UNIVERSITY OF AMSTERDAM

AMLAB Amsterdam Machine Learning Lab

Introduction to group equivariant deep learning

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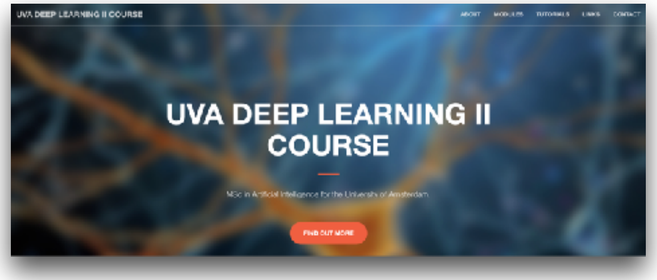
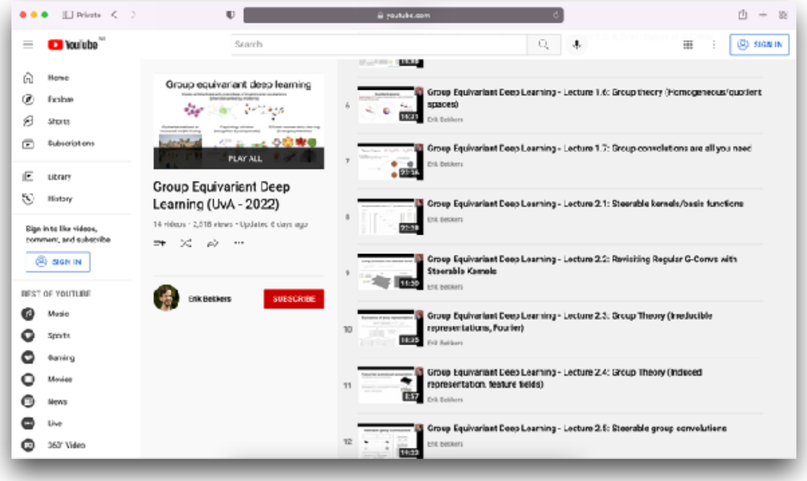
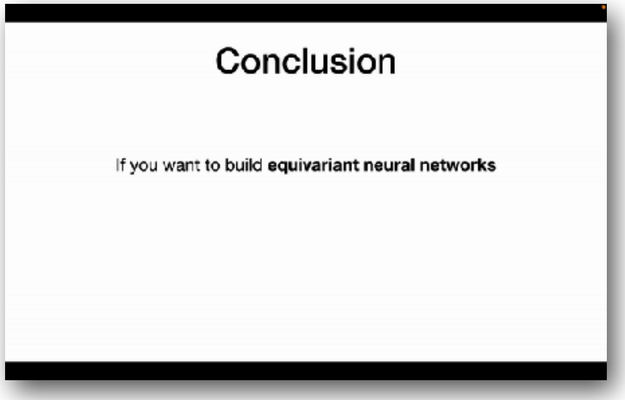
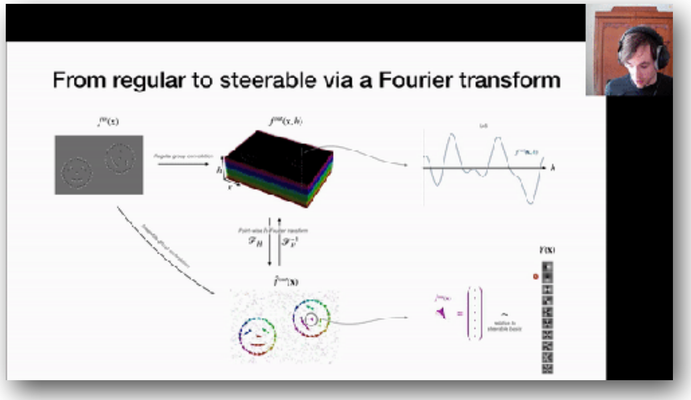
UvA course on group equivariant deep learning (https://uvagedl.github.io)



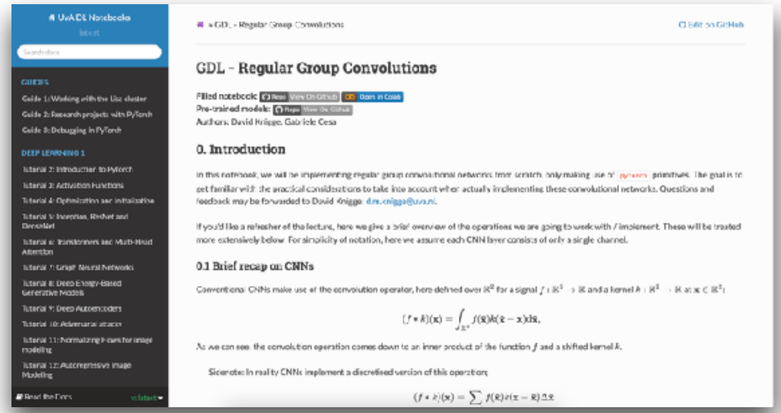
Youtube playlist

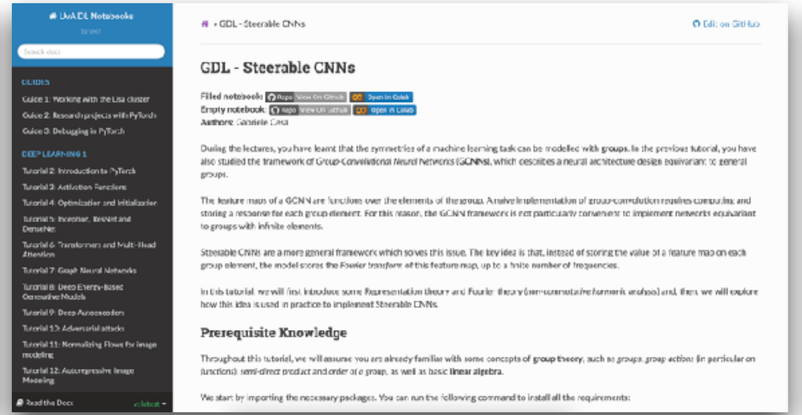


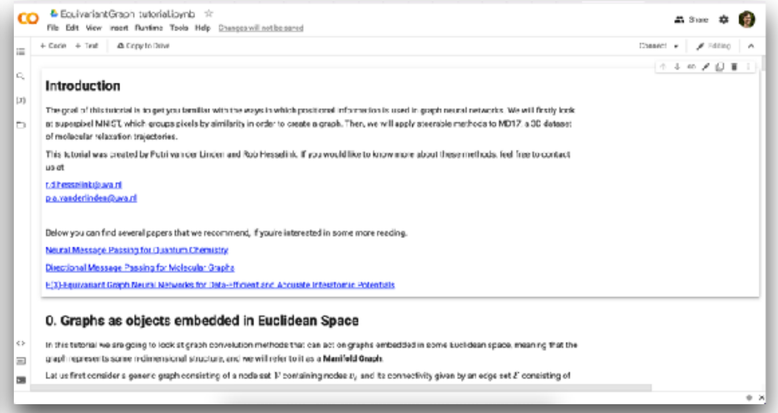




Tutorial notebooks







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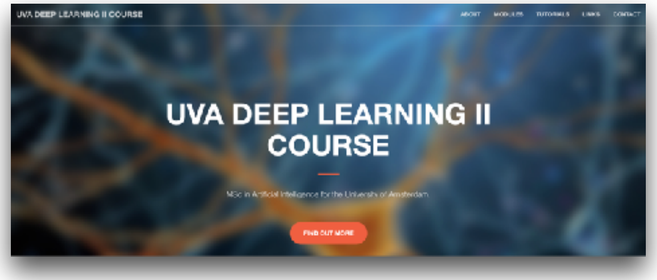

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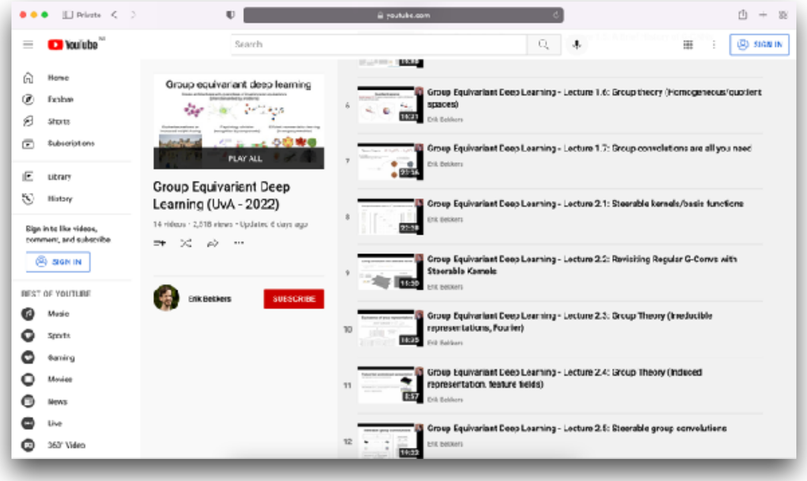

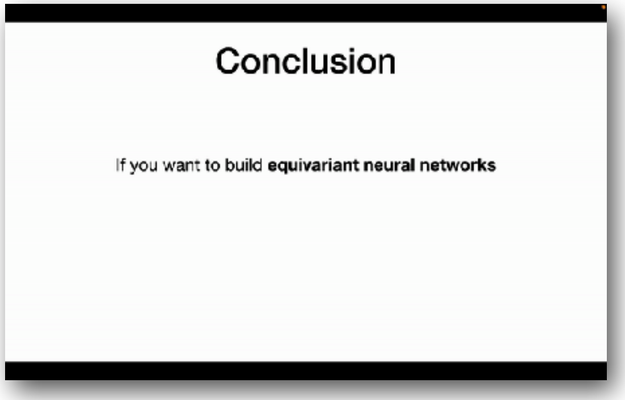

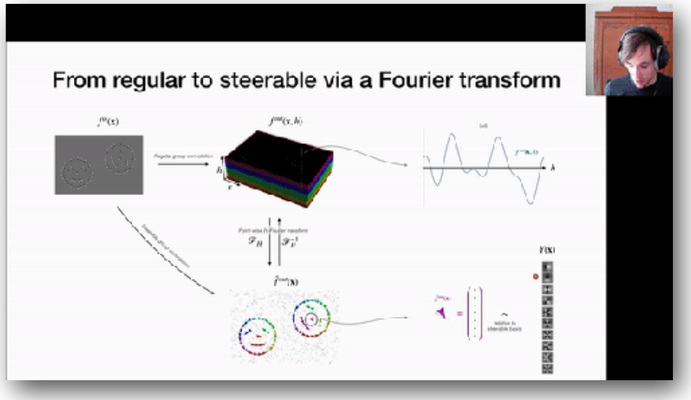

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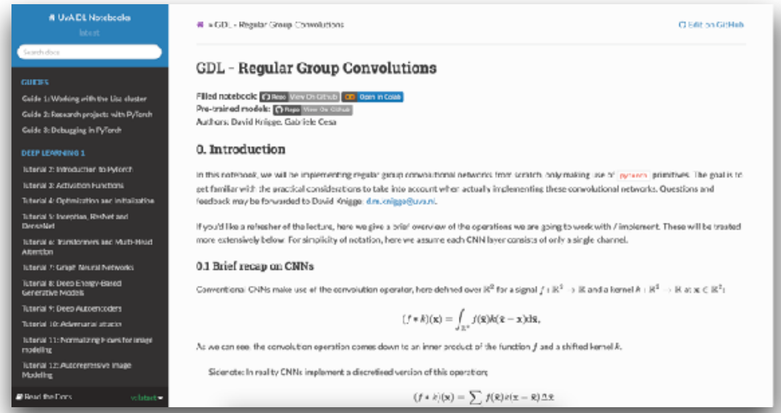

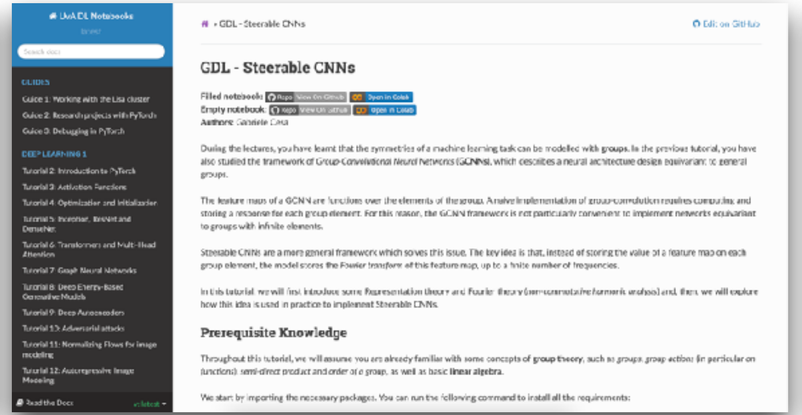

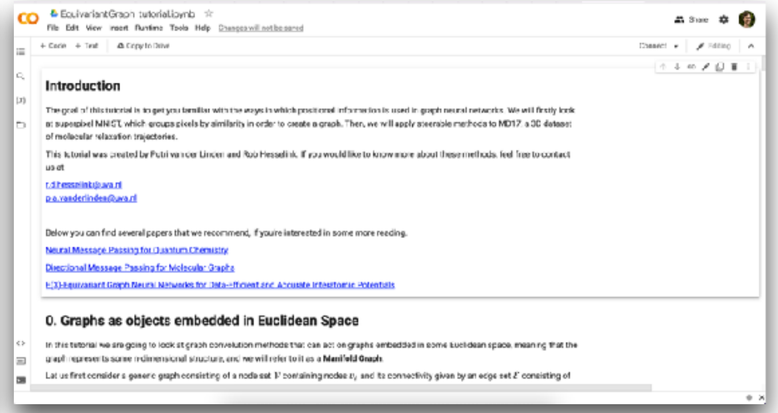

1. Motivation

2. Pattern matching using group theory

3. Group convolutions

4. Example

5. G-convs are all you need!

6. Steerable group convolutions

7. Feature fields and escnn library

8. Equivariant tensor product layers

9. Equivariant graph NNs

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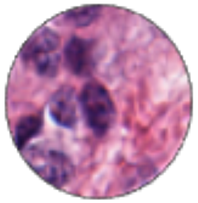
Geometric guarantees (invariance)

Example: Detection of pathological cells



Geometric guarantees (invariance)

Example: Detection of pathological cells

Healthy

?

Geometric guarantees (invariance)

Example: Detection of pathological cells

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Pathological

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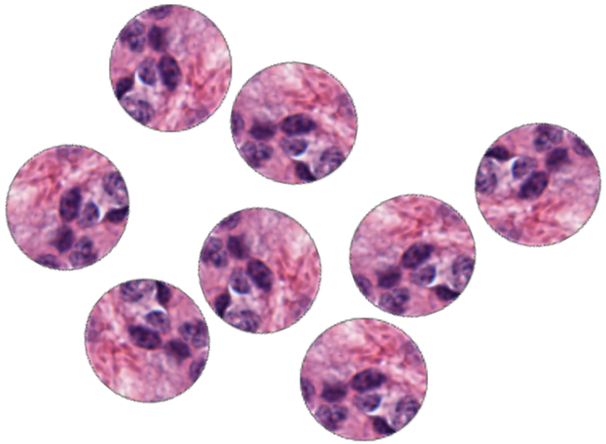
Pathological

Common approach: data-augmentation



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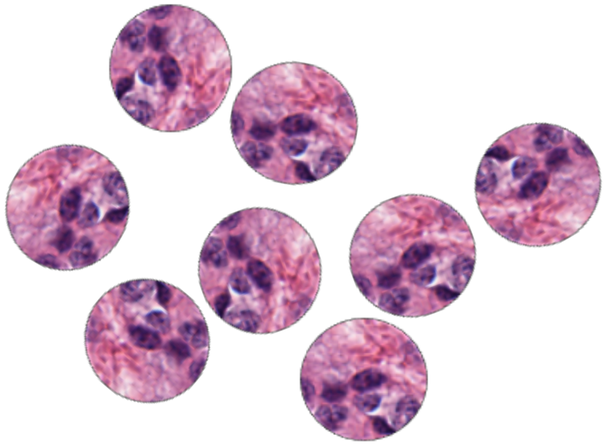

Issues:

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

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

Naturally Occurring Equivariance in Neural Networks

AUTHORS	AFFILIATIONS
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Gabriel Goh	OpenAI

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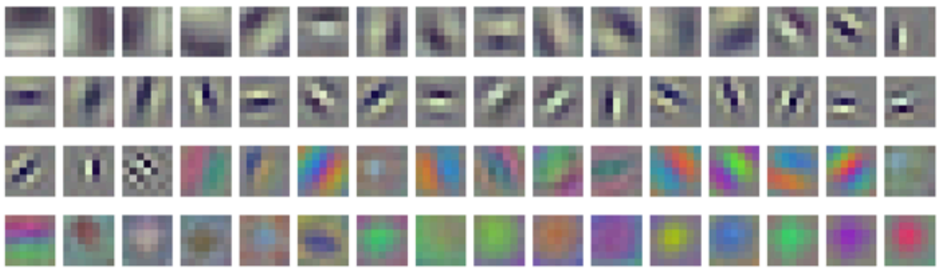
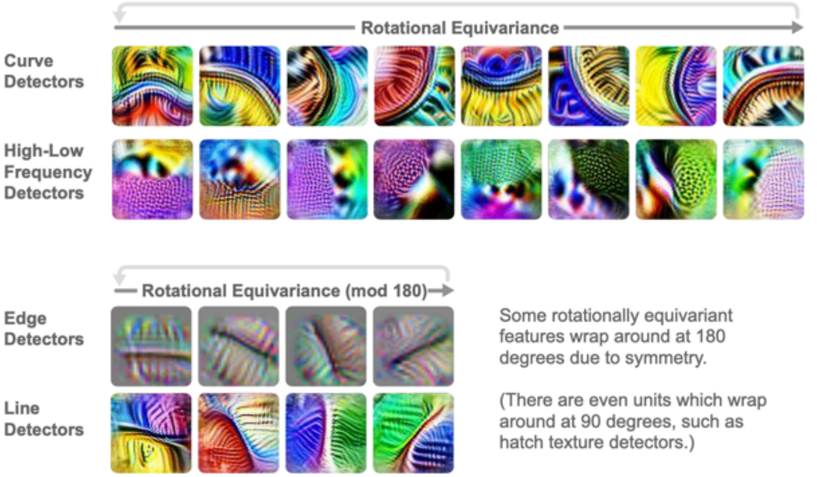


The weights for the units in the first layer of the TF-Slim [11] version of InceptionV1 [8].[5] Units are sorted by the first principal component of the adjacency matrix between the first and second layers. Note how many features are similar except for rotation, scale, and hue.

Equivariant Features

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



Geometric guarantees (equivariance)

CNNs are translation equivariant

Via convolutions

Geometric guarantees (equivariance)

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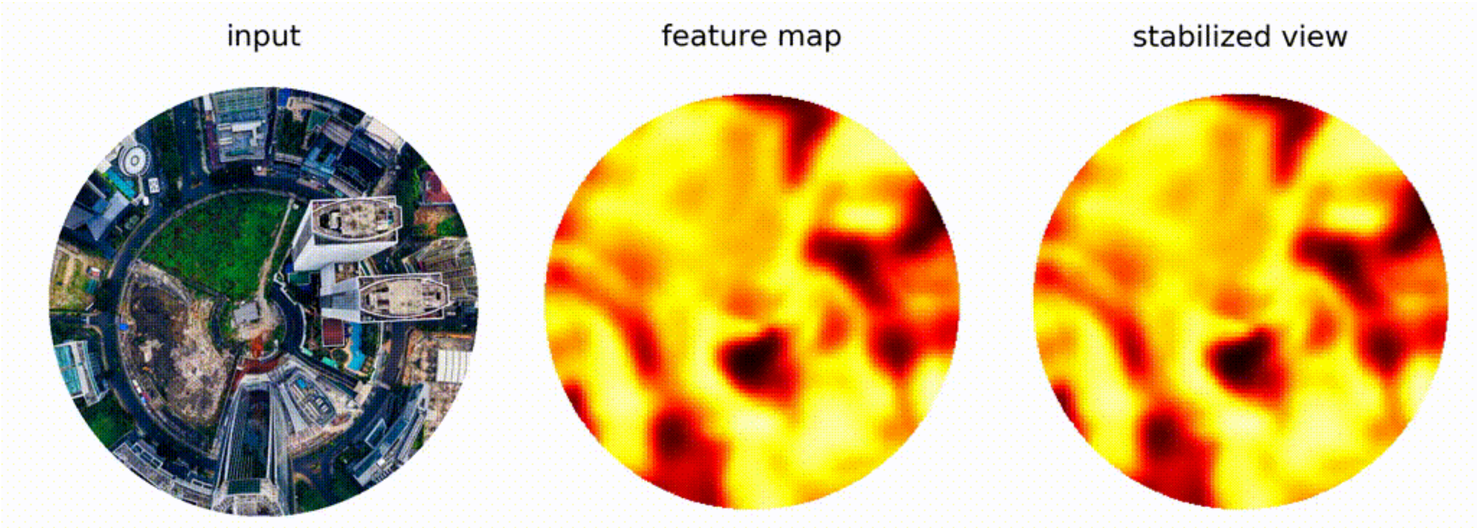
Geometric guarantees (equivariance)

Normal CNN



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

Geometric guarantees (equivariance)

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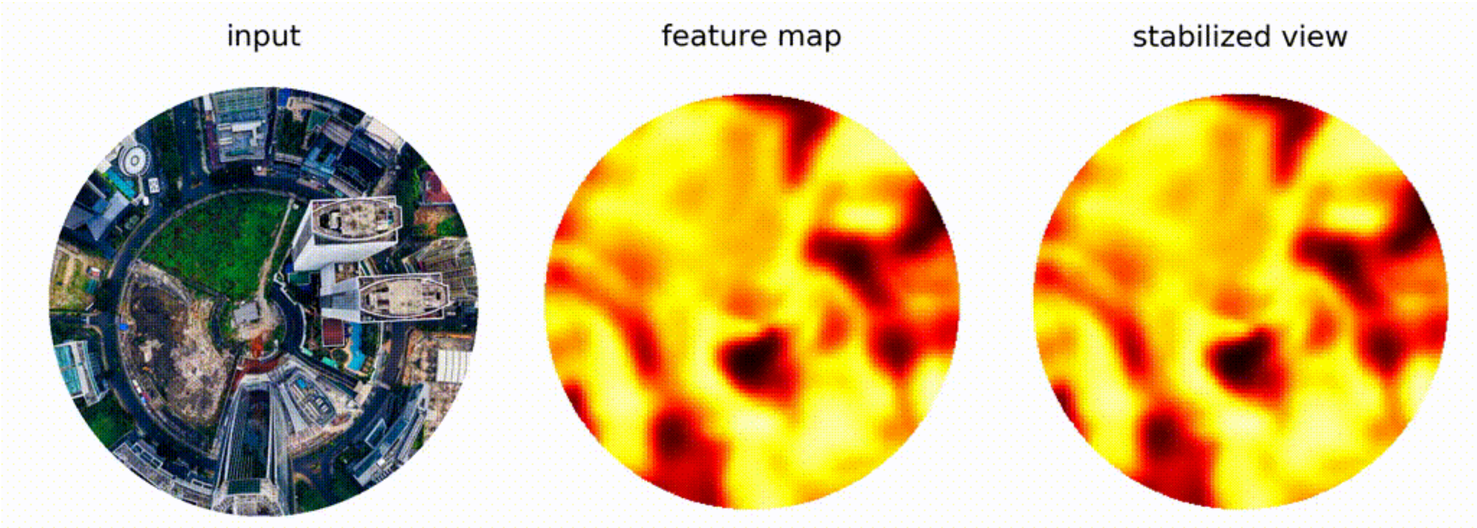

