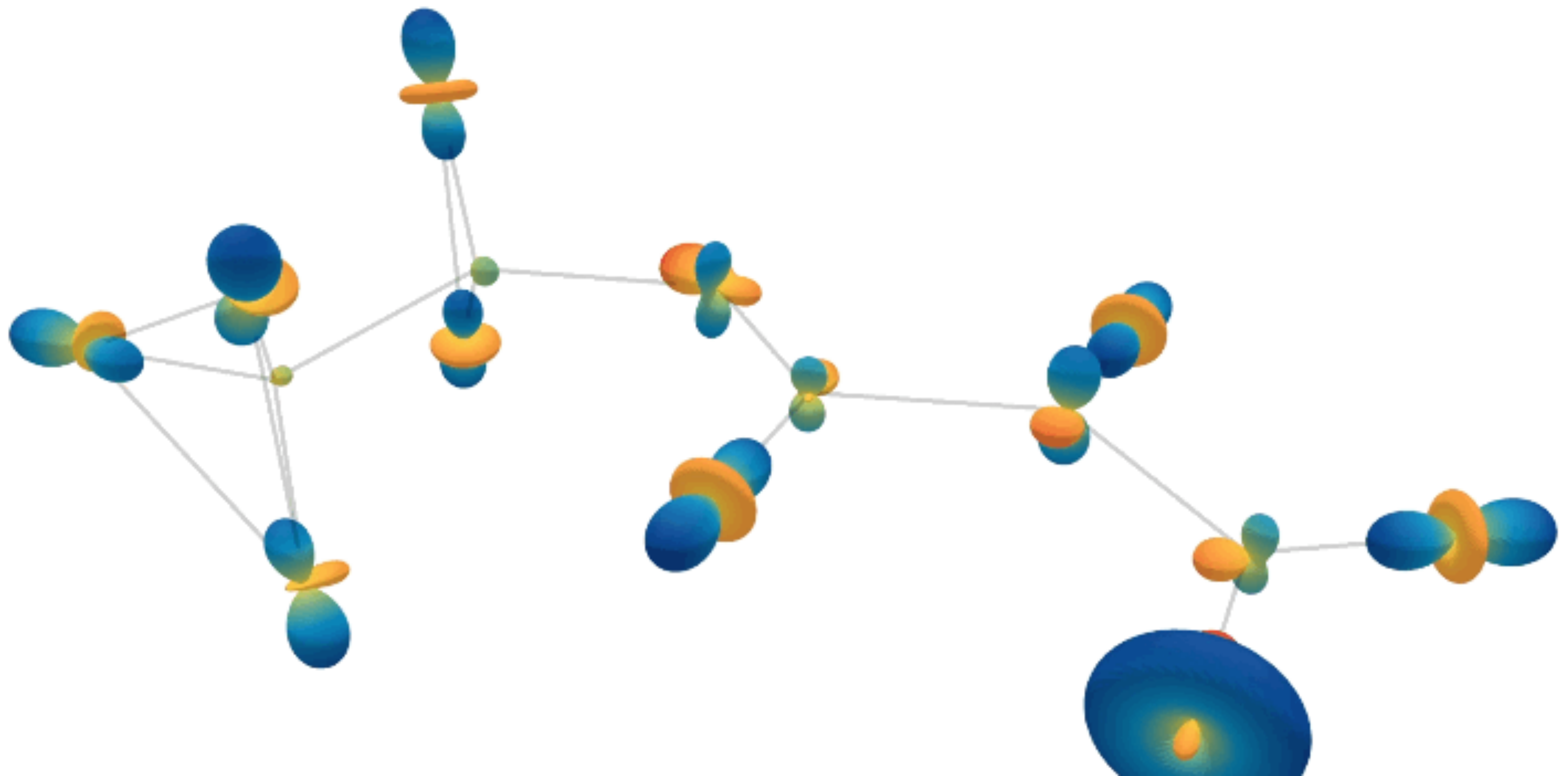
Lecture notes Section 5.2



Steerable Neural Networks

Steerable group convolutions

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Angular part of k Spatial part of k