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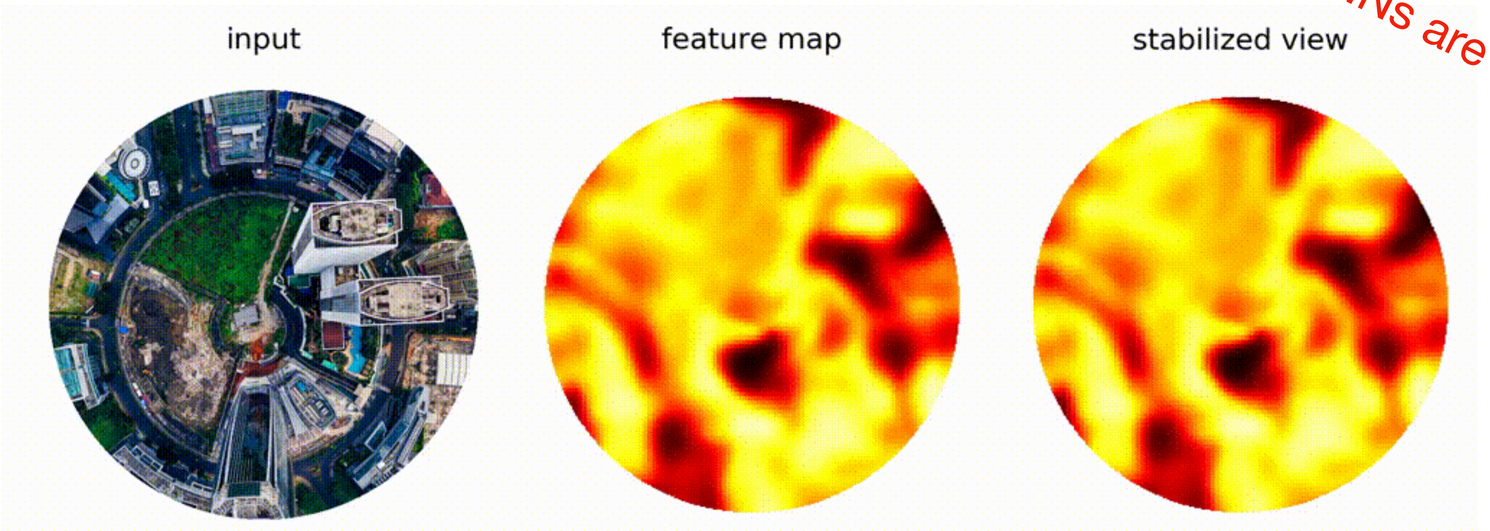

CNNs are not rotation equivariant

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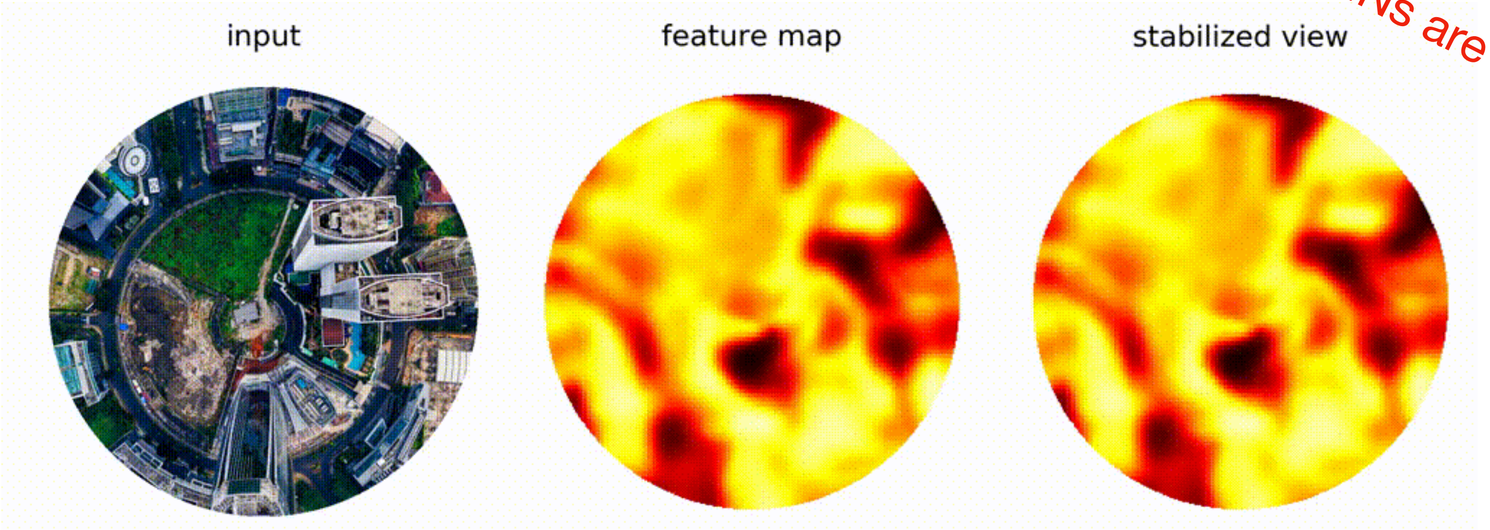
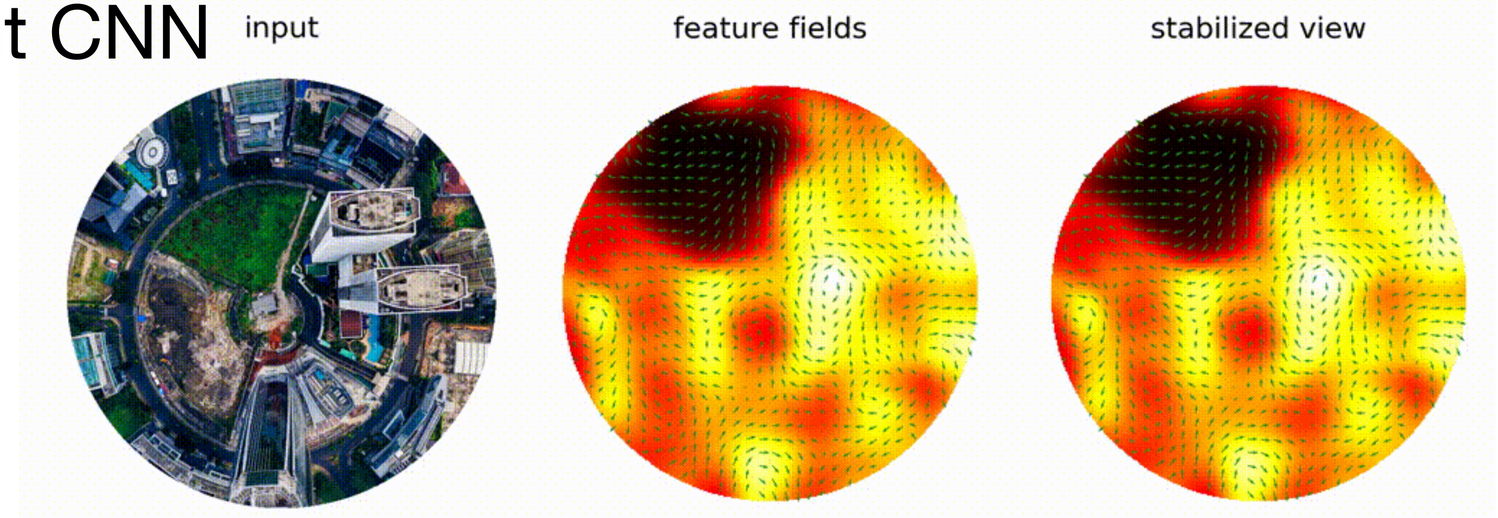


CNNs are not rotation equivariant

Group equivariant CNN



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Geometric guarantees (equivariance)

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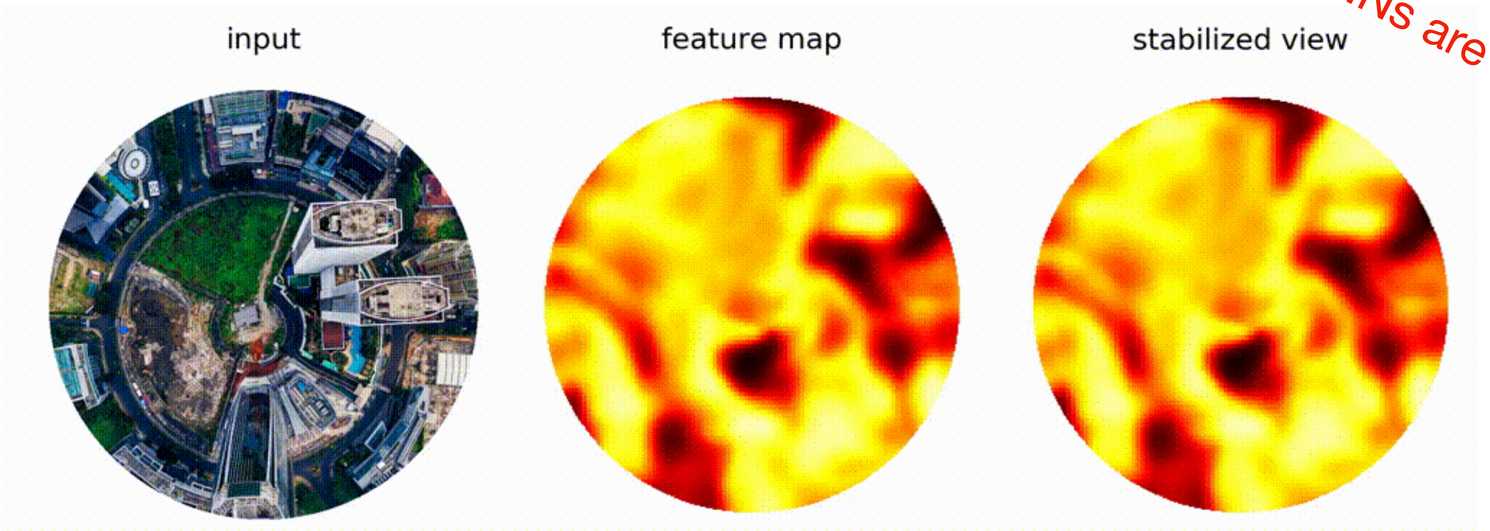
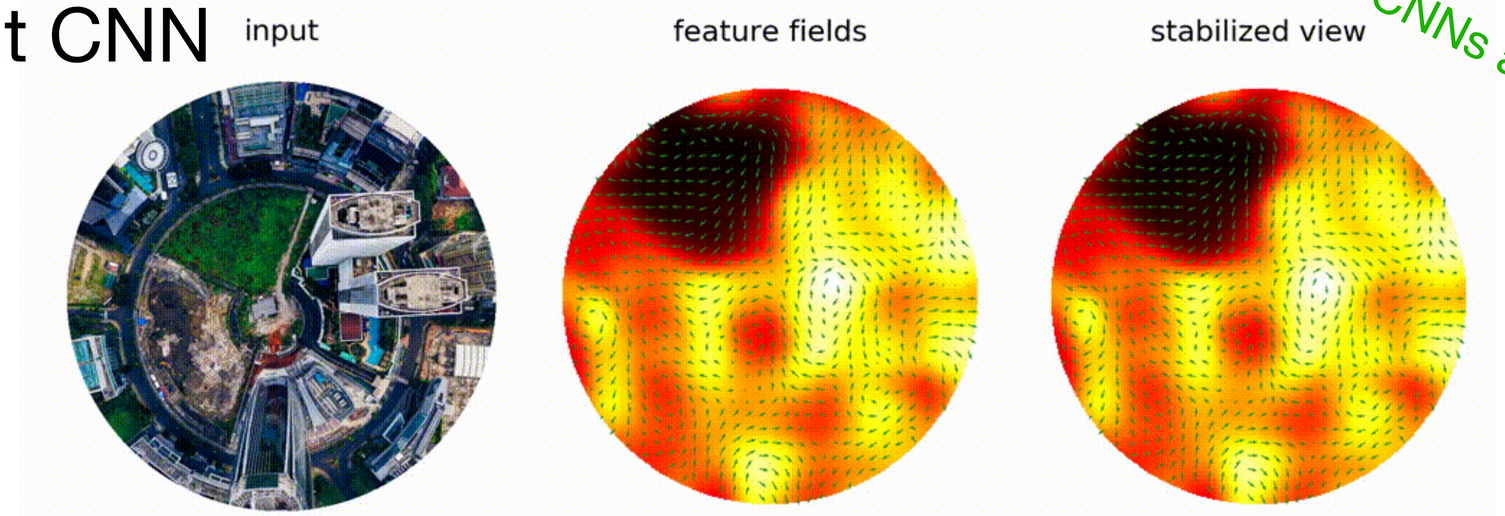


CNNs are not rotation equivariant

Group equivariant CNN



G-CNNs are rotation equivariant!

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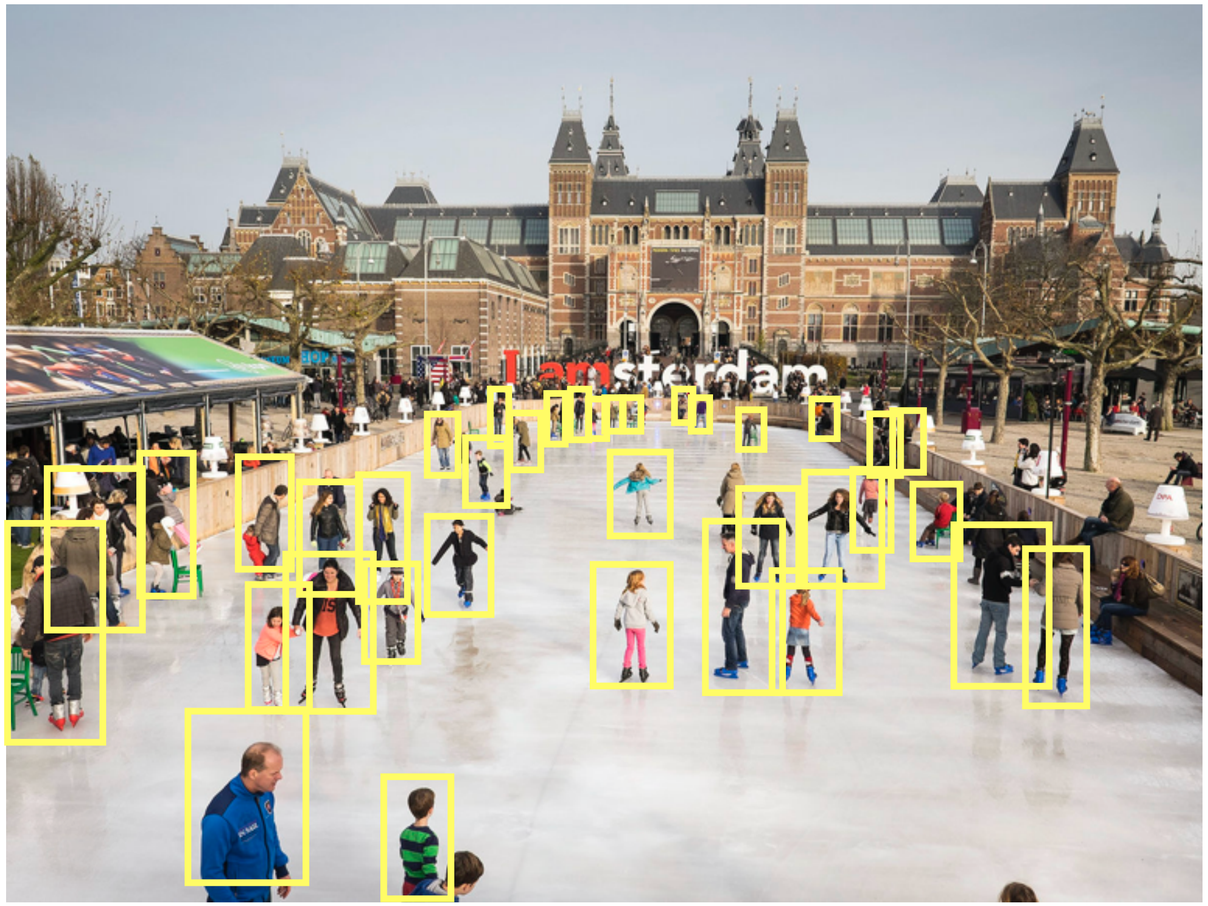
Geometric guarantees (equivariance)



Importance of equivariance:

- No information is lost when the input is transformed

- Guaranteed stability to (local + global) transformations

Group convolutions:

- Equivariance beyond translations

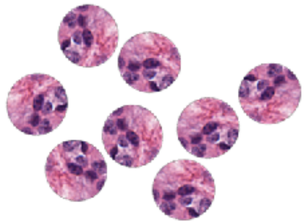
- Geometric guarantees

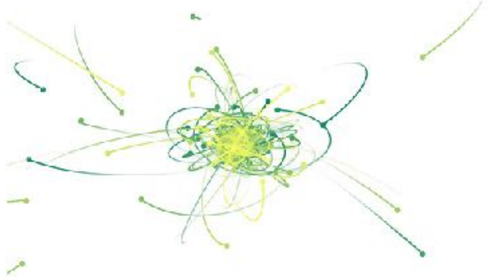
- Increased weight sharing

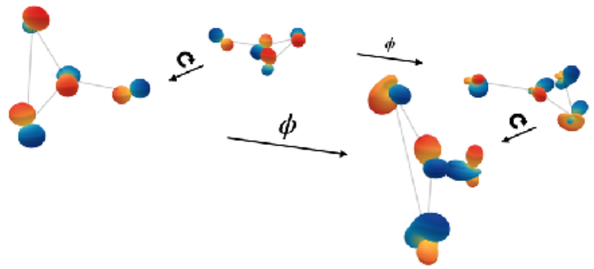
G-CNNs are not only relevant for invariant problems but for any type of structured data!

Group equivariant deep learning

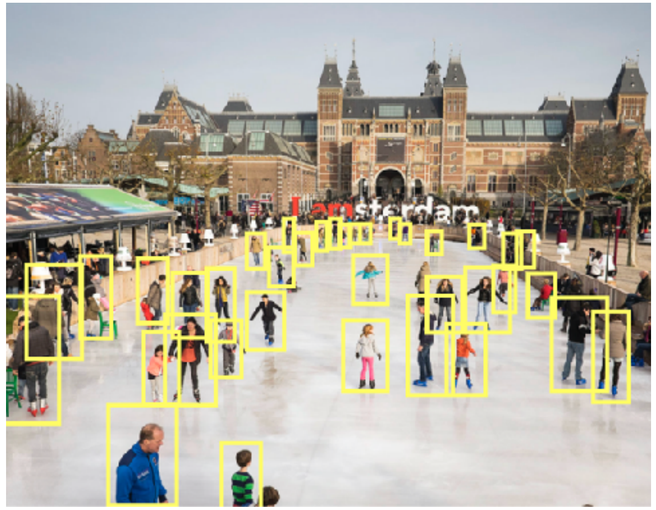
Create architectures with guarantees of invariance or equivariance
(often demanded by problems)



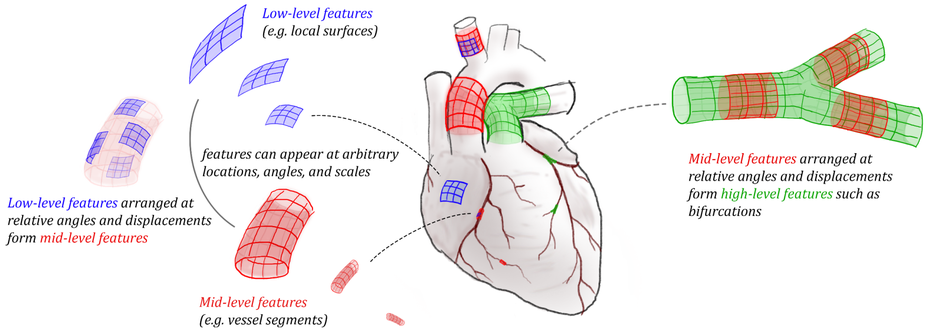




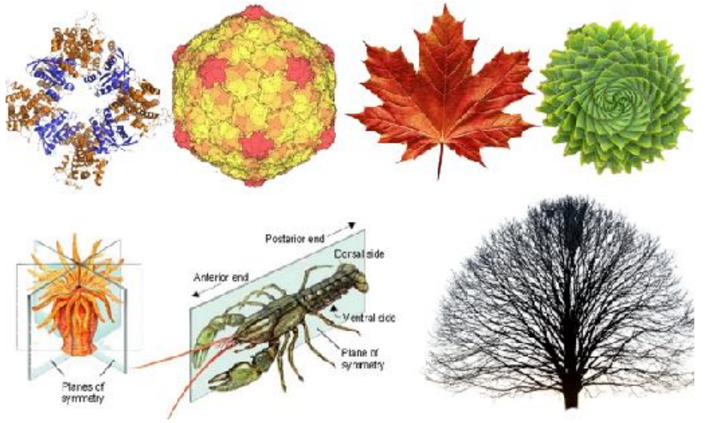
Equivariance allows for increased weight sharing



Psychology of vision (recognition by components)



Efficient representation learning (leverage symmetries)



1. Motivation — Equivariance → weight-sharing and generalization

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3. Group convolutions

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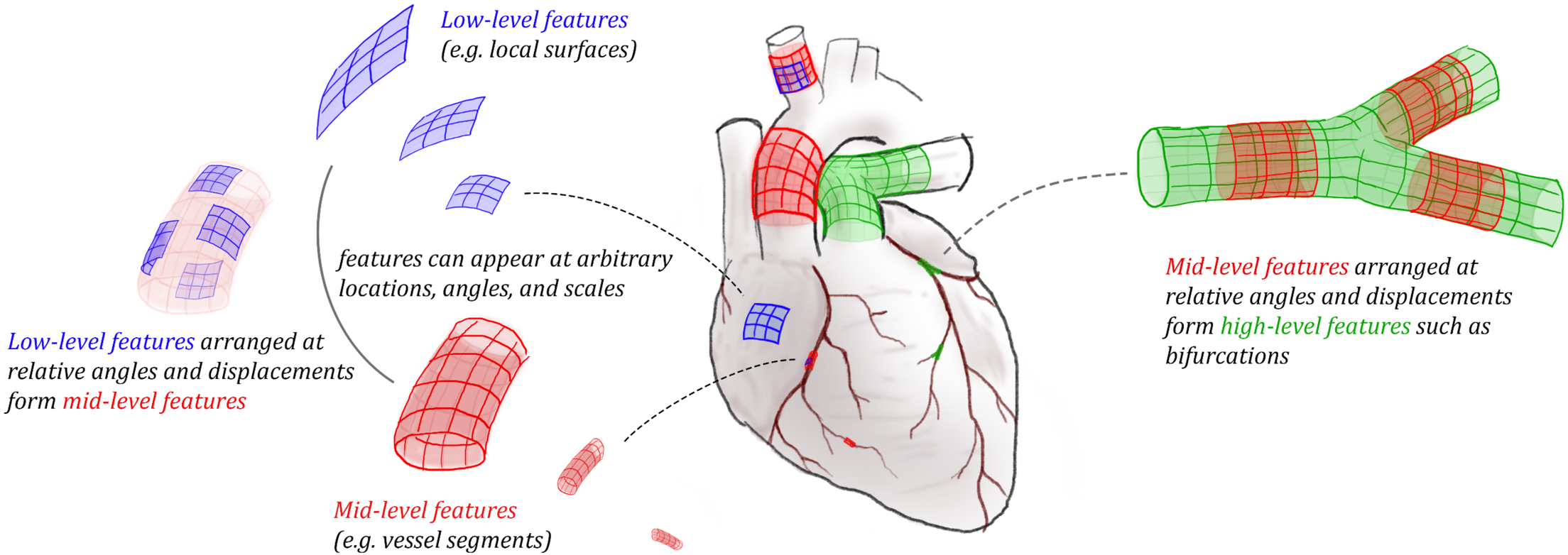
What is a group?

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. $g^{-1} \cdot g = g \cdot g^{-1} = e$.