$\Leftrightarrow$

Regular group convolutions

$$f'(\mathbf{x},\mathbf{R}) = \iint_{\mathbb{R}^3 \times SO(3)} k(\mathbf{R}^{-1}(\mathbf{x}'-\mathbf{x}), \mathbf{R}^{-1}\mathbf{R}')) f(\mathbf{x}',\mathbf{R}'))) \mathrm{d}\mathbf{x}' \mathrm{d}\mathbf{R}'$$

with $k(\mathbf{x}) = \sum_{l}^{L} \sum_{m=-l}^{l} \tilde{\mathbf{w}}_m^{(l)}(\|\mathbf{x}\|) Y_m^{(l)}\left(\frac{\mathbf{x}}{\|\mathbf{x}\|}\right)$

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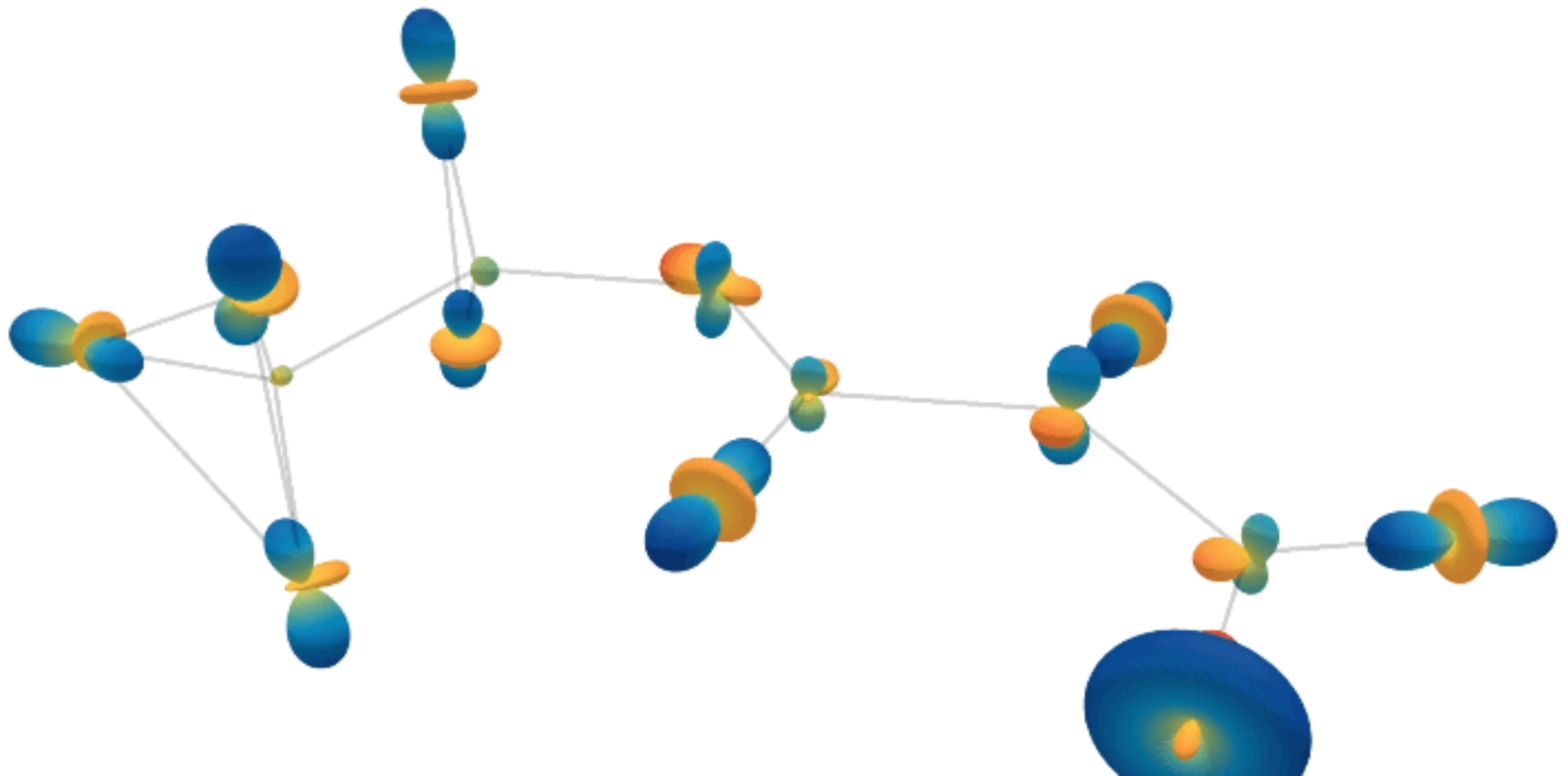
Lecture notes Section 5.2