Psychology of vision: recognition by components

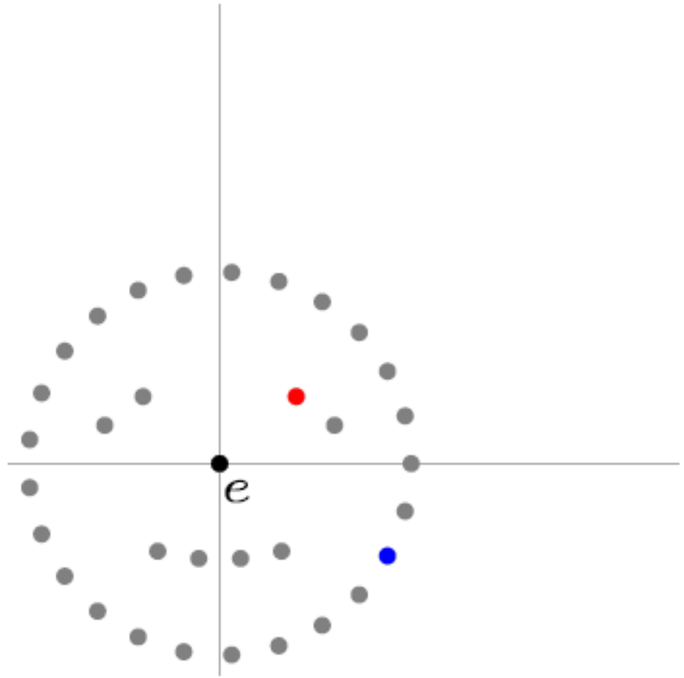


Translation group $(\mathbb{R}^2, +)$

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



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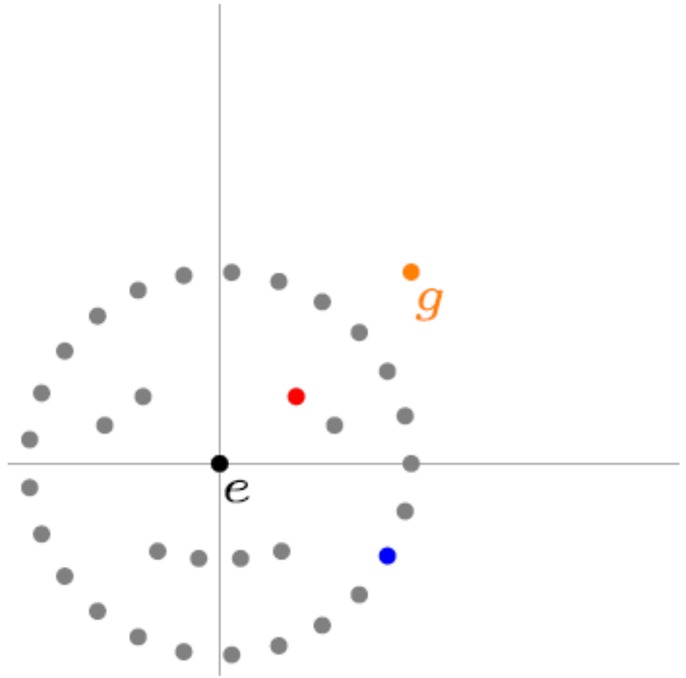

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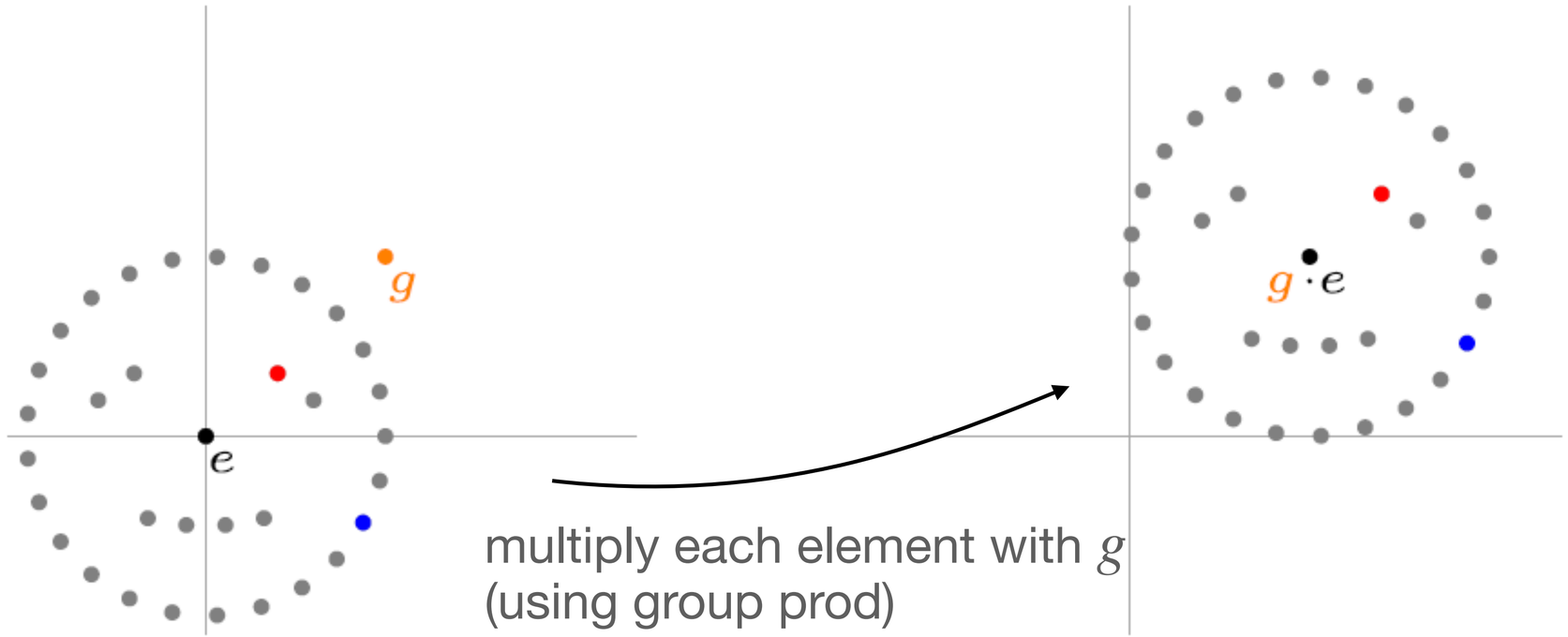

Roto-ranslation group $SE(2)$

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

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

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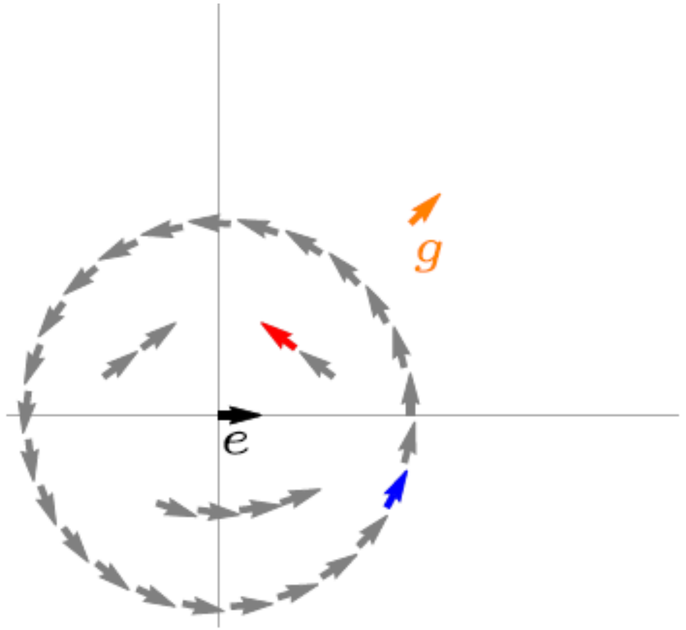

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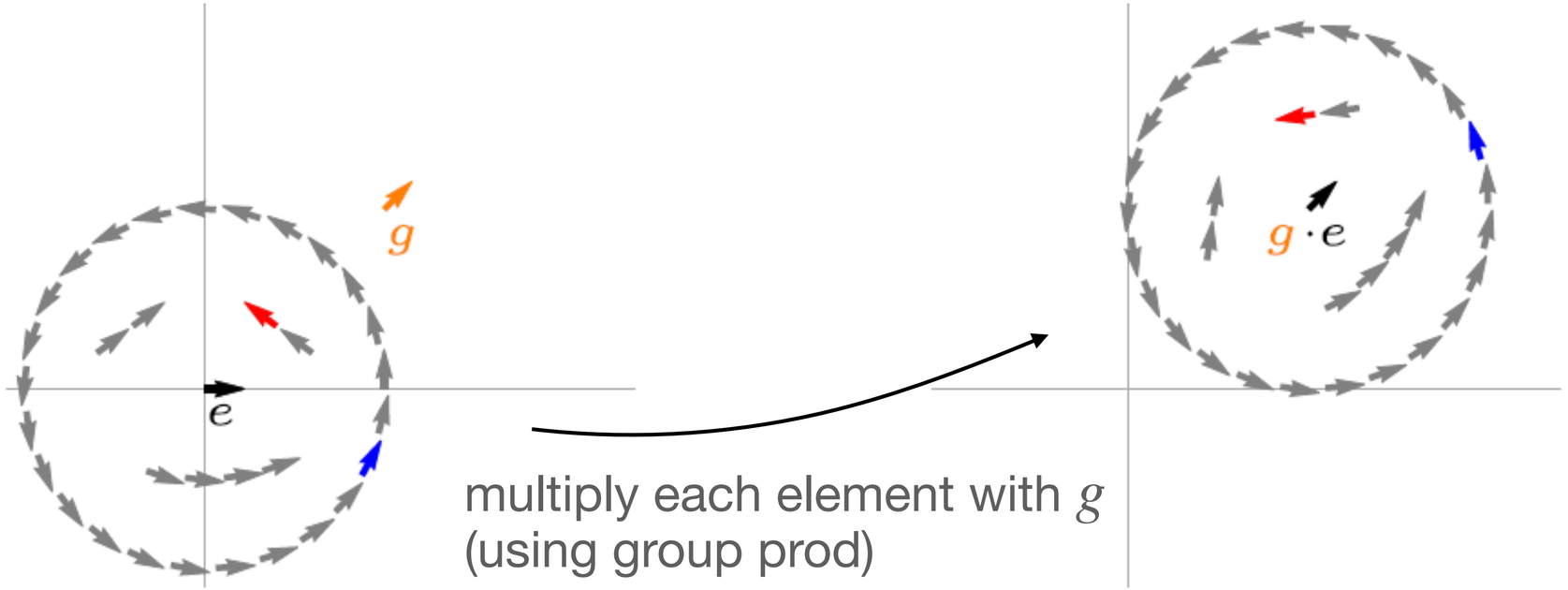
$$g^{-1} = (-\mathbf{R}_\theta^{-1}\mathbf{x}, \mathbf{R}_\theta^{-1})$$

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



Roto-ranslation group $SE(2)$

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

Matrix representation: The group can also be represented by matrices

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

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

In parametric form:

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

$$\leftrightarrow$$

In matrix form:

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

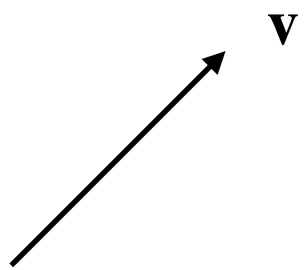
Representations

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

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

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

Representations



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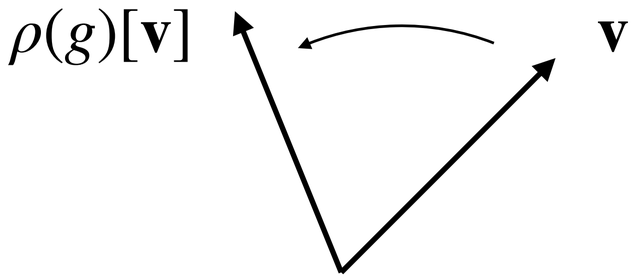

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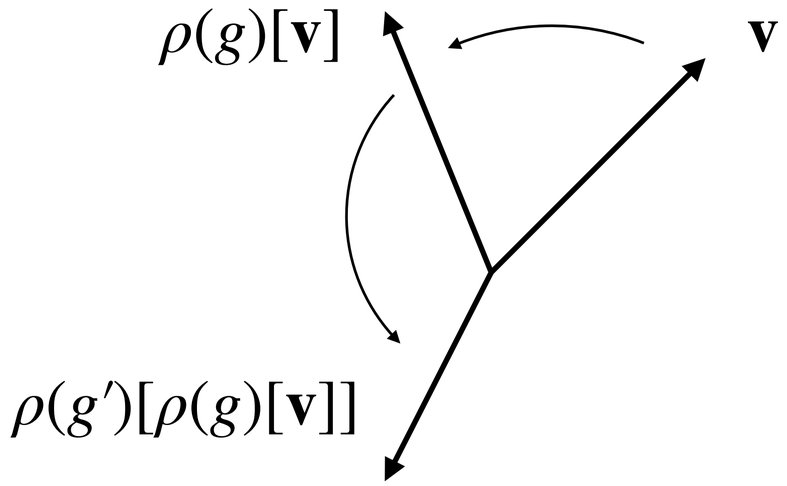

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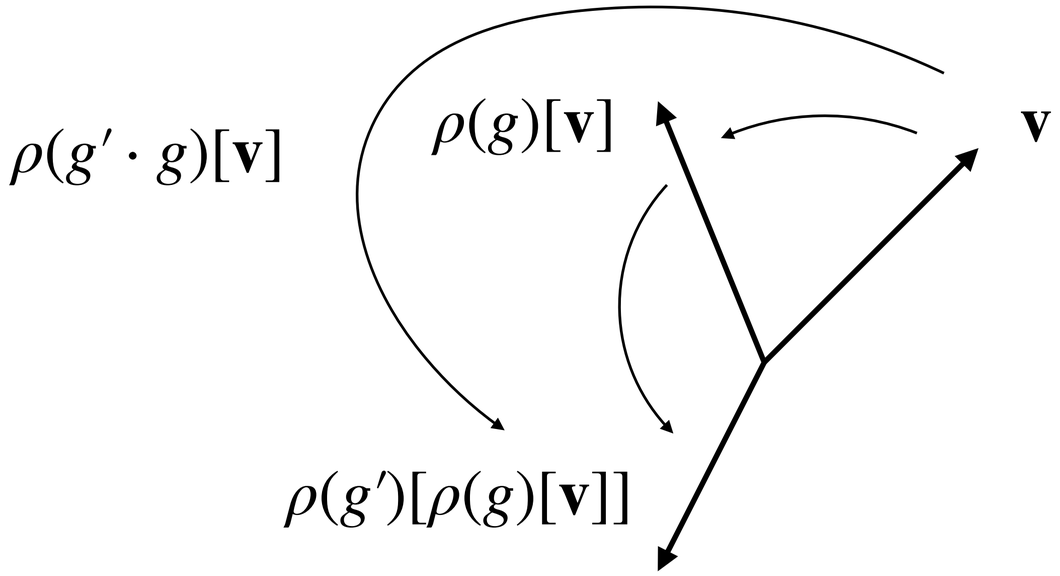

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Left-regular Representations

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

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

"group action" equals group product when domain is G

Left-regular Representations

Example:

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

- a 2D image

$G = SE(2)$

- the roto-translation group

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

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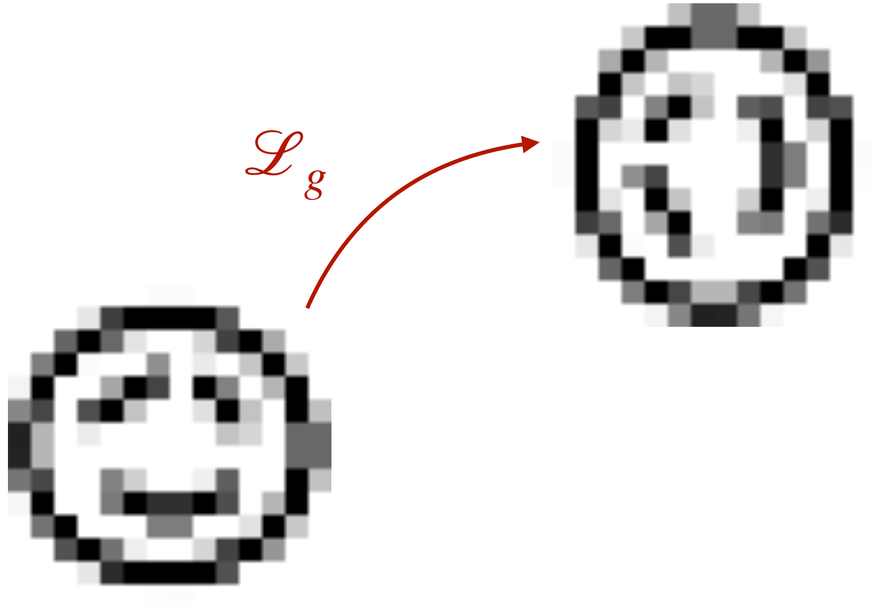

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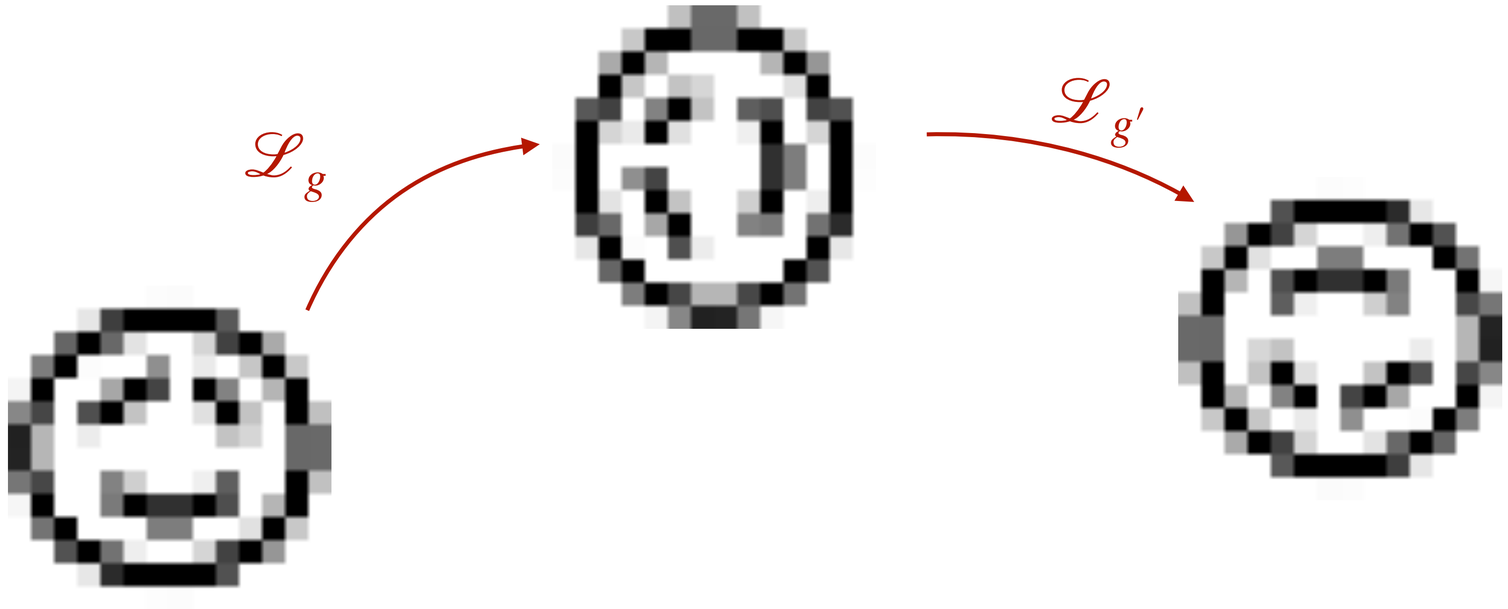

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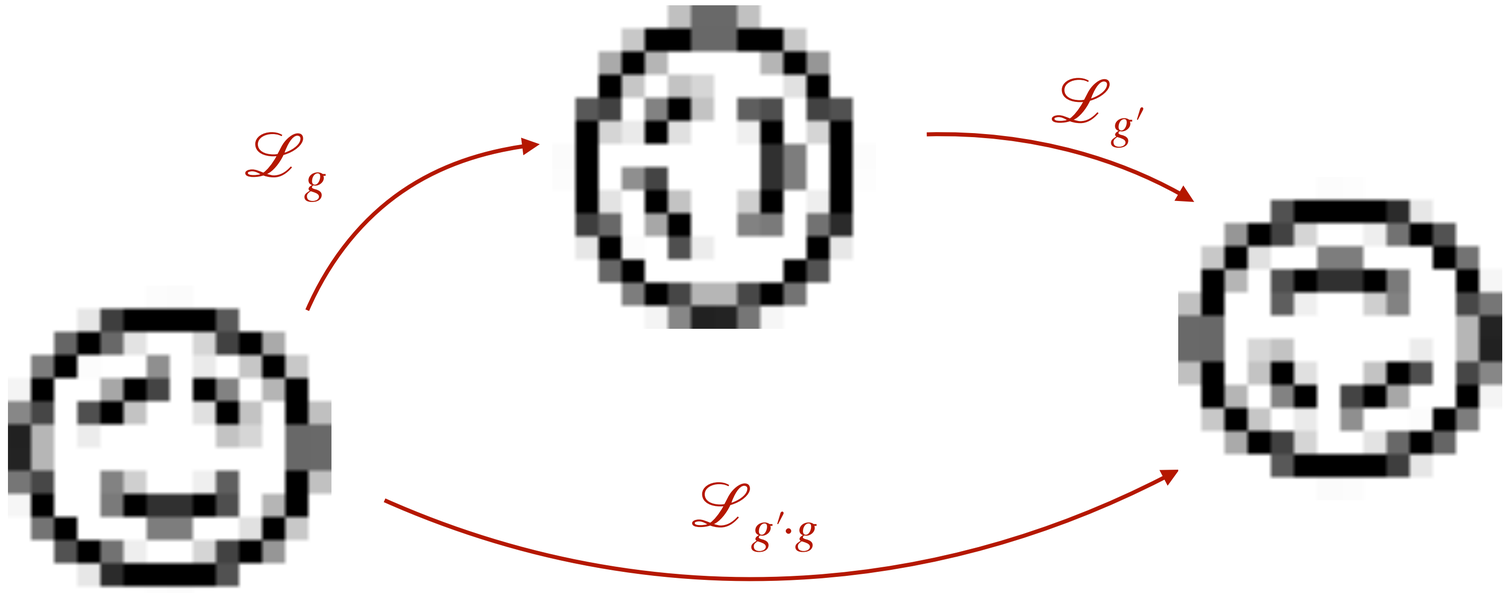

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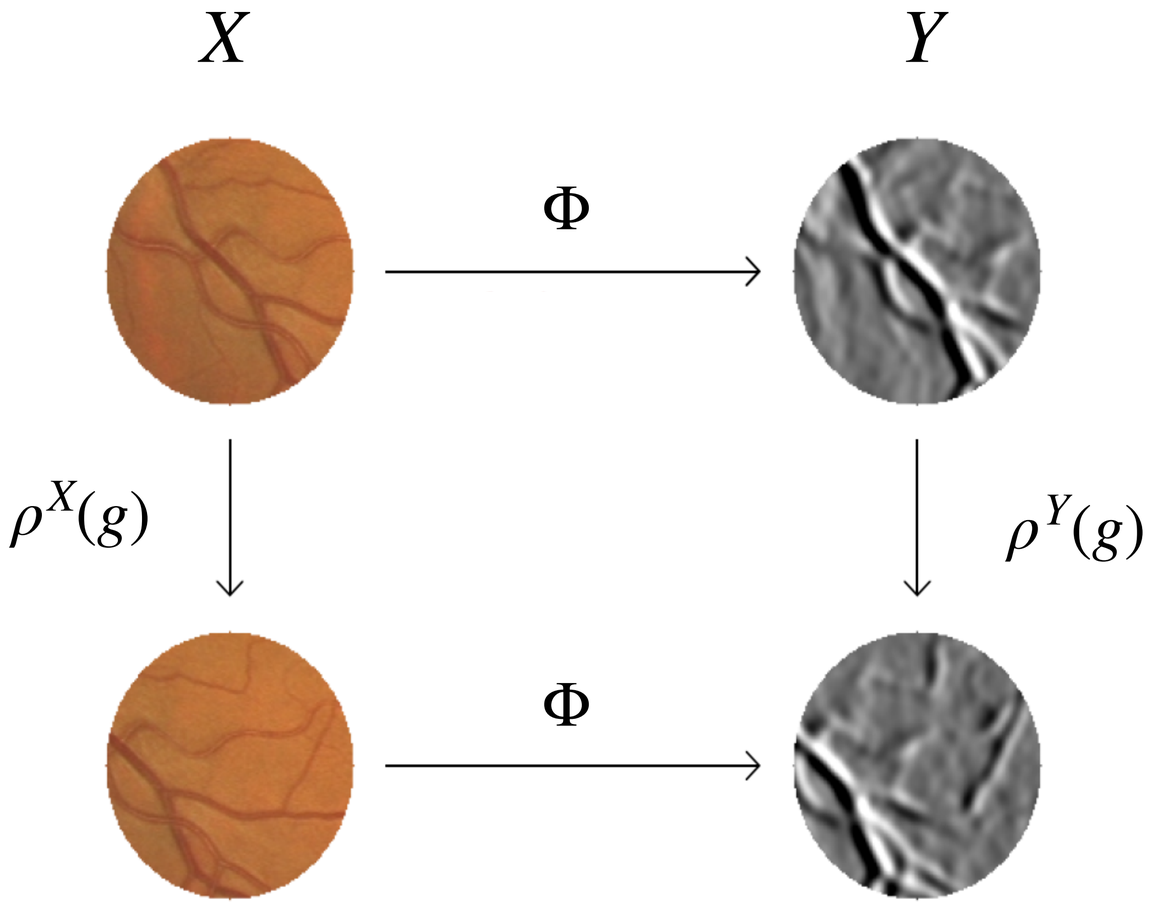
Equivariance

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

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

group representation action on X



1. Motivation — Equivariance → weight-sharing and generalization

2. Pattern matching using group theory — Group theory: symmetries & recognition by components
(features have “poses”)

3. Group convolutions

4. Example

5. G-convs are all you need!

6. Steerable group convolutions

7. Feature fields and escnn library

8. Equivariant tensor product layers

9. Equivariant graph NNs

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Cross-correlations

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

Cross-correlations

Representation of the translation group!

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

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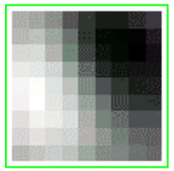
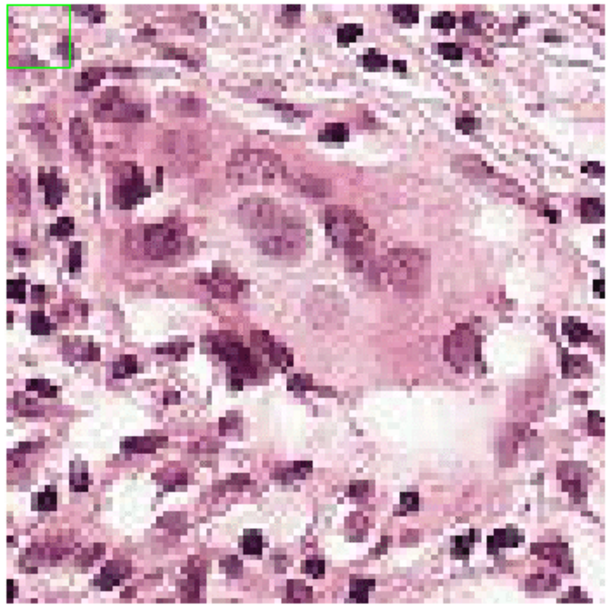


$\star_{\mathbb{R}^2}$



$=$

k
2D convolution kernel

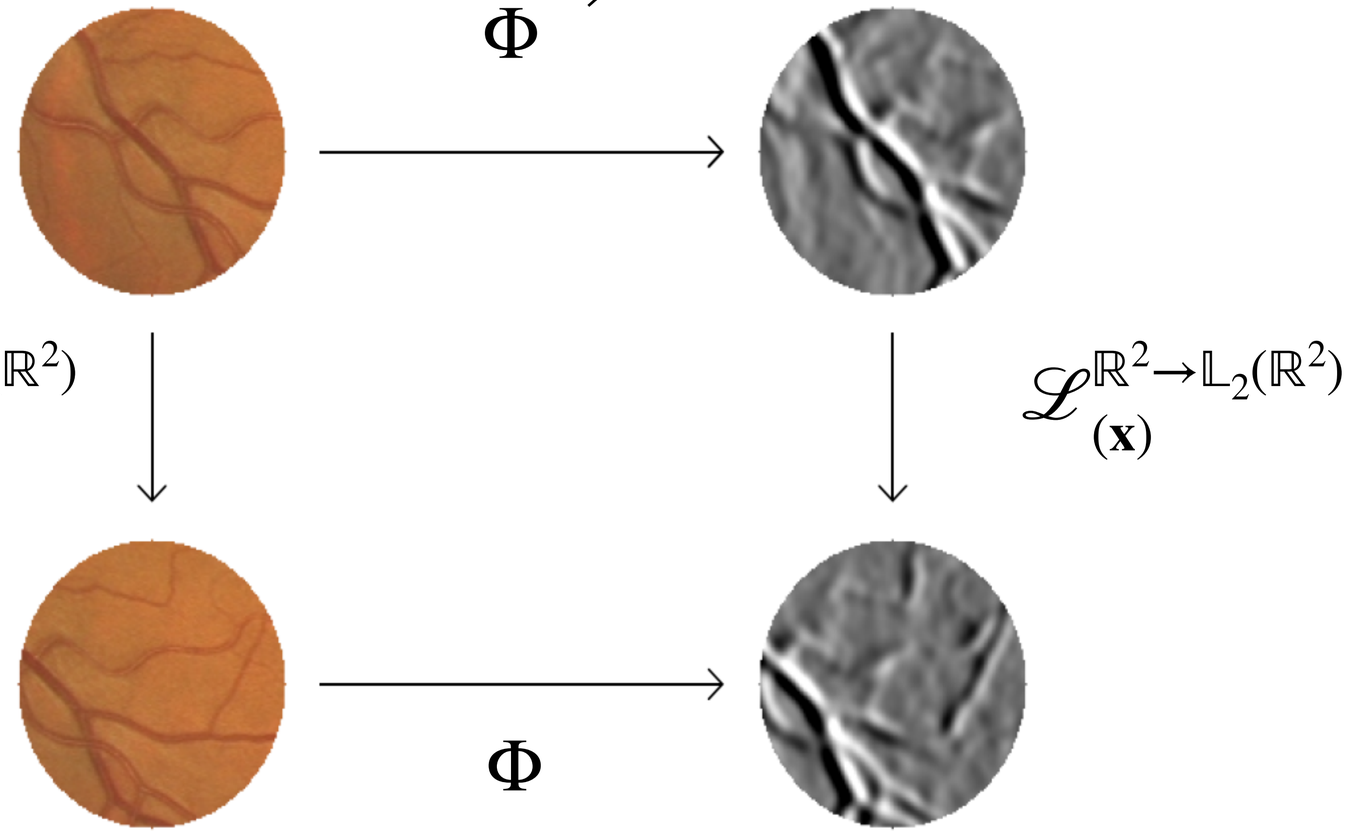
f^{in}
2D feature map

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

Equivariance

Convolutions/cross-correlations are translation equivariant

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



Representation of the translation group

Equivariance

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

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

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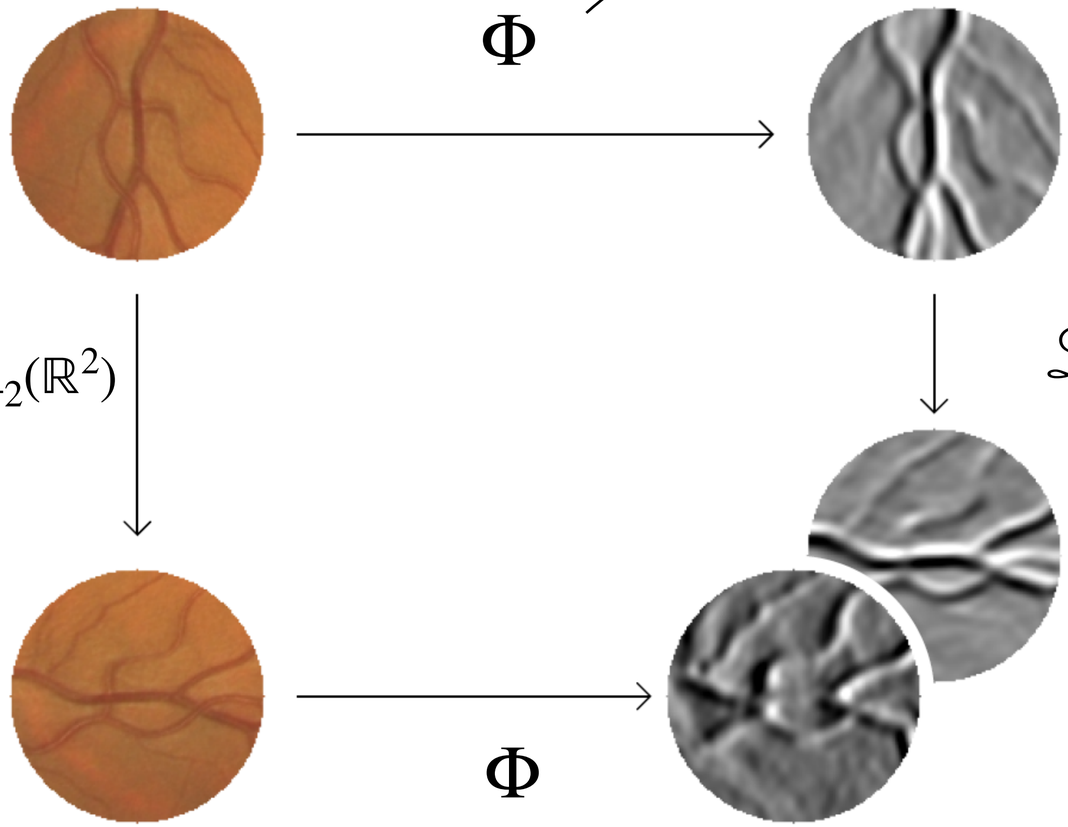

Representation of the rotation group

SE(2) equivariant cross-correlations

Representation of the roto-translation group!

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

SE(2) equivariant cross-correlations

Representation of the roto-translation group!

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translation *rotation*

SE(2) equivariant cross-correlations

Representation of the roto-translation group!

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

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

translation *rotation*

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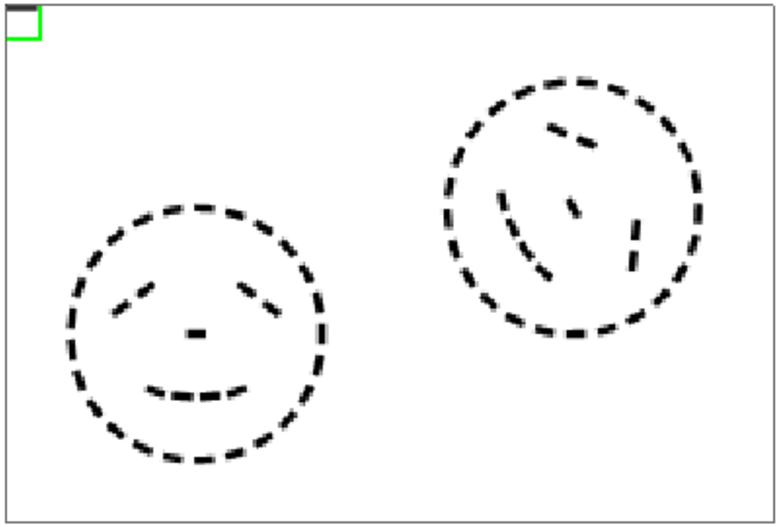
translation *rotation*

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



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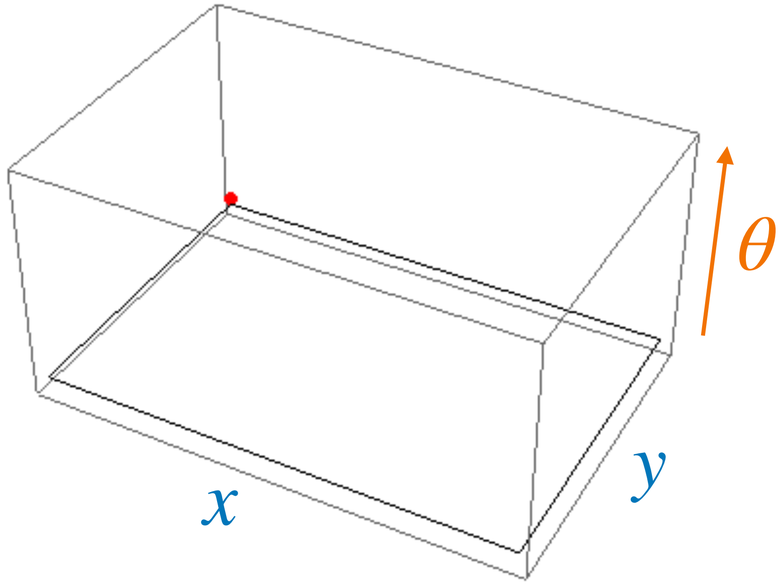

$\mathscr{L}_\theta^{SO(2)\to\mathbb{L}_2(\mathbb{R}^2)}k$
Rotated 2D convolution kernel

f^{in}
2D feature map

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

SE(2) equivariant cross-correlations

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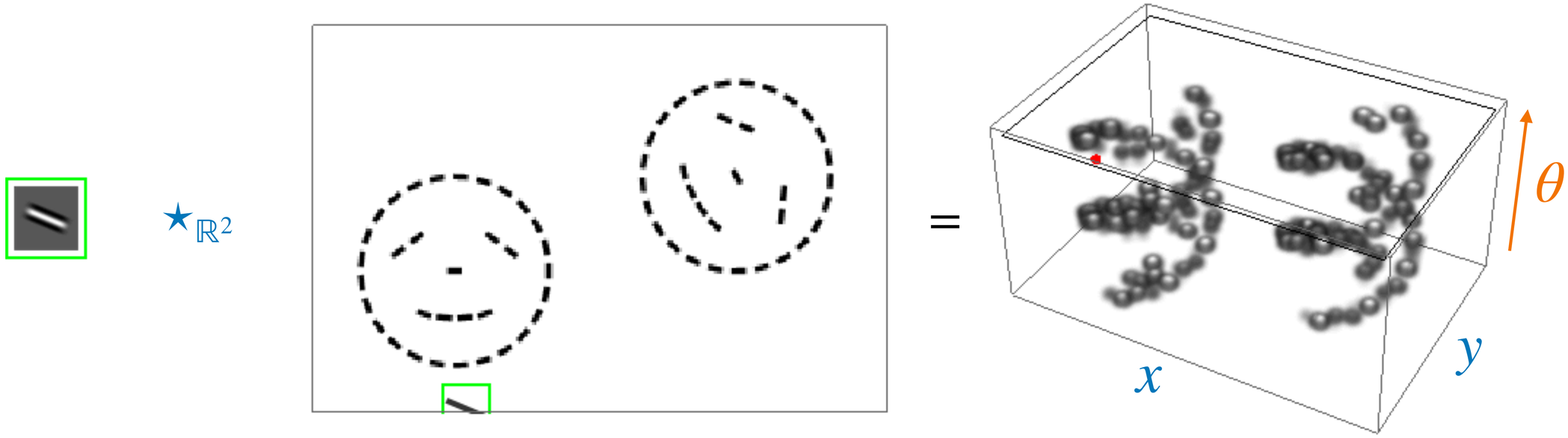
translation *rotation*



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Equivariance

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

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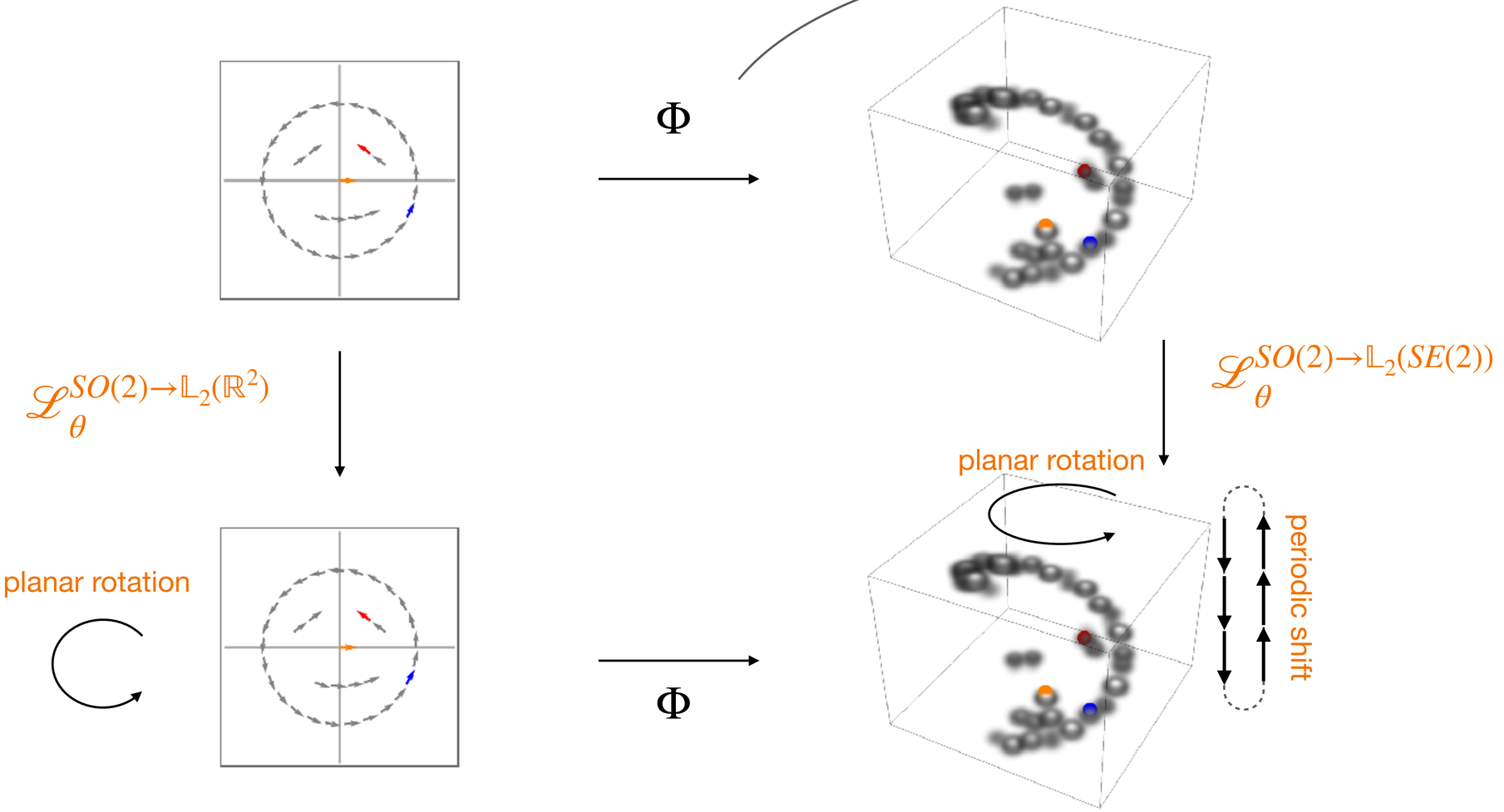

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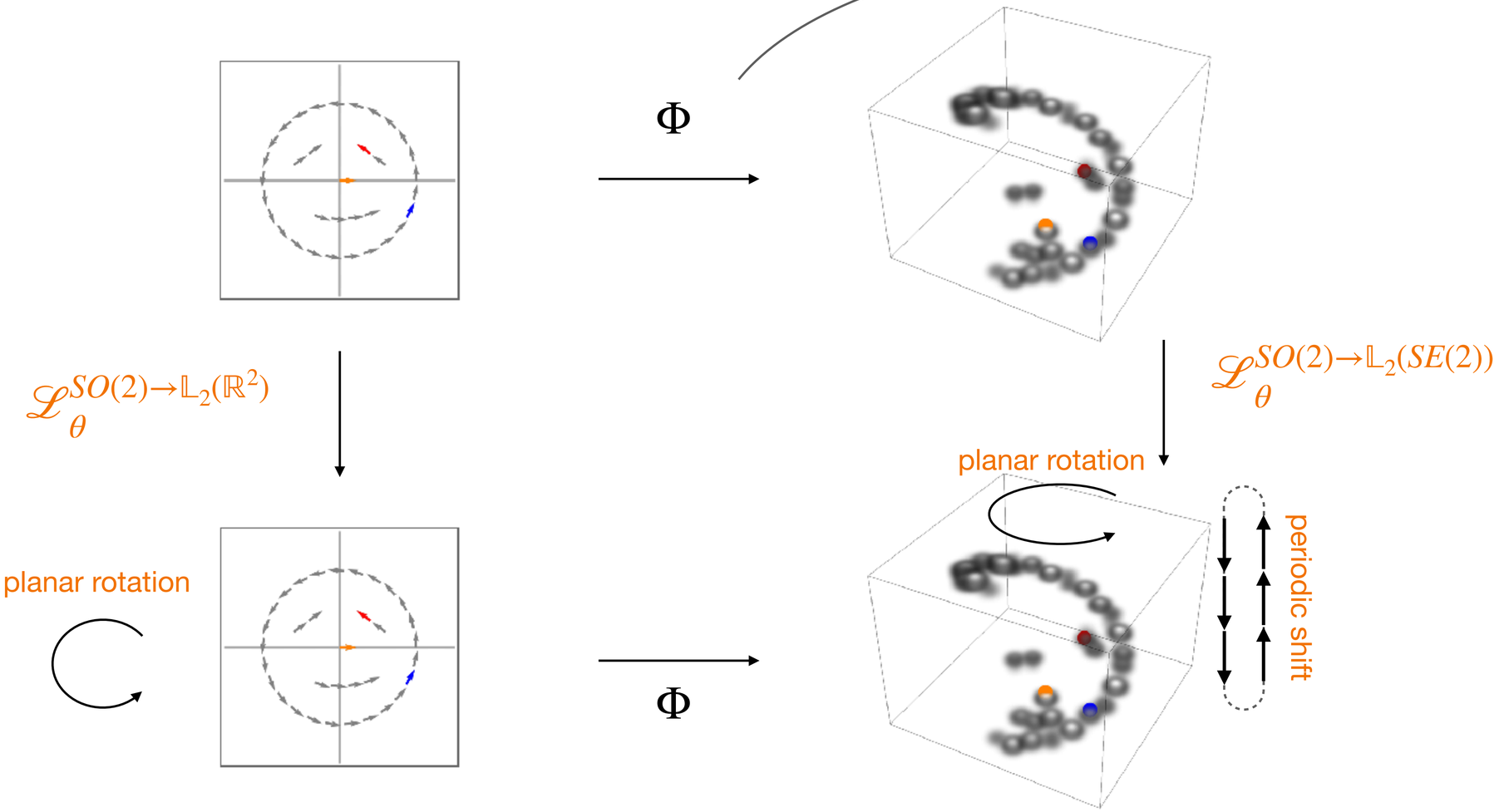