Steerable Neural Networks

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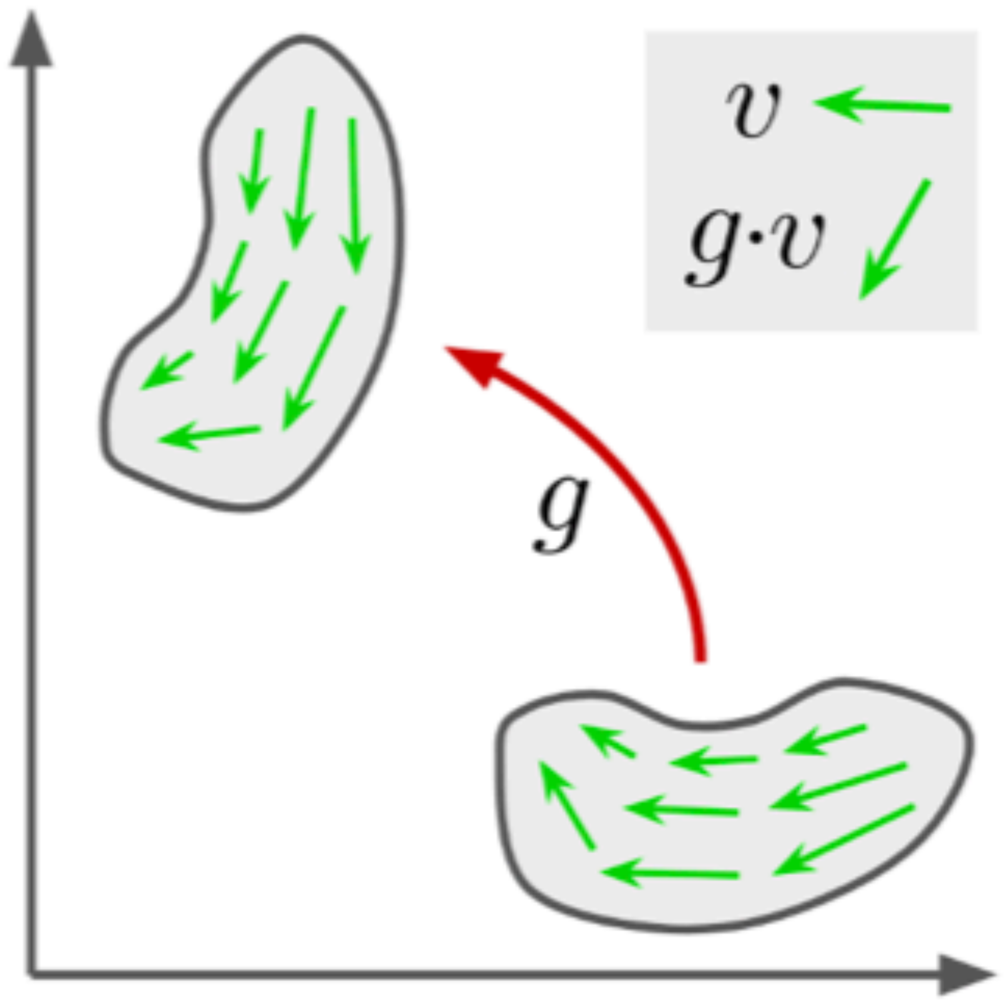