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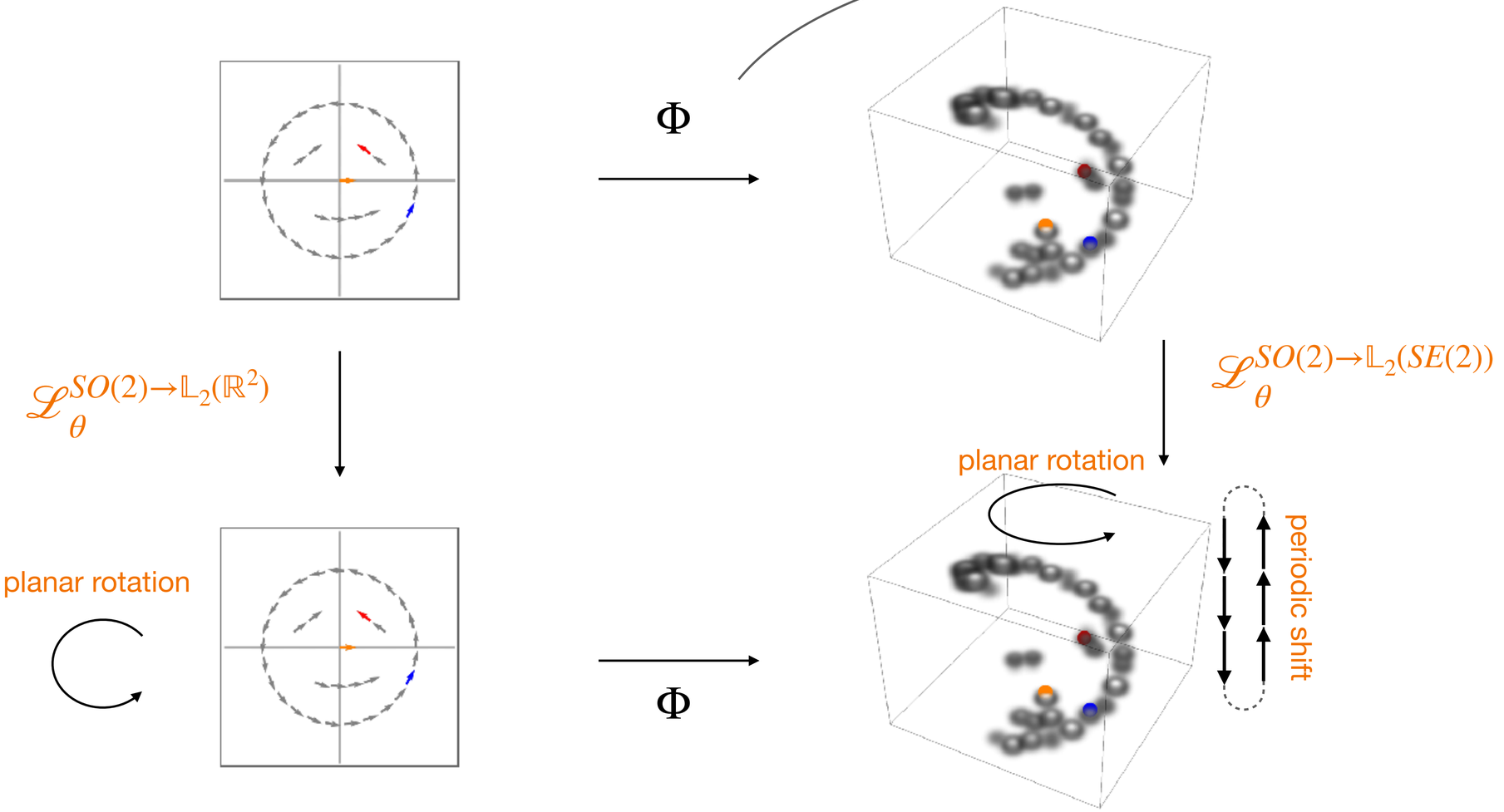

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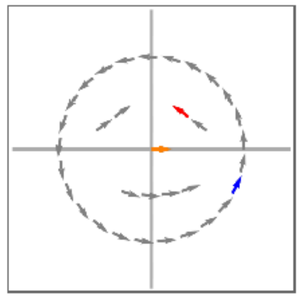

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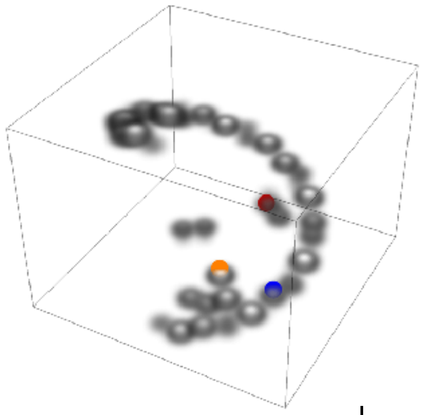
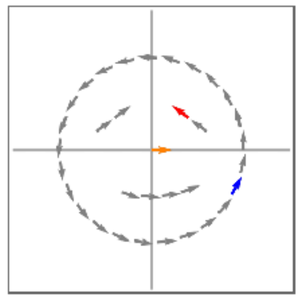


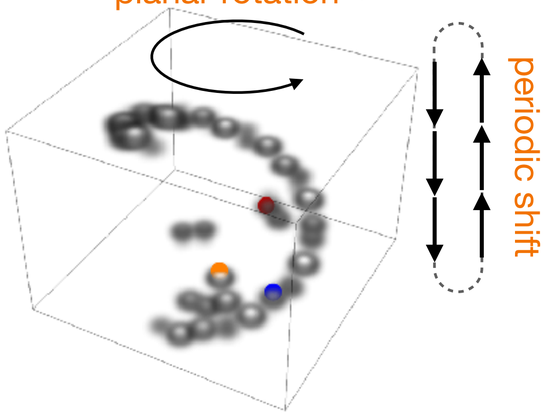
$\mathscr{L}_{\theta}^{SO(2) \to \mathbb{L}_2(\mathbb{R}^2)}$

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

planar rotation



Φ



periodic shift

What about subsequent layers?

SE(2) equivariant cross-correlations

Group correlations:

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

SE(2) equivariant cross-correlations

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

translation *rotation*

SE(2) equivariant cross-correlations

Group correlations:

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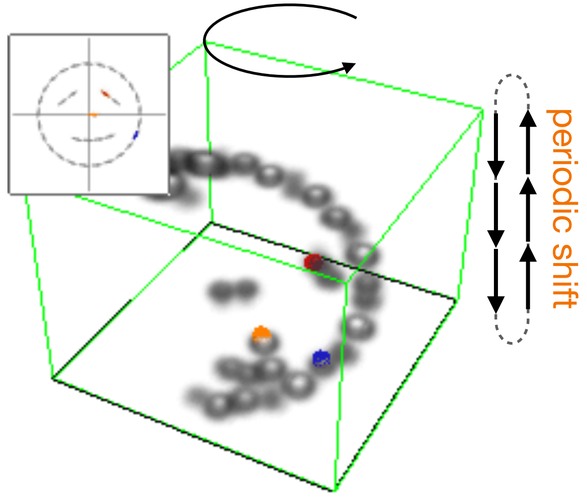
translation *rotation*



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

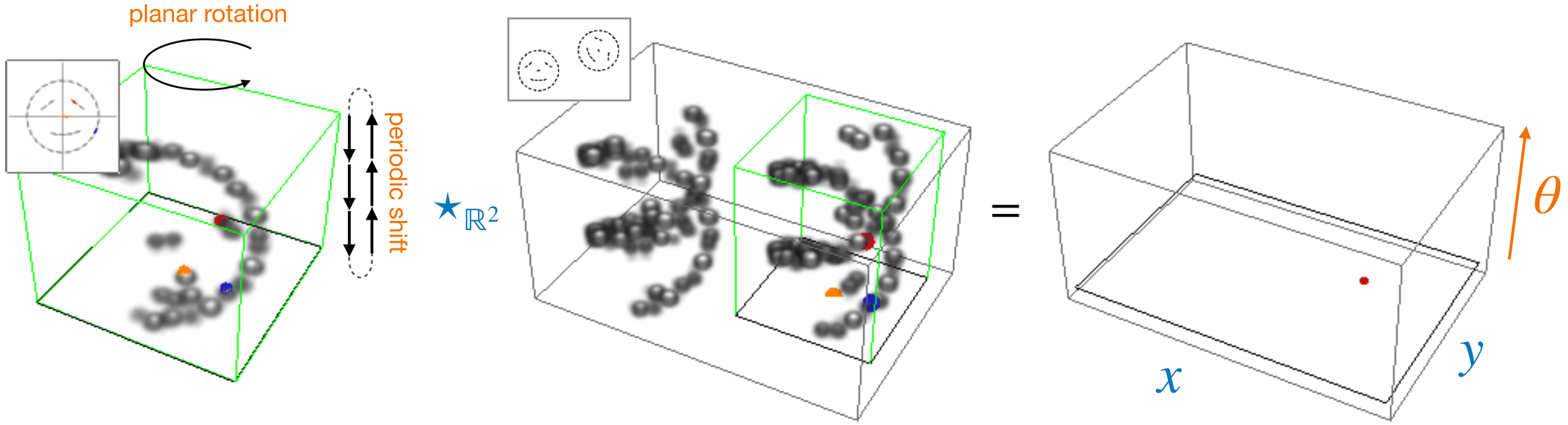
Rotated SE(2) convolution kernel

SE(2) equivariant cross-correlations

Group correlations:

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

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)

SE(2) equivariant cross-correlations

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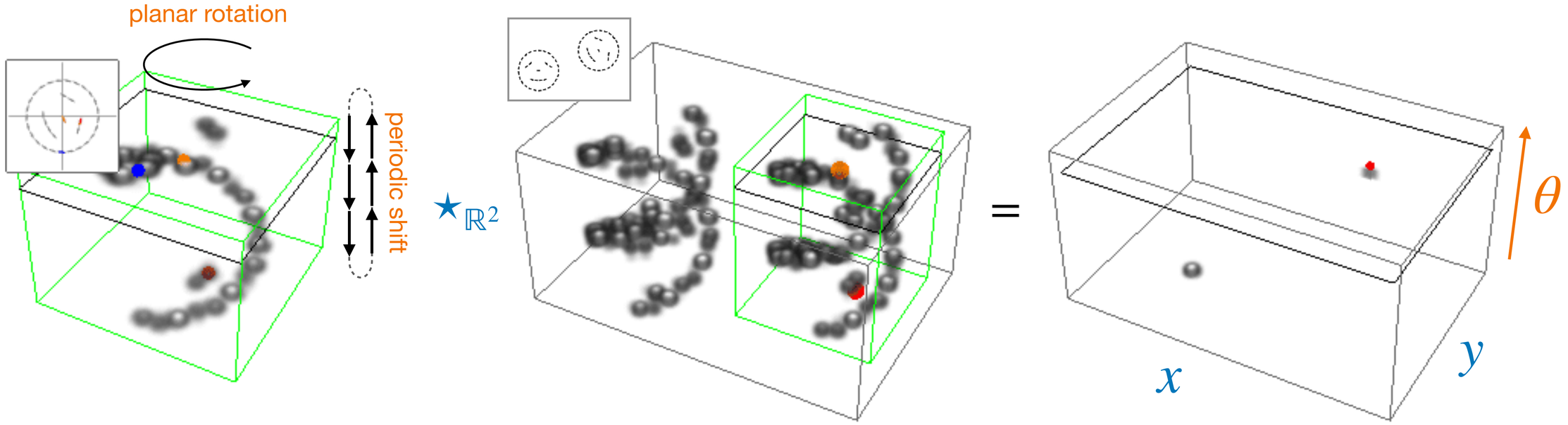
translation *rotation*



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SE(2) feature map

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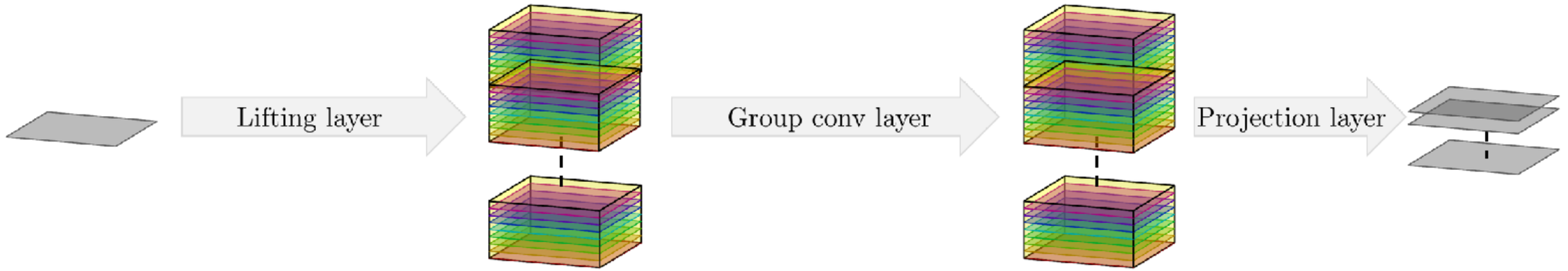
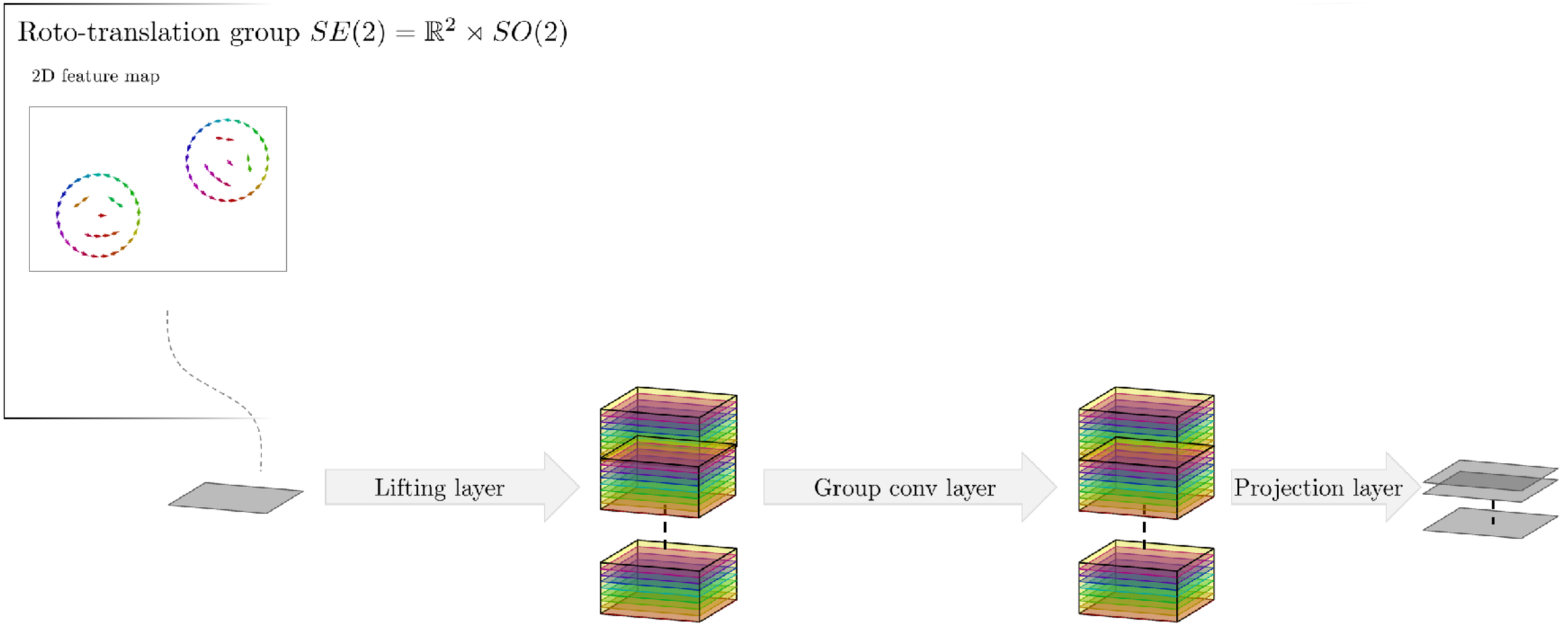
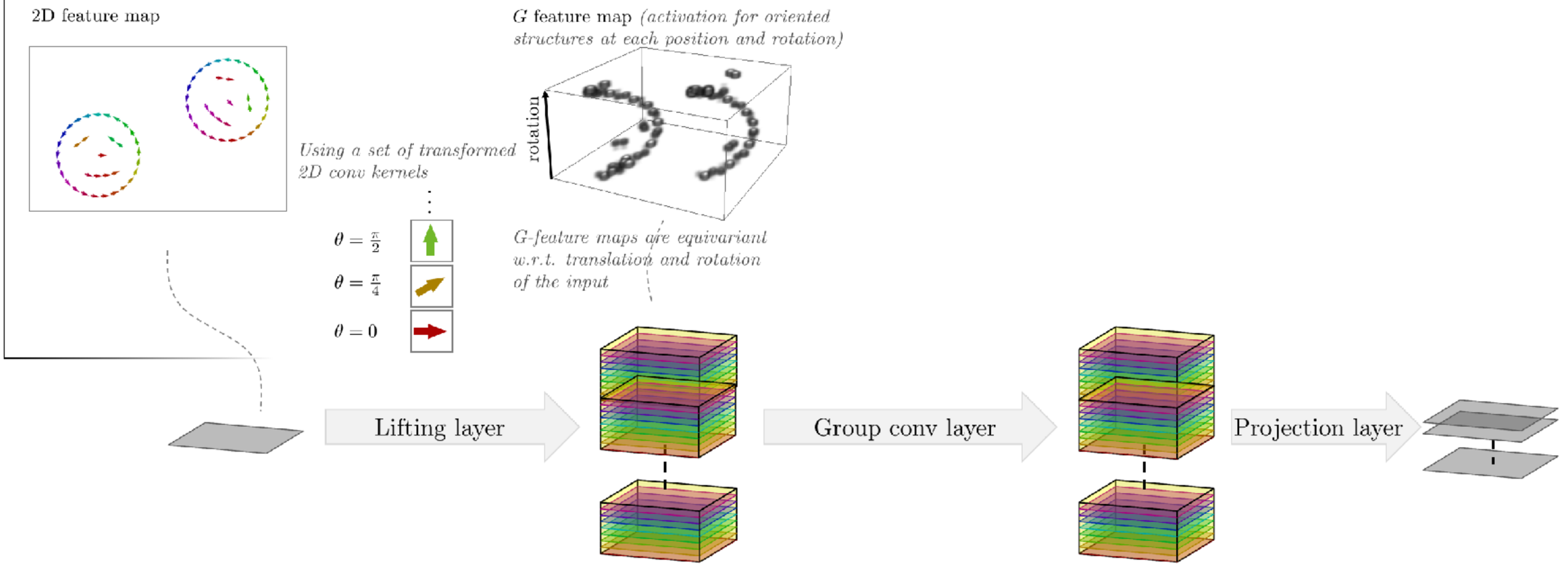
SE(2) feature map (after ReLU)

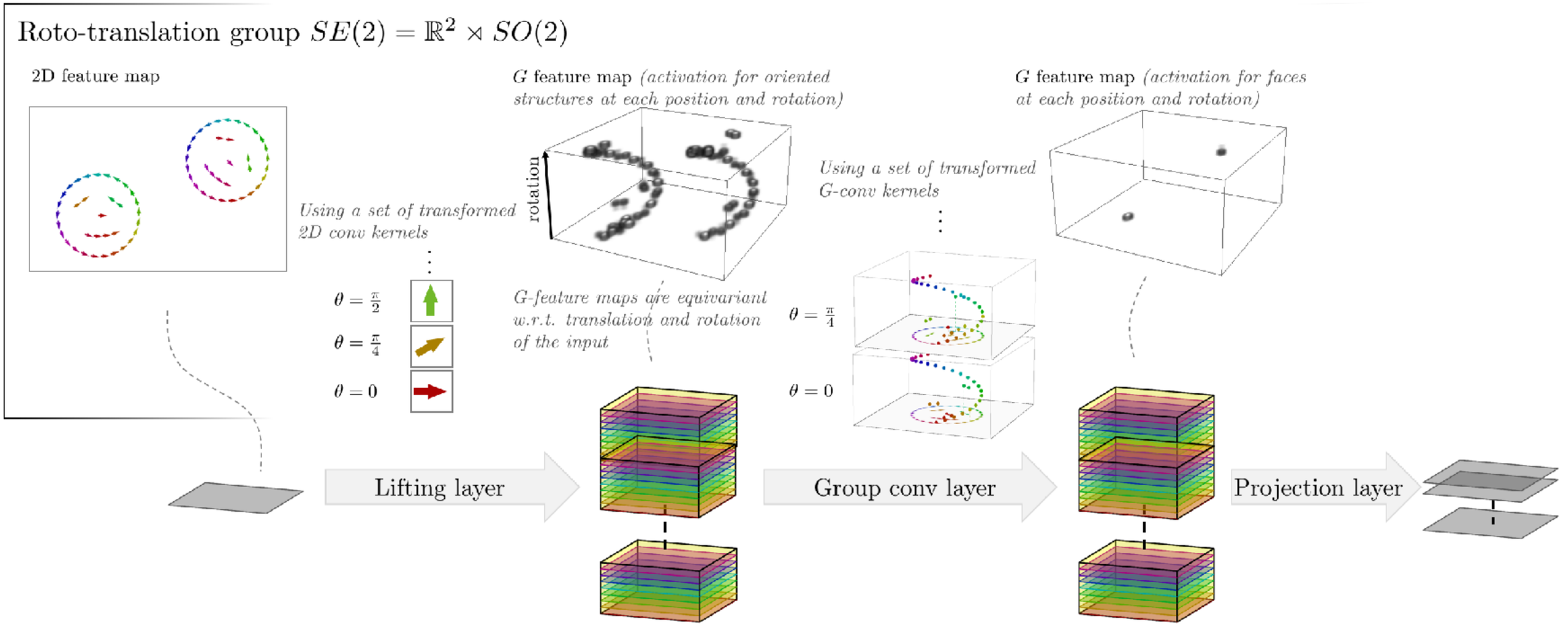

Lifting layer
Group conv layer
Projection layer

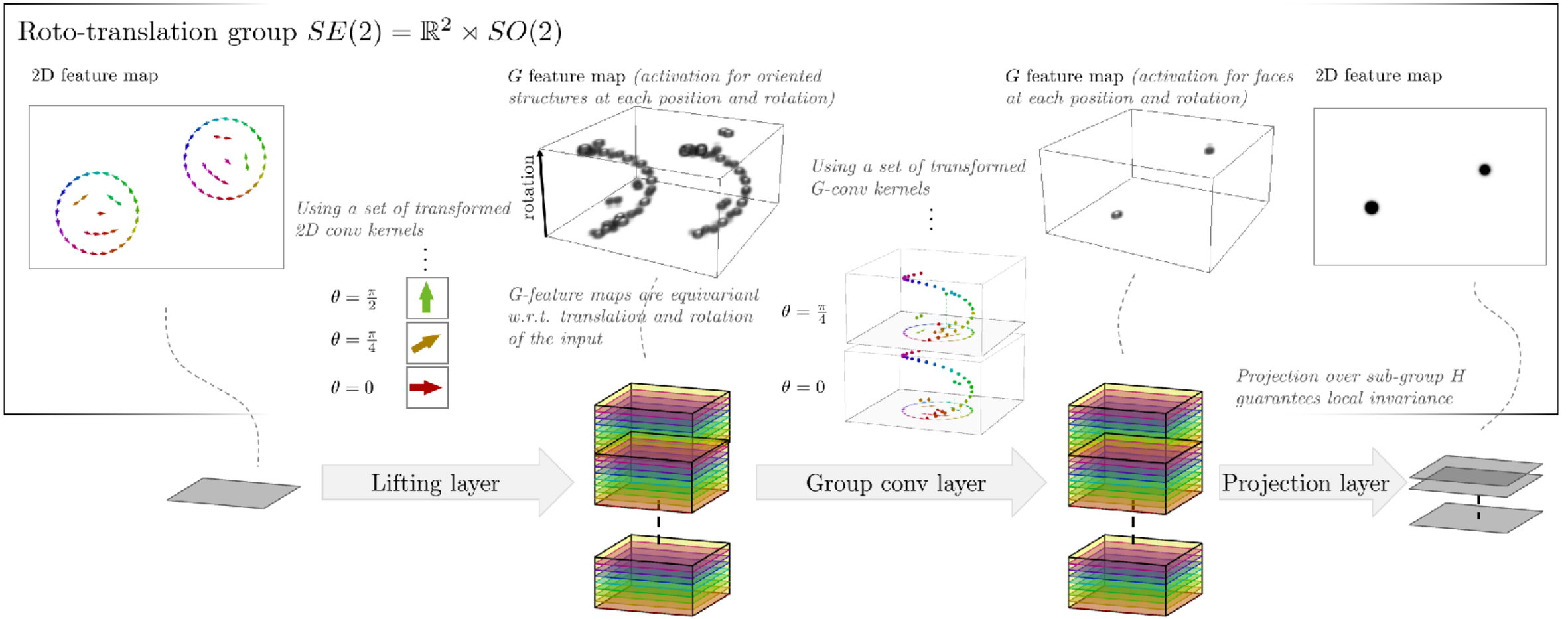
Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$



Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$




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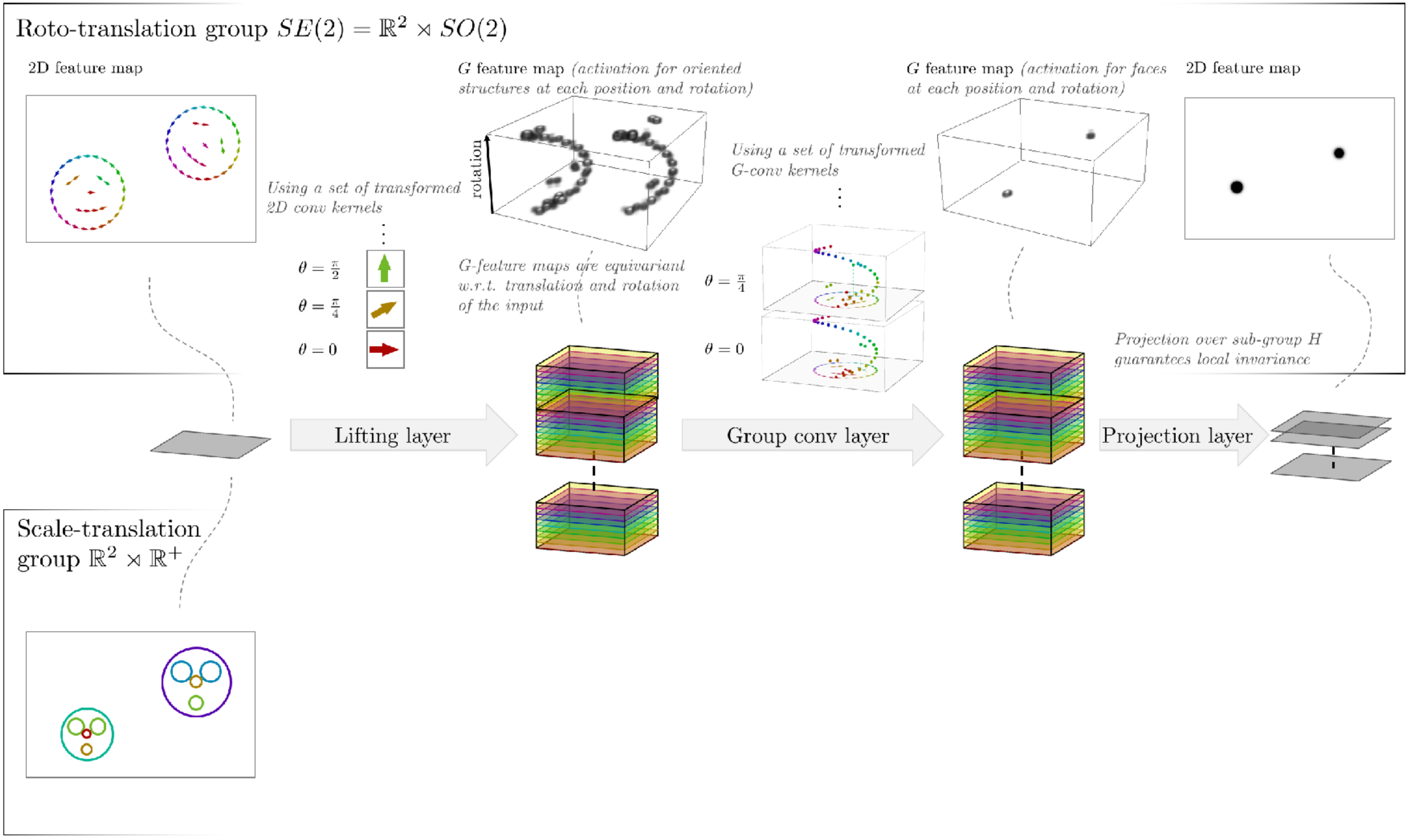
G feature map (activation for faces at each position and rotation)
2D feature map
Projection over sub-group H guarantees local invariance
Lifting layer
Group conv layer
Projection layer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$\theta = \frac{\pi}{2}$
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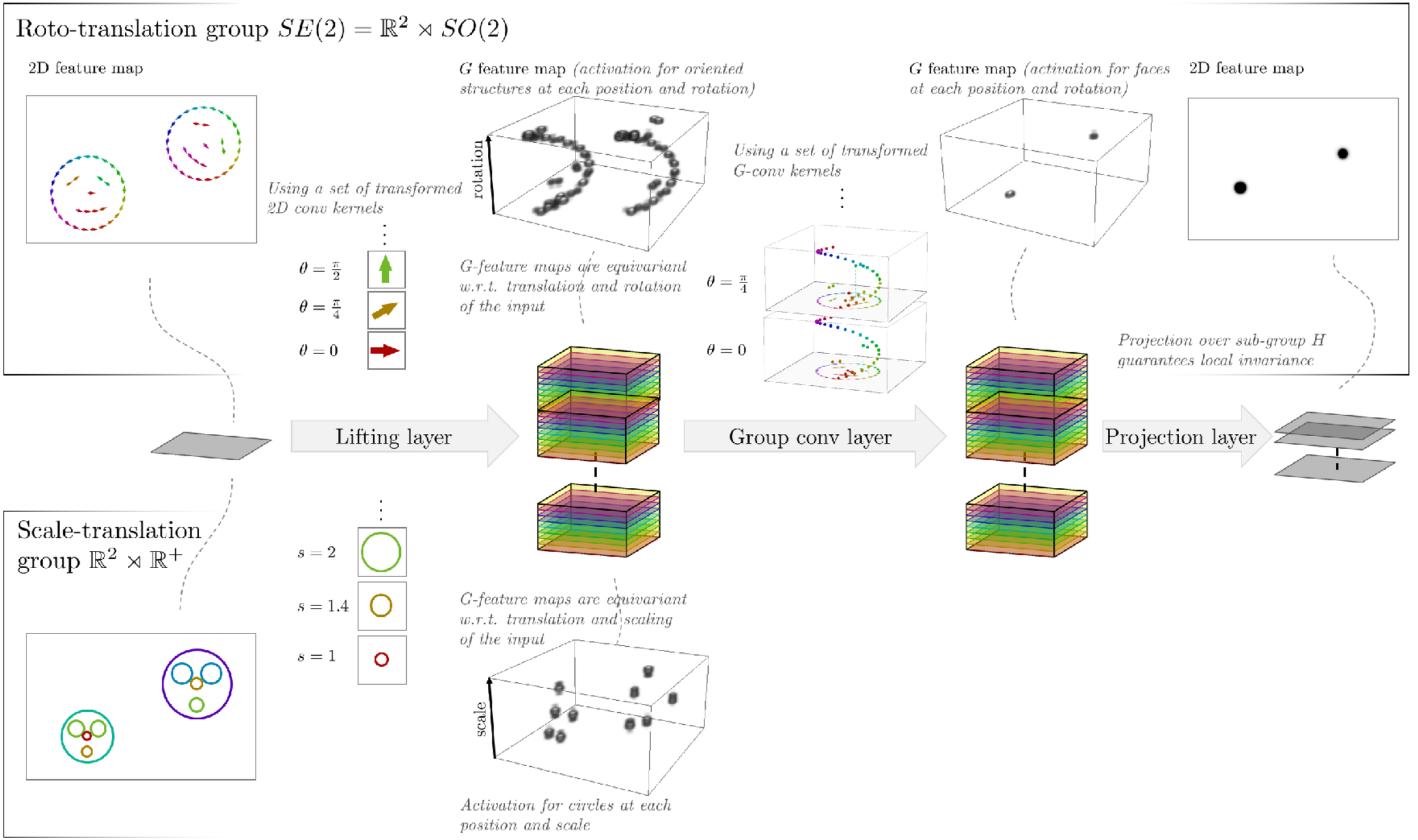
2D feature map
Projection over sub-group H guarantees local invariance
Lifting layer
Group conv layer
Projection layer
Scale-translation group $\mathbb{R}^2 \rtimes \mathbb{R}^+$


Roto-translation group $SE(2) = \mathbb{R}^2 \rtimes SO(2)$
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Using a set of transformed 2D conv kernels
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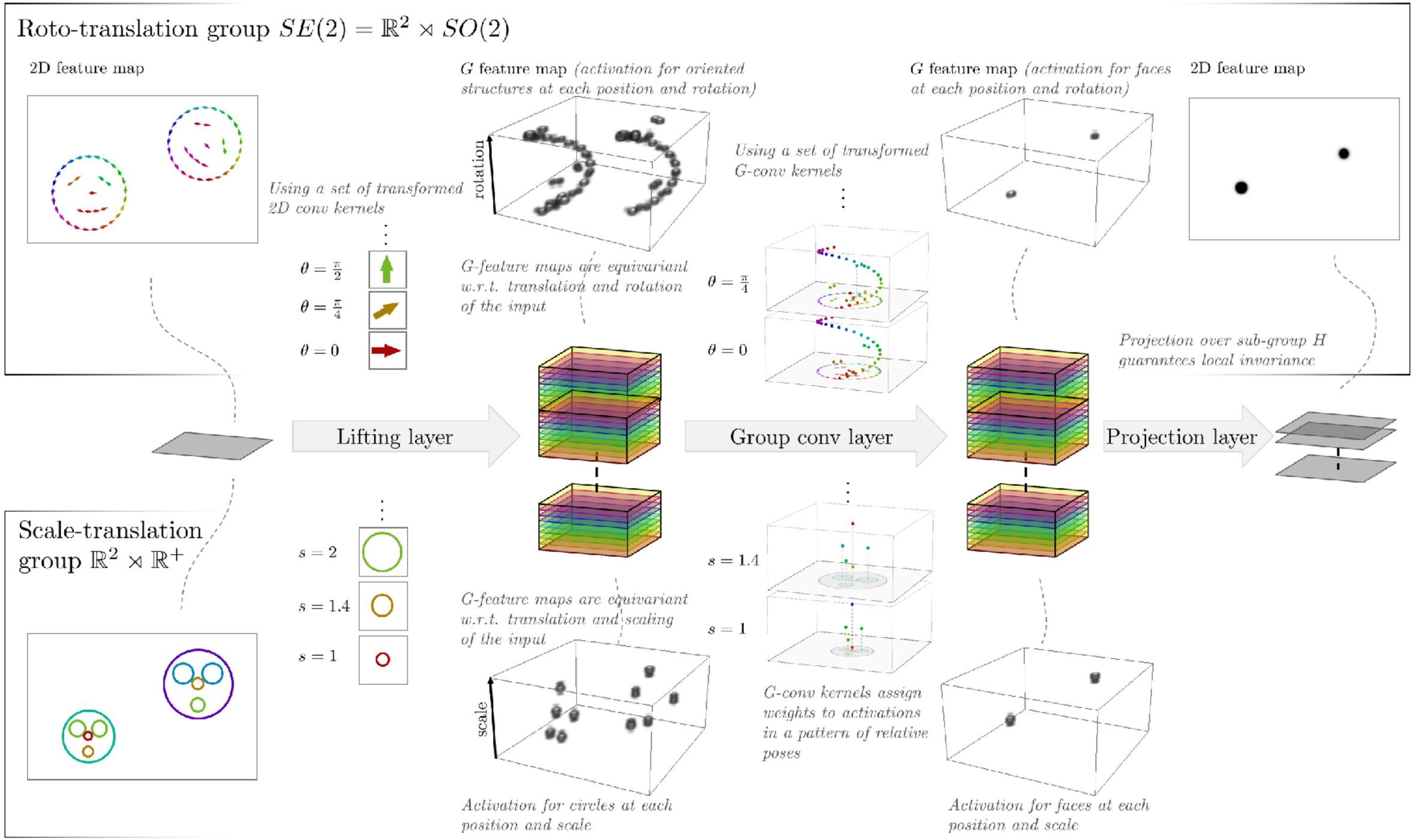
Scale-translation group $\mathbb{R}^2 \rtimes \mathbb{R}^+$
$s = 2$
$s = 1.4$
$s = 1$
G-feature maps are equivariant w.r.t. translation and scaling of the input
scale
Activation for circles at each position and scale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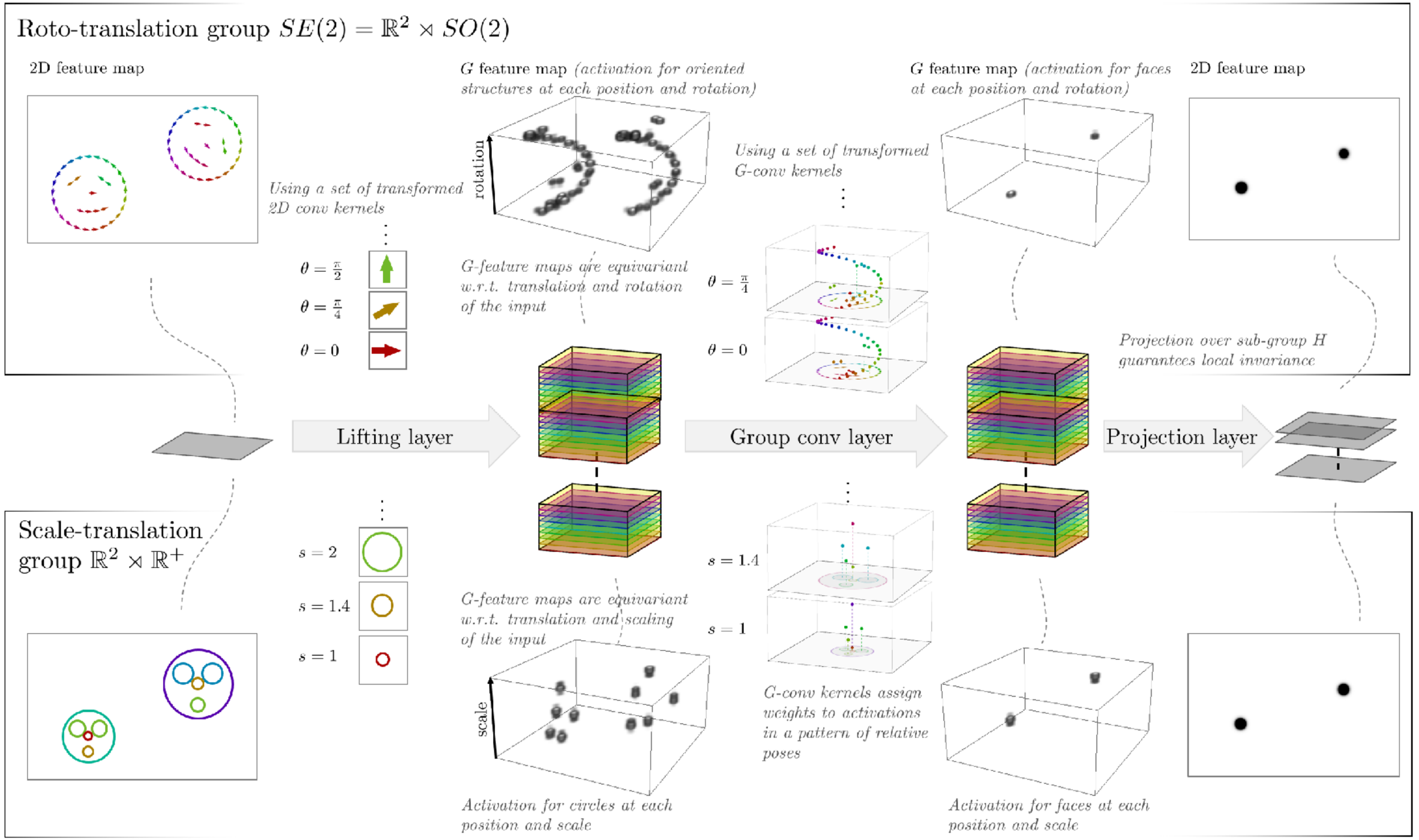
G-feature maps are equivariant w.r.t. translation and scaling of the input
scale
Activation for circles at each position and scale
$s = 1.4$
$s = 1$
G-conv kernels assign weights to activations in a pattern of relative poses
Activation for faces at each position and scale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1. Motivation — Equivariance → weight-sharing and generalization

2. Pattern matching using group theory — Group theory: symmetries & recognition by components
(features have “poses”)

3. Group convolutions — Template matching over groups

4. Example

5. G-convs are all you need!

6. Steerable group convolutions

7. Feature fields and escnn library

8. Equivariant tensor product layers

9. Equivariant graph NNs

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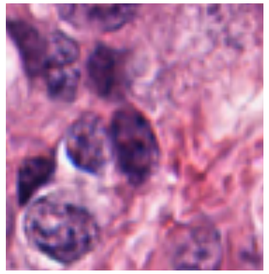
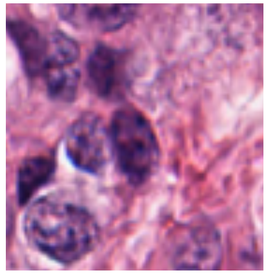
Architecture for rotation invariant mitotic cell detection

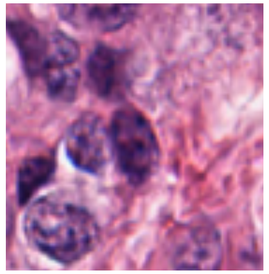


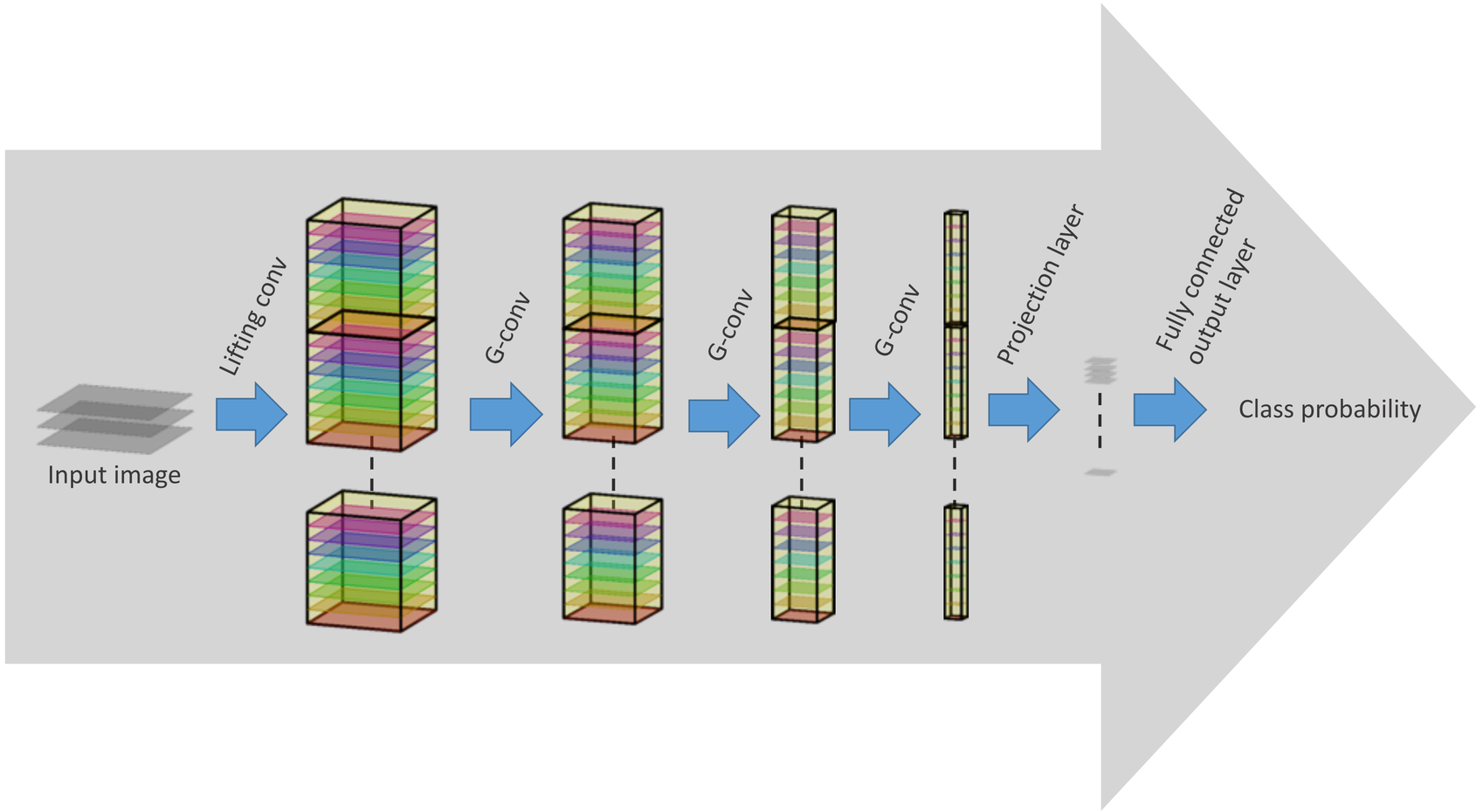
Architecture for rotation invariant mitotic cell detection



“normal” (0)
vs
“mitotic” (1)

Architecture for rotation invariant mitotic cell detection





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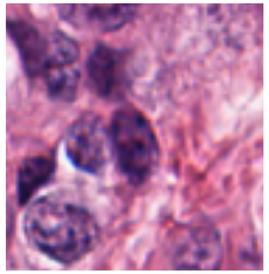