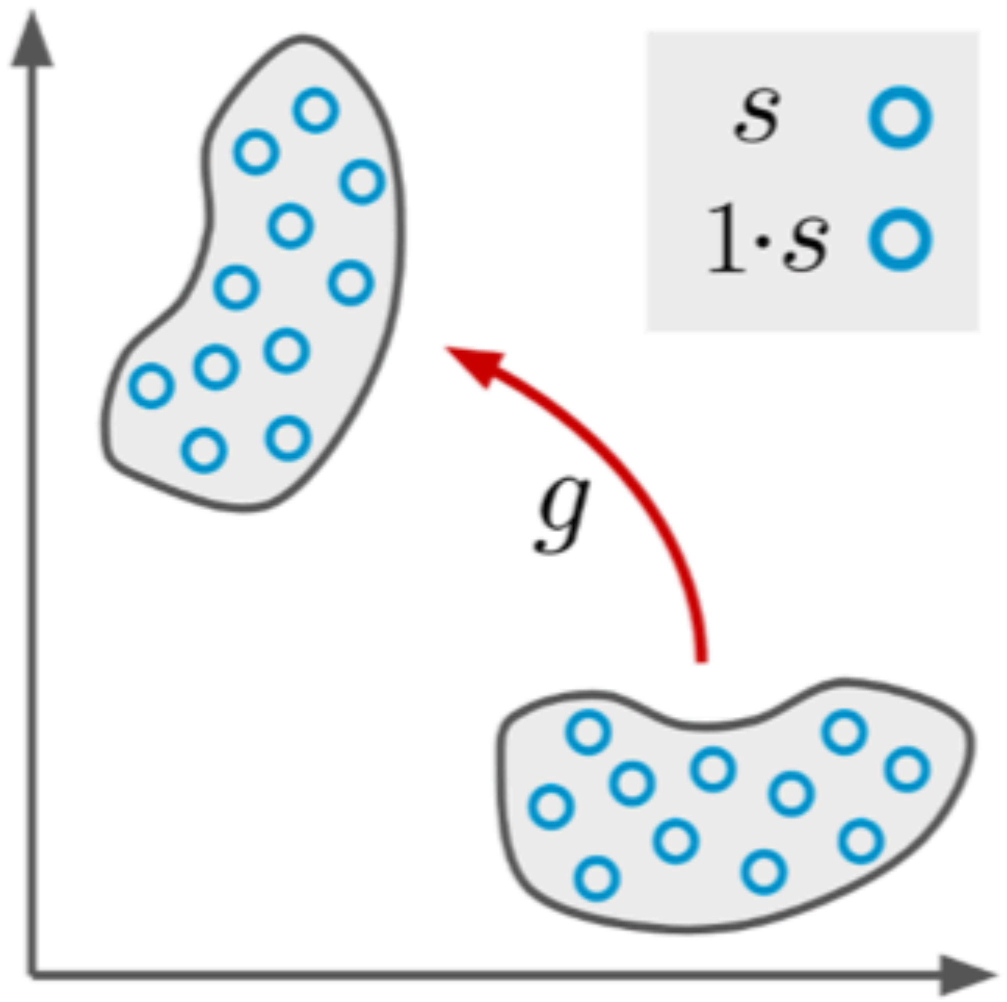
Feature maps: $f : \mathbb{R}^3 \rightarrow V_0 \oplus V_1 \oplus \ldots$