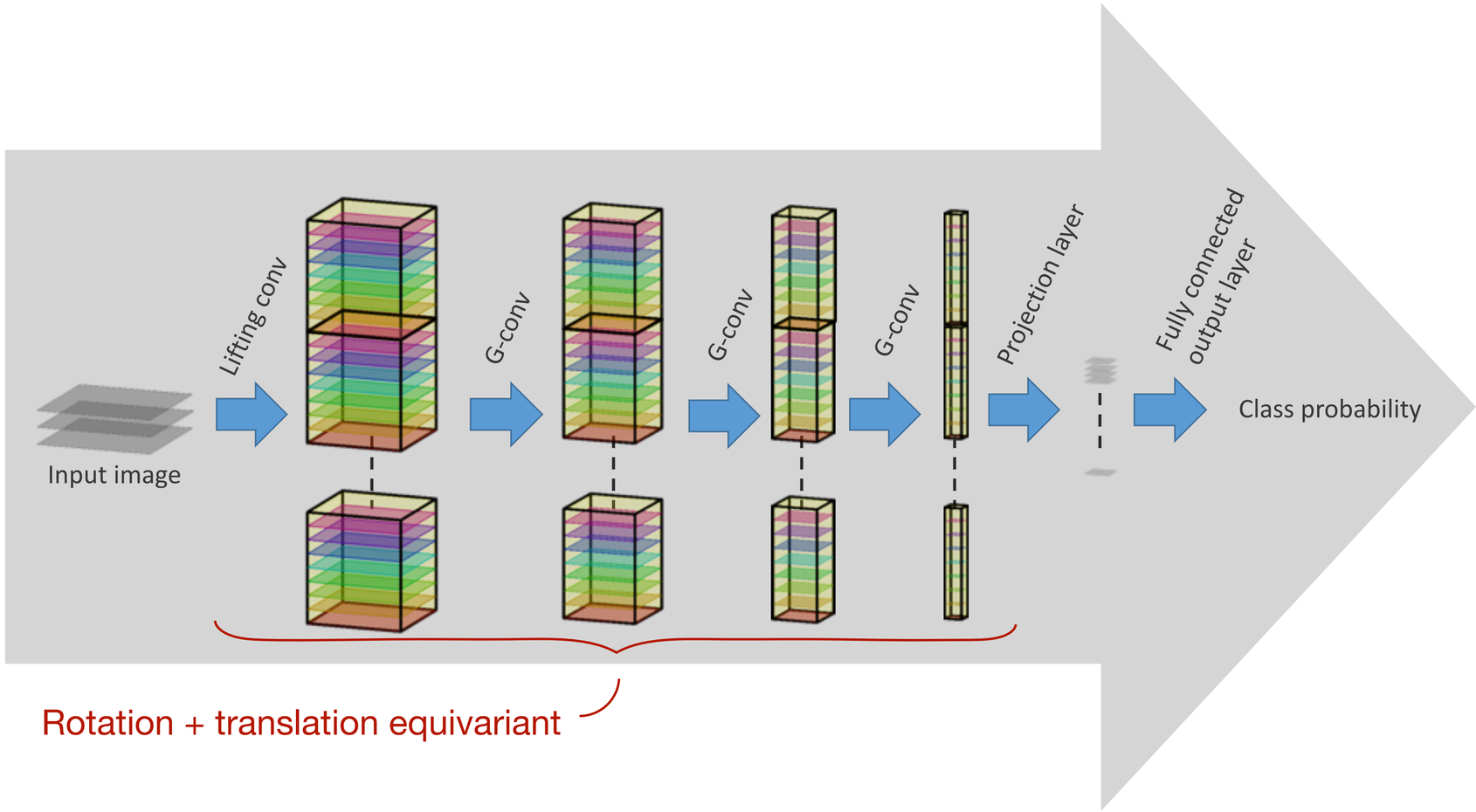

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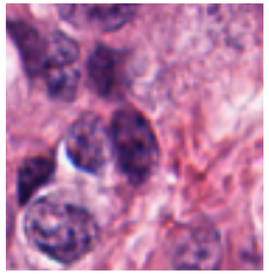
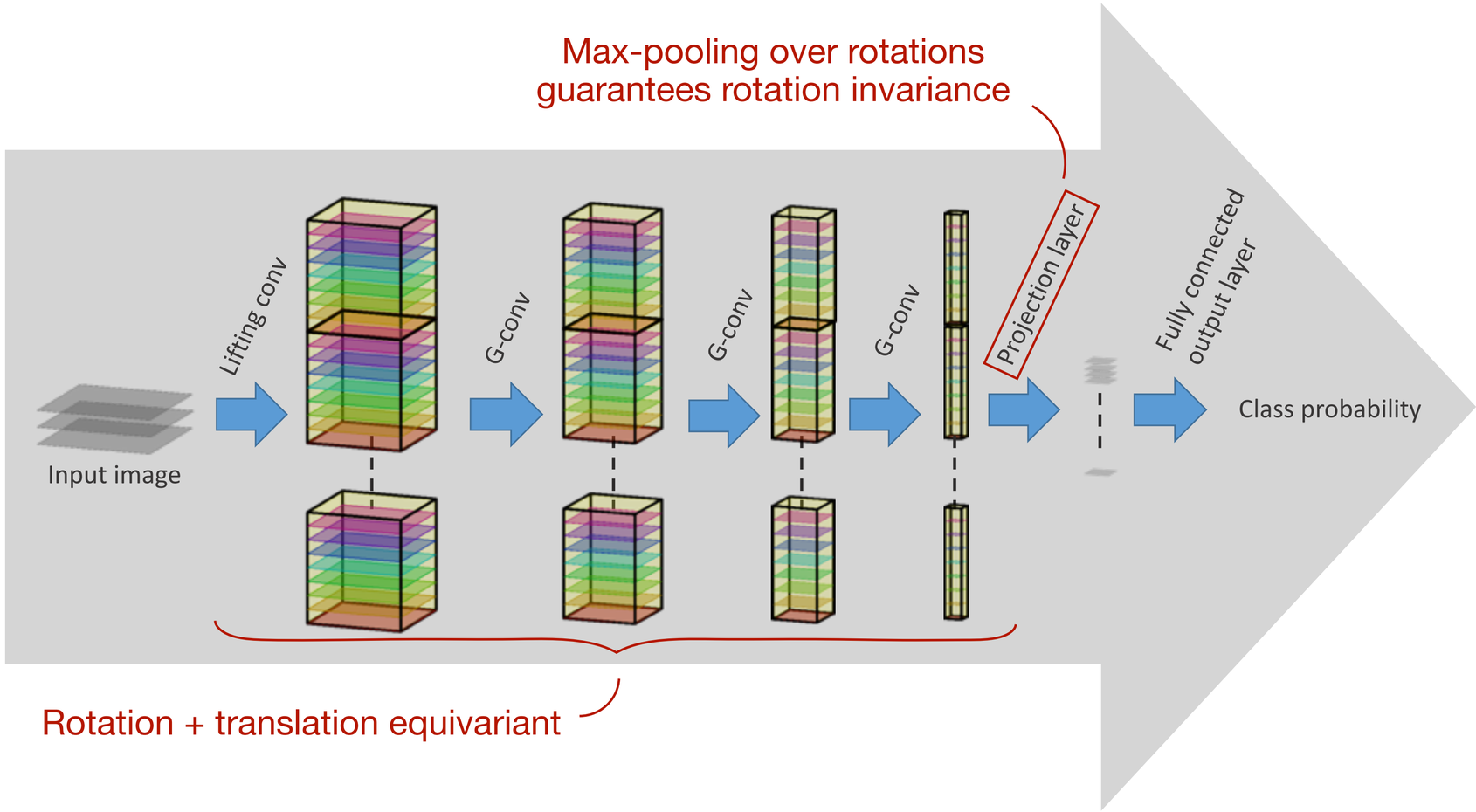
Architecture for rotation invariant mitotic cell detection





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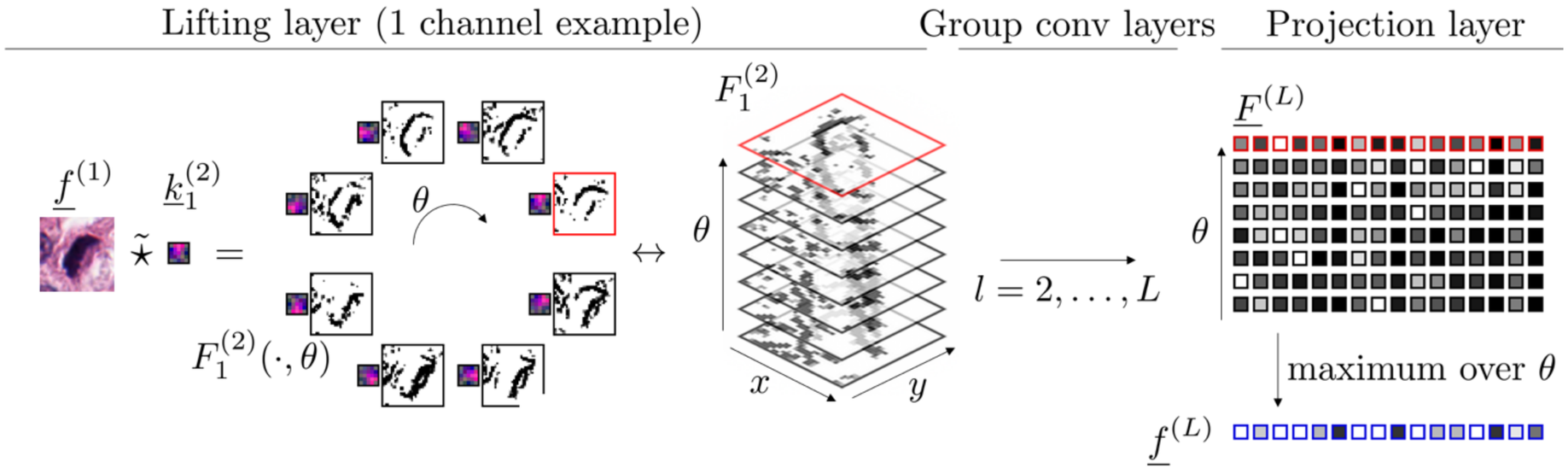
Bekkers & Lafarge et al. MICCAI 2018

Architecture for rotation invariant mitotic cell detection



Bekkers & Lafarge et al. MICCAI 2018

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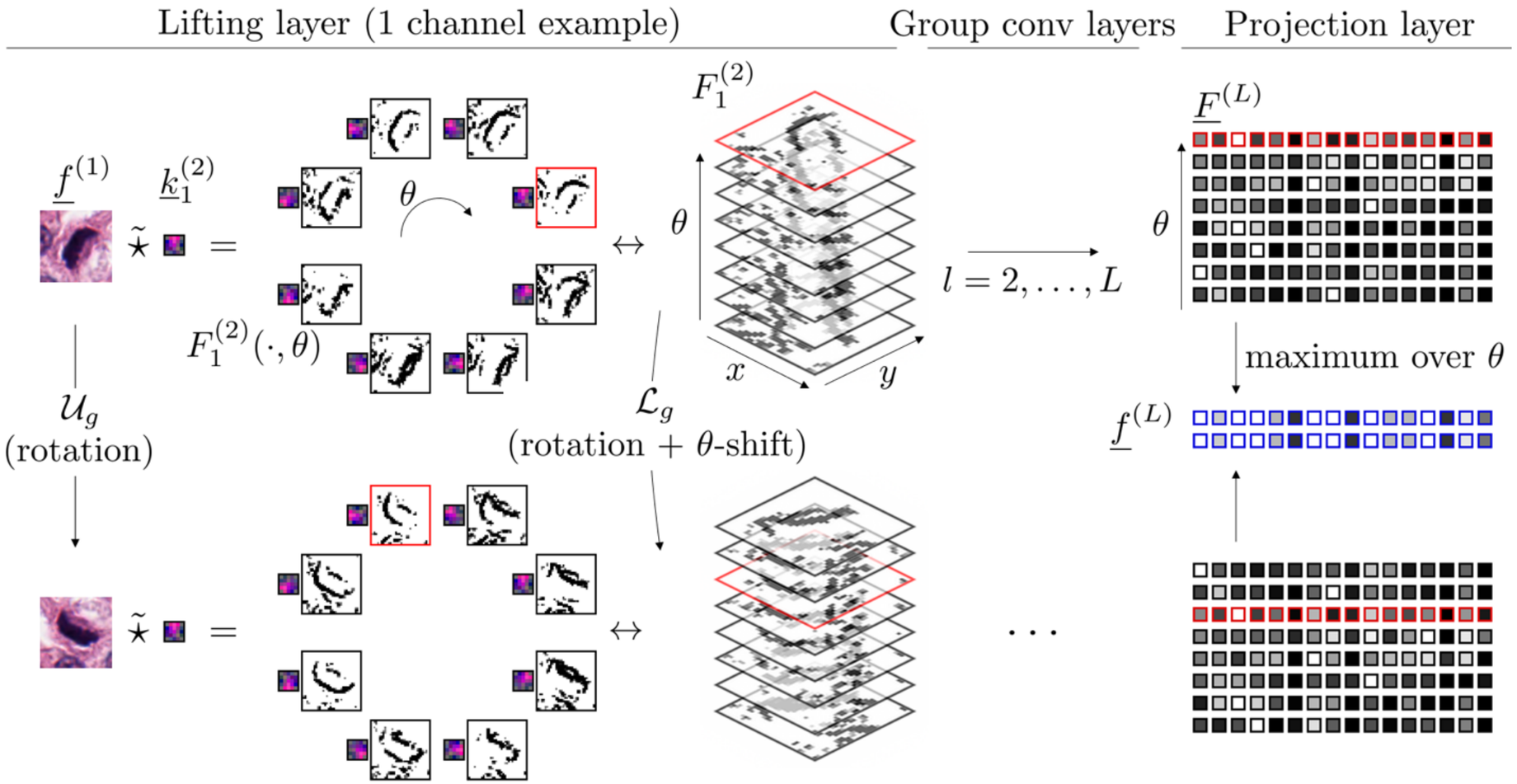
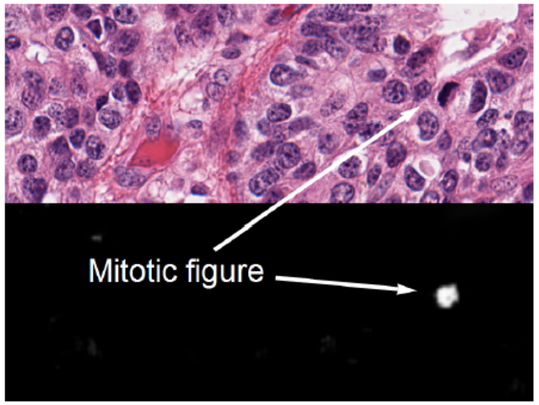
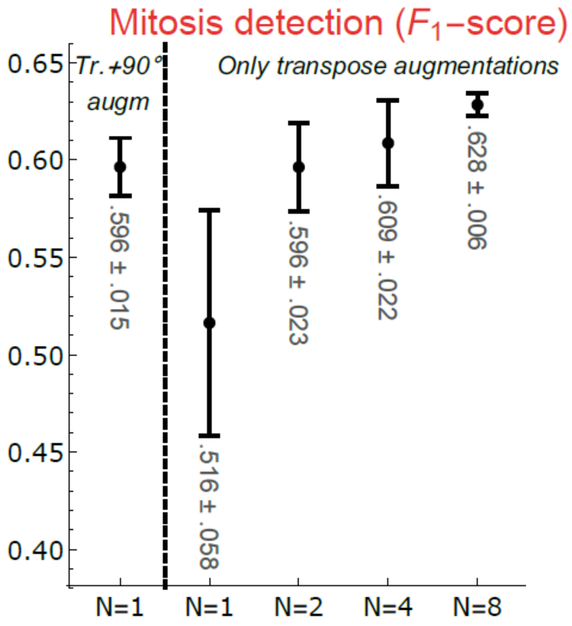


Architecture for rotation invariant mitotic cell detection

Bekkers & Lafarge et al. MICCAI 2018

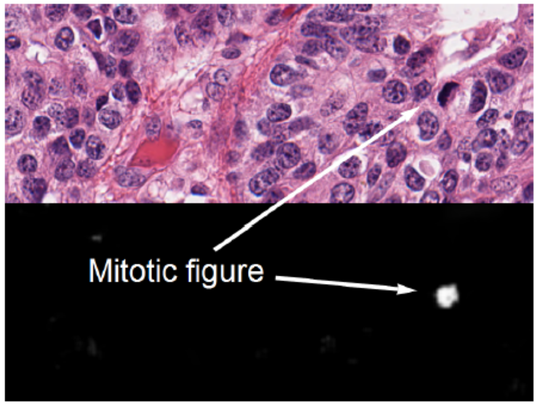


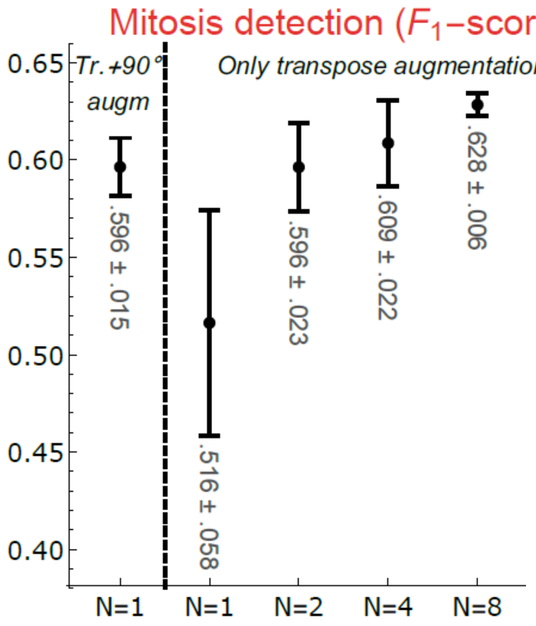


G-CNNs without data-augmentation
outperform
CNNs with data-augmentation

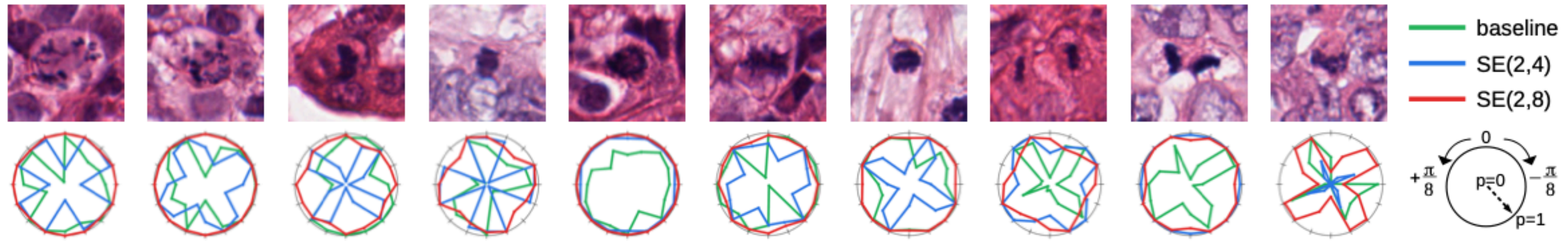
Architecture for rotation invariant mitotic cell detection

Bekkers & Lafarge et al. MICCAI 2018





Lafarge et al. MedIA 2020

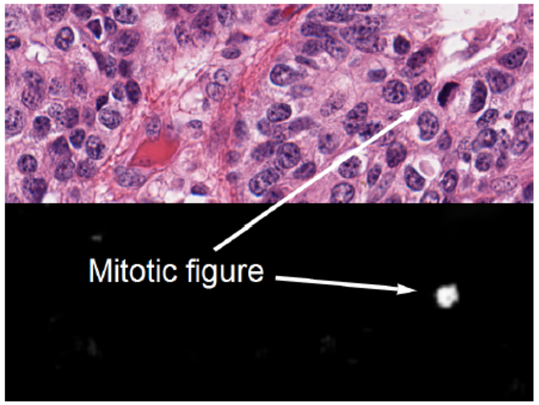


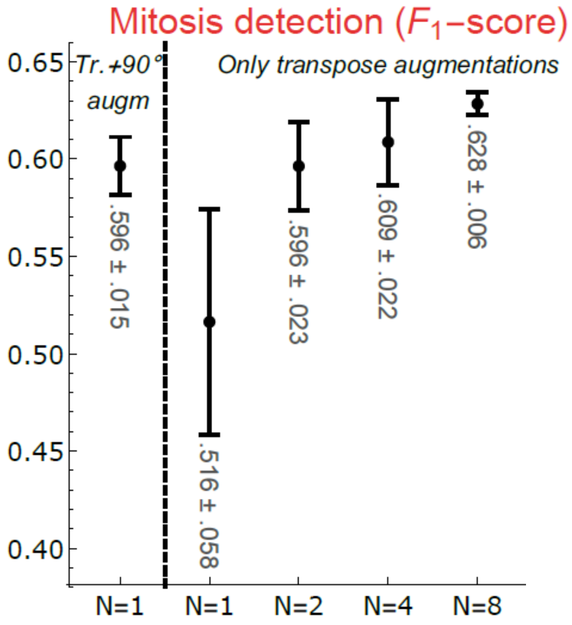
*G-CNNs guarantee geometric stability. They are **robust to input distortions**, regular CNNs aren't…*

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

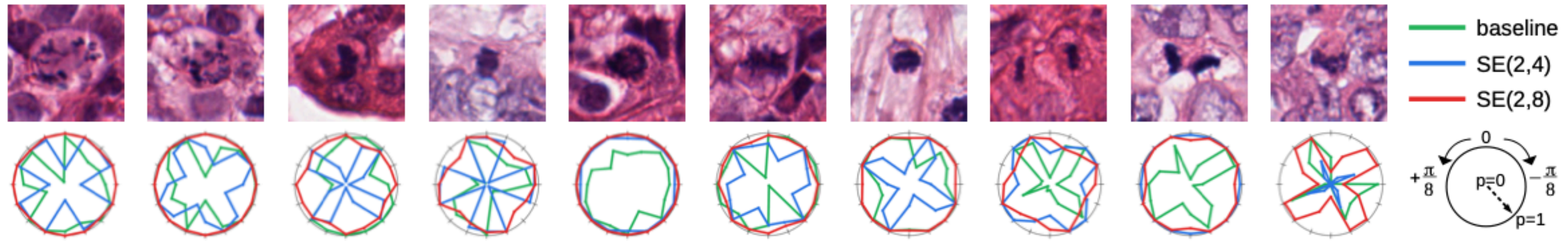
Architecture for rotation invariant mitotic cell detection

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

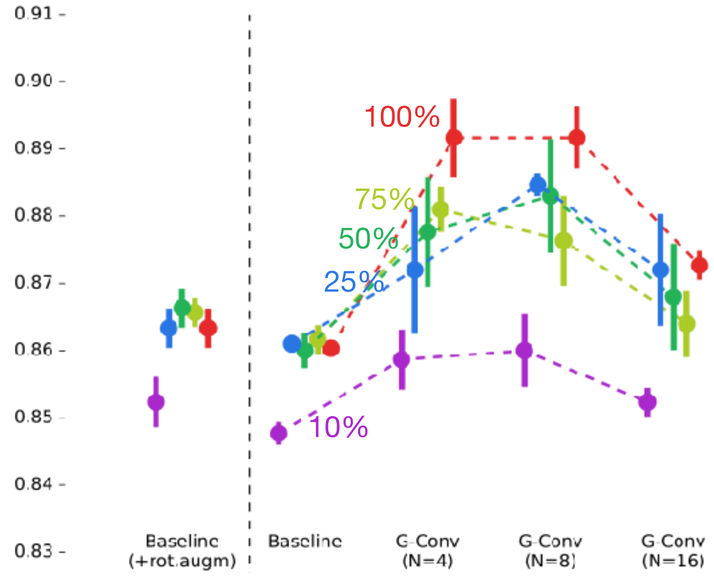


Figure 7: Mean and Standard Deviation plots summarizing the accuracy of the tumor classification models. Mean ± standard deviation is indicated. Color identifies the different data regime (red: 100%; lime: 75%; green: 50%; blue: 25%; purple: 10%).