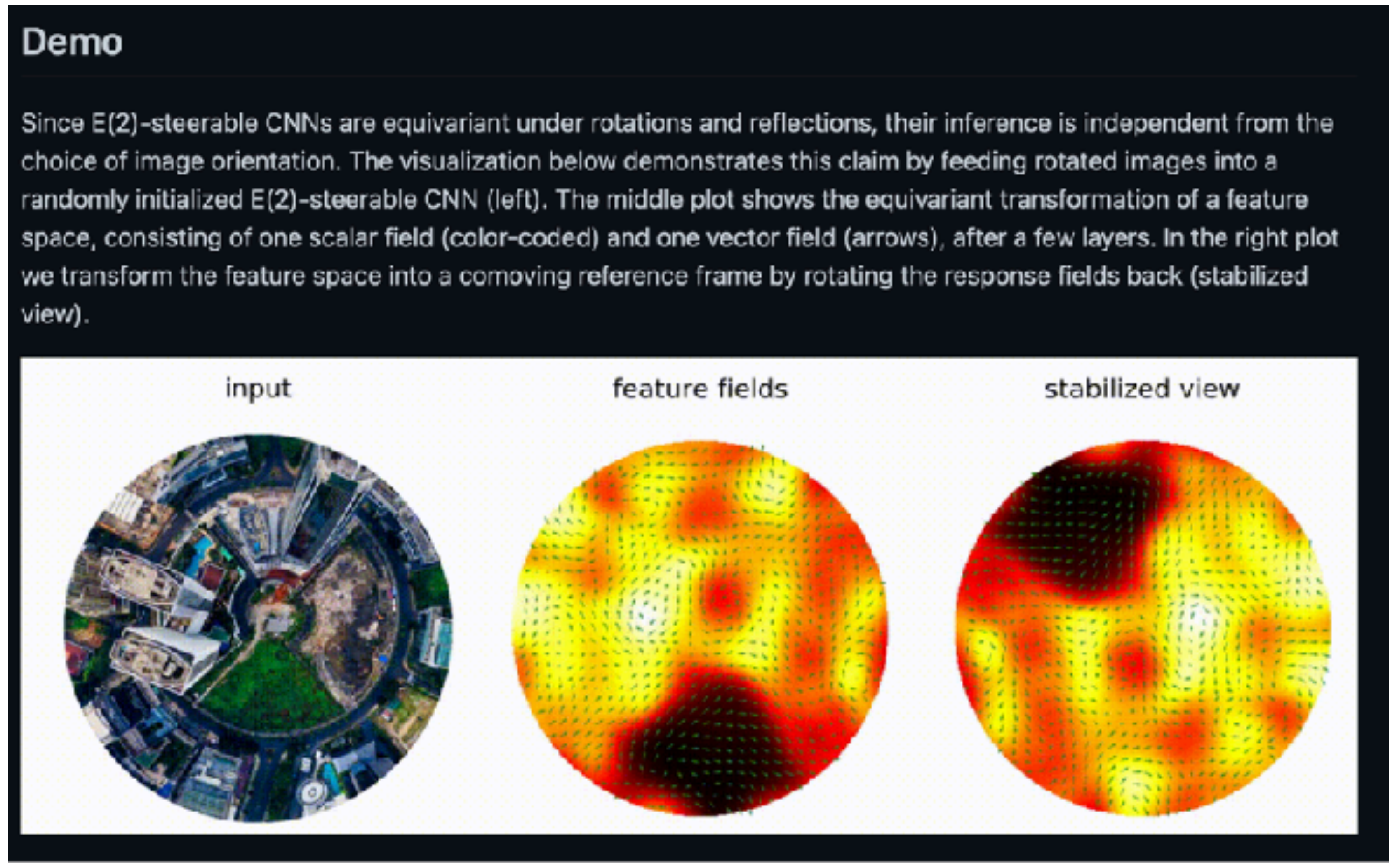


Feature maps: $f : \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R}$



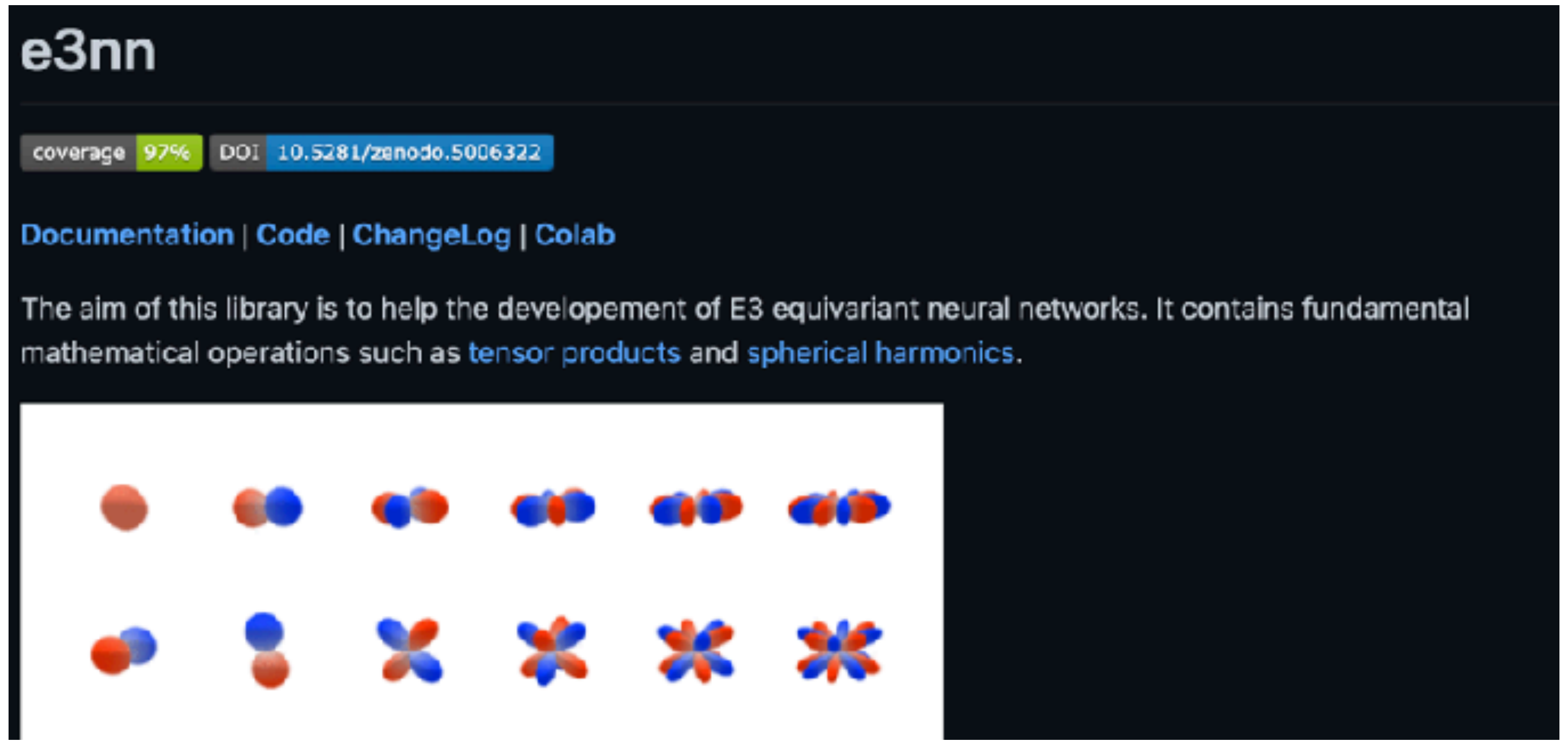
Figures: https://github.com/QUVA-Lab/e2cnn

Libraries and repositories



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

e3nn: https://github.com/e3nn/e3nn



e3cnn (released soon)

Conclusion

Conclusion

- **G-CNNs naturally arise** from NNs under equivariance constraints
- **G-CNNs improve upon classic CNNs** by
  - Making data augmentation w.r.t. the group obsolete
  - No valuable network capacity needs to be spend on dealing w geometry
  - The added geometric structure allows to deal with context (recognition by components, relative poses)
  - The added geometric structure enables to reach performances that cannot be achieved with data augmentation alone
  - Have guaranteed geometric stability
  - Can be applied to many types of signal data (not covered today: equivariance to Lie groups and gauge equivariant methods