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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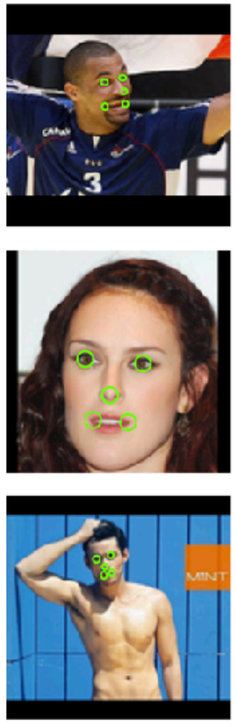
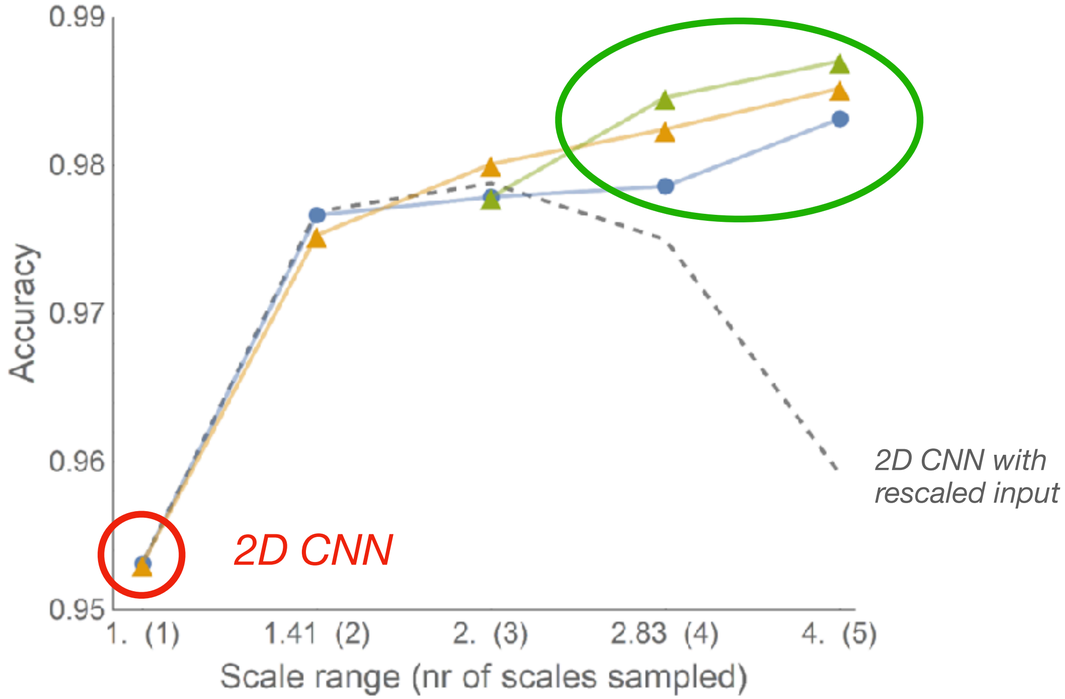
From rotation to scale equivariant CNNs

Bekkers ICLR 2020

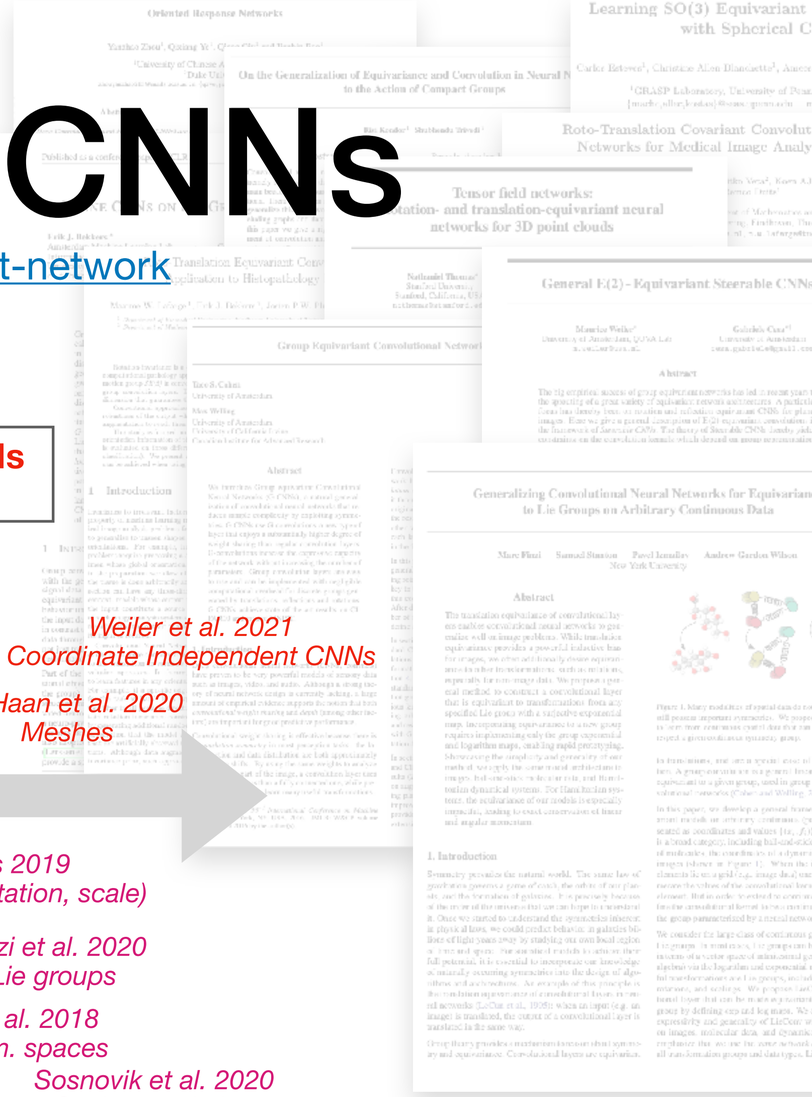
Translation + *scale equivariant G-CNNs*





A brief history of G-CNNs

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



Discrete G-CNNs
(square/cube symmetries)

Gauge-equivariant CNNs
(manifolds)

NNs

CNNs

G-CNNs

LeCun et al. 1990

Cohen-Welling 2016
p4m

Winkels-Cohen 2018
3D discrete roto-transl.

Hoogeboom et al. 2018
SE(2,6)

Dieleman et al. 2016
p4m

Worrall-Brostow 2018
3D discrete roto-transl.

Cohen et al. 2019
Icosahedron

Weiler et al. 2021
Coordinate Independent CNNs

de Haan et al. 2020
Meshes

Mallat et al. 2013, 2015
SE(2)

Worrall et al. 2017
SE(2)

Cohen et al. 2018
SE(3)

Bekkers 2019
Lie groups (rotation, scale)

Esteves 2017
SO(3)

Kondor-Trivedi 2018
SE(3)

Bekkers et al. 2014-2018
SE(2)

Weiler et al. 2018
SE(3)

Finzi et al. 2020
Lie groups

Kondor 2018
SE(3)

Weiler et al. 2017
SE(2)

Chakraborty et al. 2018
Riemannian Hom. spaces

Zhou et al. 2017
SE(2)

Thomas et al. 2018
SE(3)

Weiler-Cesa 2019
SE(2)

Sosnovik et al. 2020
Scale-translation

Continuous rotation G-CNNs
(regular discretizations)

Continuous rotation G-CNNs
(steerable)

Continuous G-CNNs
(Lie groups)

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

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

1. Motivation — Equivariance → weight-sharing and generalization

2. Pattern matching using group theory — Group theory: symmetries & recognition by components
(features have “poses”)

3. Group convolutions — Template matching over groups

4. Example — Effective representation learning and generalization

5. G-convs are all you need!

6. Steerable group convolutions

7. Feature fields and escnn library

8. Equivariant tensor product layers

9. Equivariant graph NNs

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Theorem (G-convs are all you need)

Bekkers ICLR 2020, Thm. 1*

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 $H = \text{Stab}_G(y_0)$ for some chosen origin $y_0 \in Y$ and let $g_y \in G$ such that $\forall_{y \in Y} : y = g_y y_0$.

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

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

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

*Work with Remco Duits at TU/e.

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

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Steerable basis

A vector $Y(x) = \begin{pmatrix} \vdots \\ Y_l(x) \\ \vdots \end{pmatrix} \in \mathbb{K}^L$ with (basis) functions $Y_l \in \mathbb{L}_2(X)$ is steerable if

$$\forall_{g \in G}: \quad Y(g\,x) = \rho(g) Y(x),$$

where $g\,x$ denotes the action of G on X and $\rho(g) \in \mathbb{K}^{L \times L}$ is a representation of G.

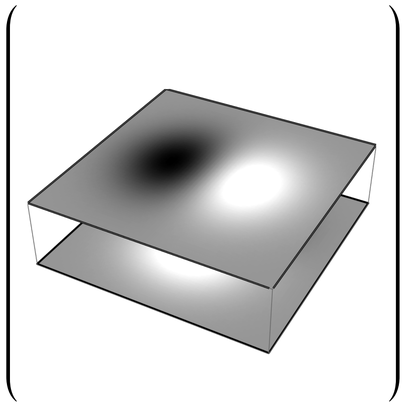
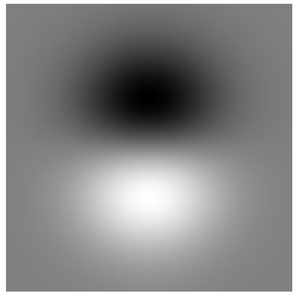
I.e., we can transform all basis functions simply by taking a linear combination of the original basis functions.

Function in steerable basis

Let $f(x \mid \hat{\mathbf{w}}) = \hat{\mathbf{w}}^{\dagger} Y(x)$ ($Y(x)$ a steerable basis)

Then we can steer/shift this function by transforming the weights $\hat{\mathbf{w}}$

$$f(h^{-1}x \mid \hat{\mathbf{w}}) = f(x \mid \rho(h)\hat{\mathbf{w}})$$

$(\rho(h)\hat{\mathbf{w}})^{\dagger}$  $=$ 

$\|$

$Y(x)$

$\|$

$f(x \mid \rho(h)\hat{\mathbf{w}})$

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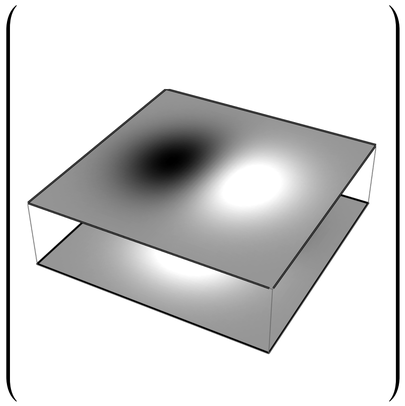
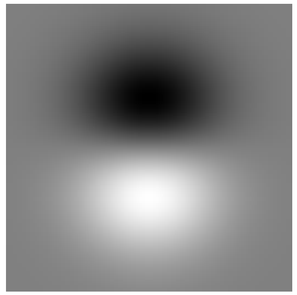
$(\rho(h)\hat{\mathbf{w}})^{\dagger}$  $=$ 

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$Y(x)$

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$f(x \mid \rho(h)\hat{\mathbf{w}})$

Example: Steerable basis on S^1 (circular harmonics)

Basis functions (for $\mathbb{L}_2(S^1)$): $Y_l(\alpha) = e^{i\,l\,\alpha}$

Are steered by representations: $\rho_l(\theta) = e^{i\,l\,\theta}$

Proof: $Y_l(\alpha - \theta) = e^{i\,l\,(\alpha-\theta)}$
$= e^{-i\,l\,\theta}\, e^{i\,l\,\alpha}$
$= \rho_l(-\theta)\, Y_l(\alpha)$

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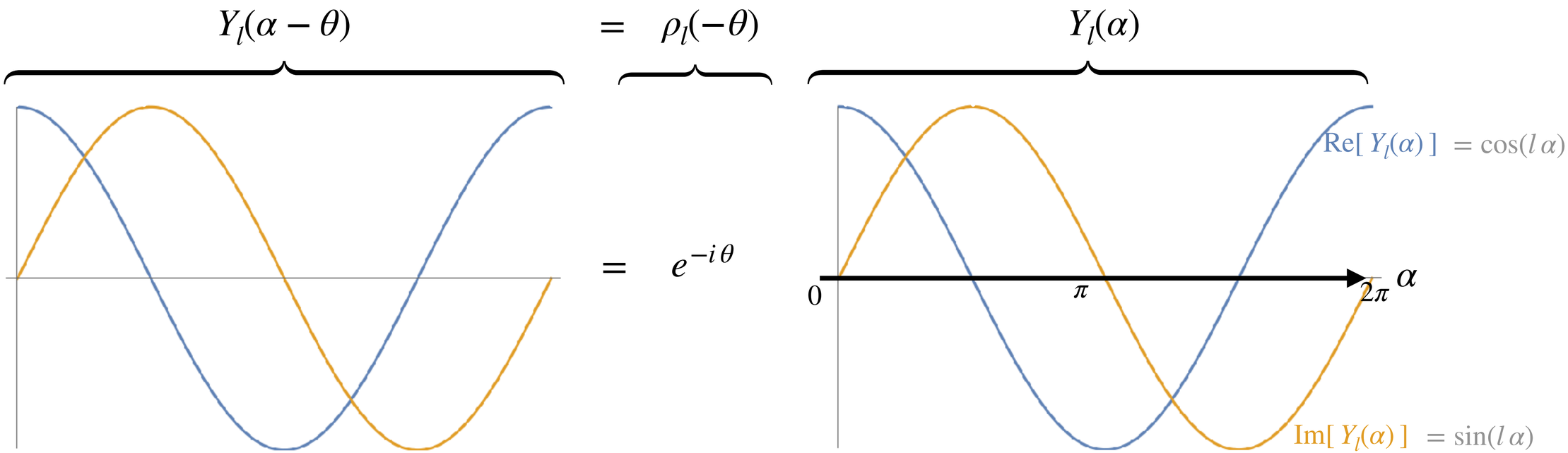

Example: Steerable basis on S^1 (circular harmonics)

$Y(\alpha - \theta)$

$$\rho(-\theta) = \bigoplus_{l=-L}^{L} \rho_l(-\theta)$$

$Y(\alpha)$

$$\begin{pmatrix} \\ \\ \\ \\ \\ \\ \\ \end{pmatrix} = \begin{pmatrix} e^{i3\theta} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{i2\theta} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & e^{i1\theta} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{-i1\theta} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{-i2\theta} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & e^{-i3\theta} \end{pmatrix} \begin{pmatrix} \\ \\ \\ \\ \\ \\ \\ \end{pmatrix}$$

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Basis functions (for $\mathbb{L}_2(S^1)$):

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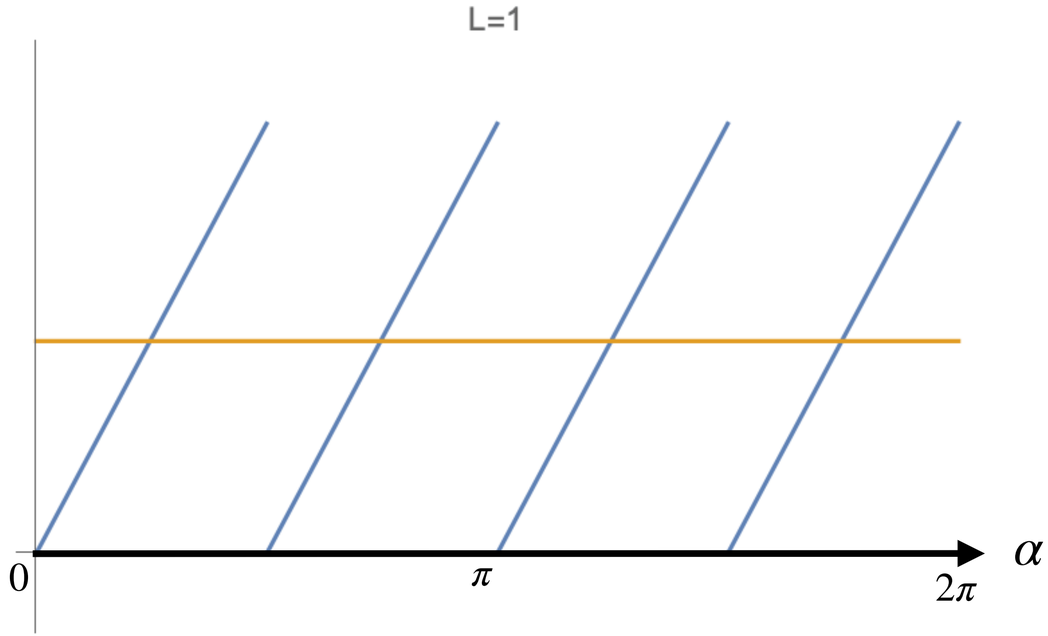
Form a complete orthonormal (Fourier) basis:

$$f(\alpha \,|\, \hat{\mathbf{w}}) = \sum_{l=-\infty}^{\infty} \overline{\hat{w}_l}\; Y_l(\alpha)$$

Y_l are given by the irreps of $SO(2)$ and hence form orthogonal basis (Peter-Weyl Theorem)



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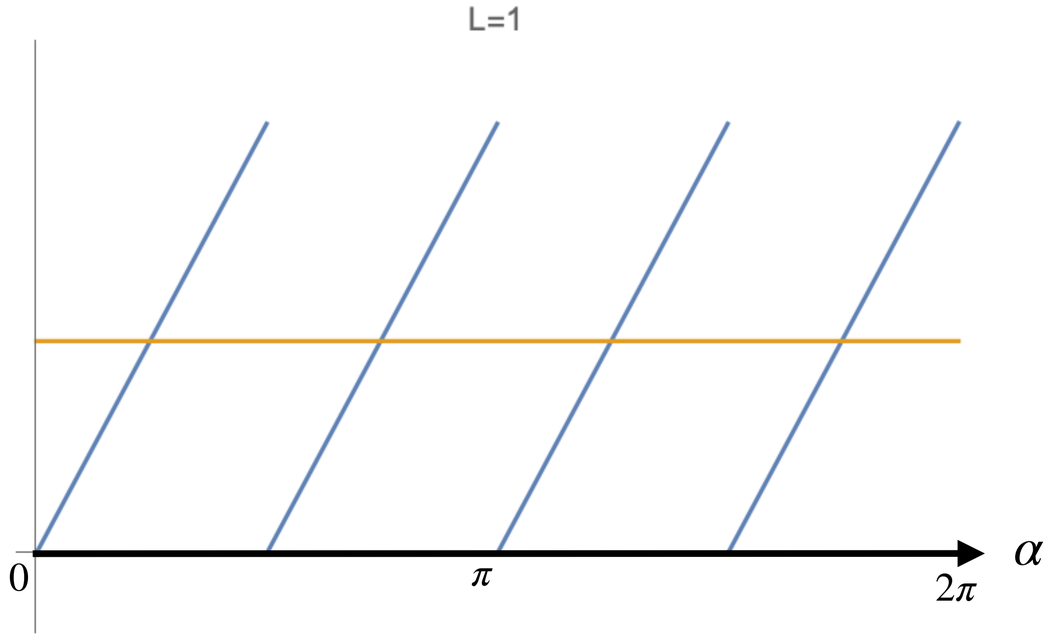

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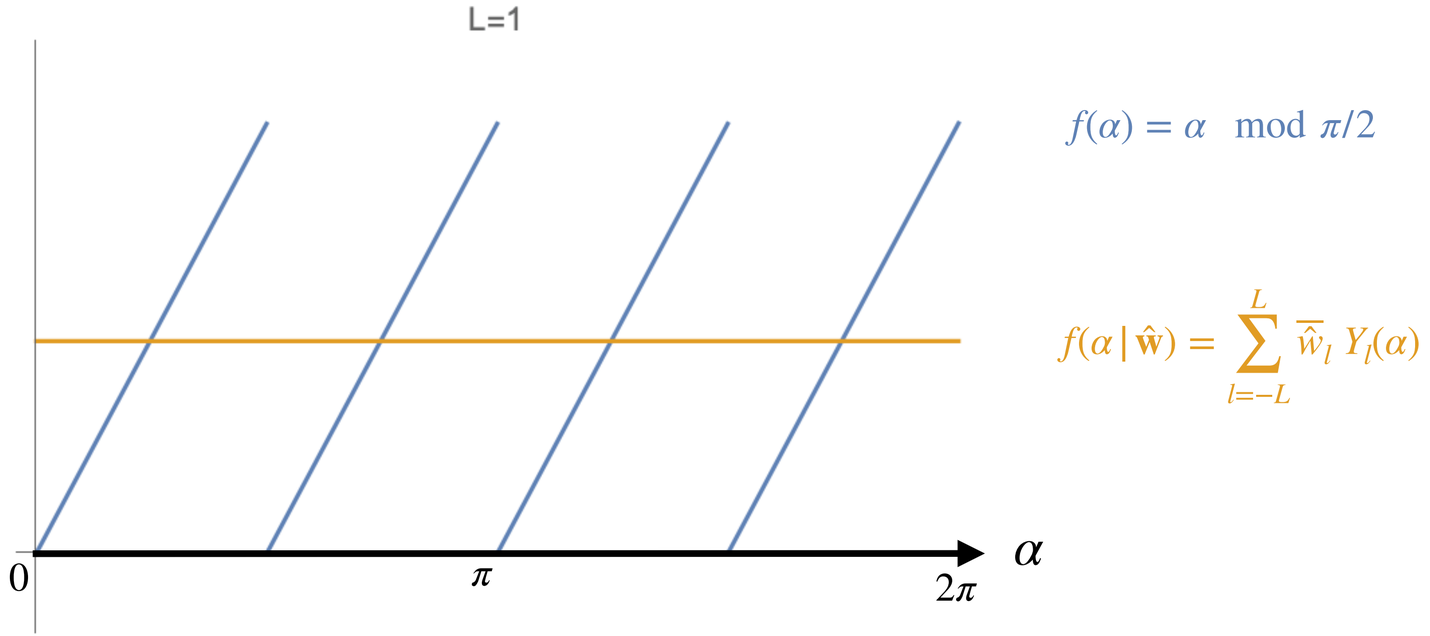

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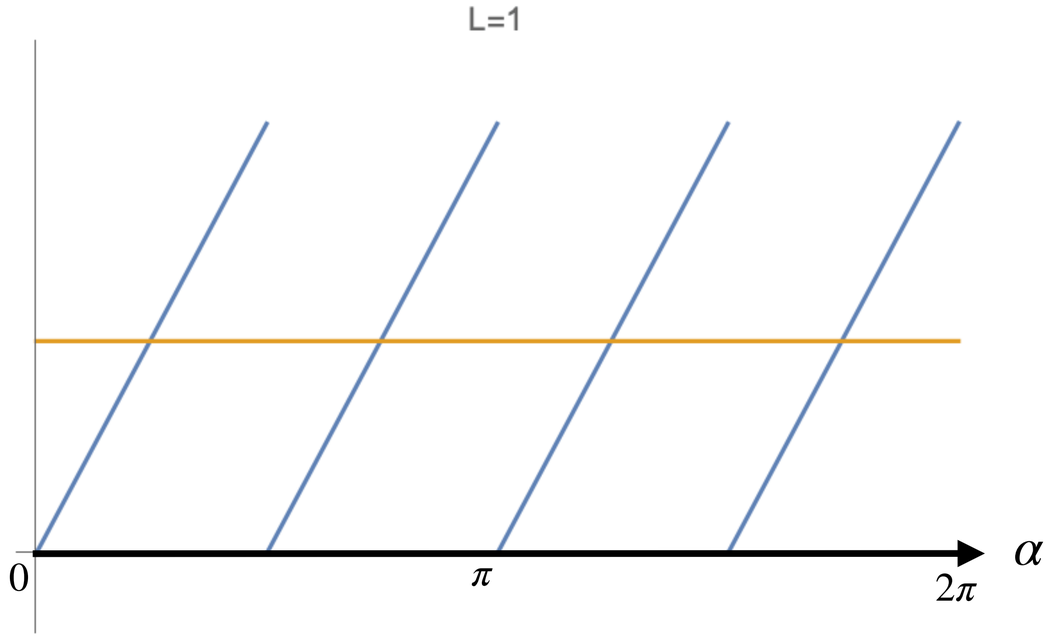

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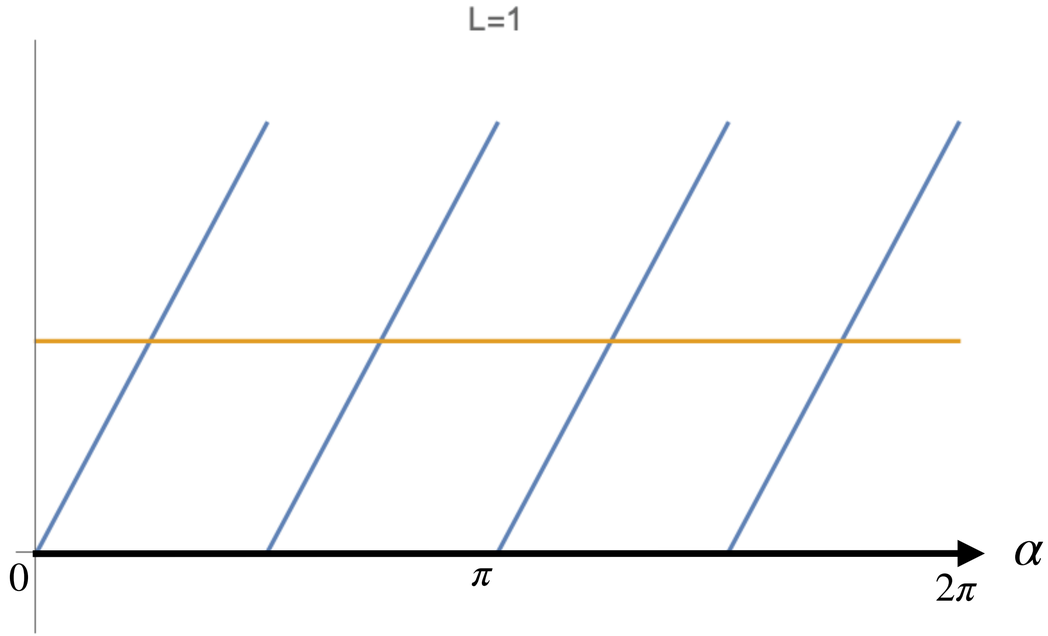

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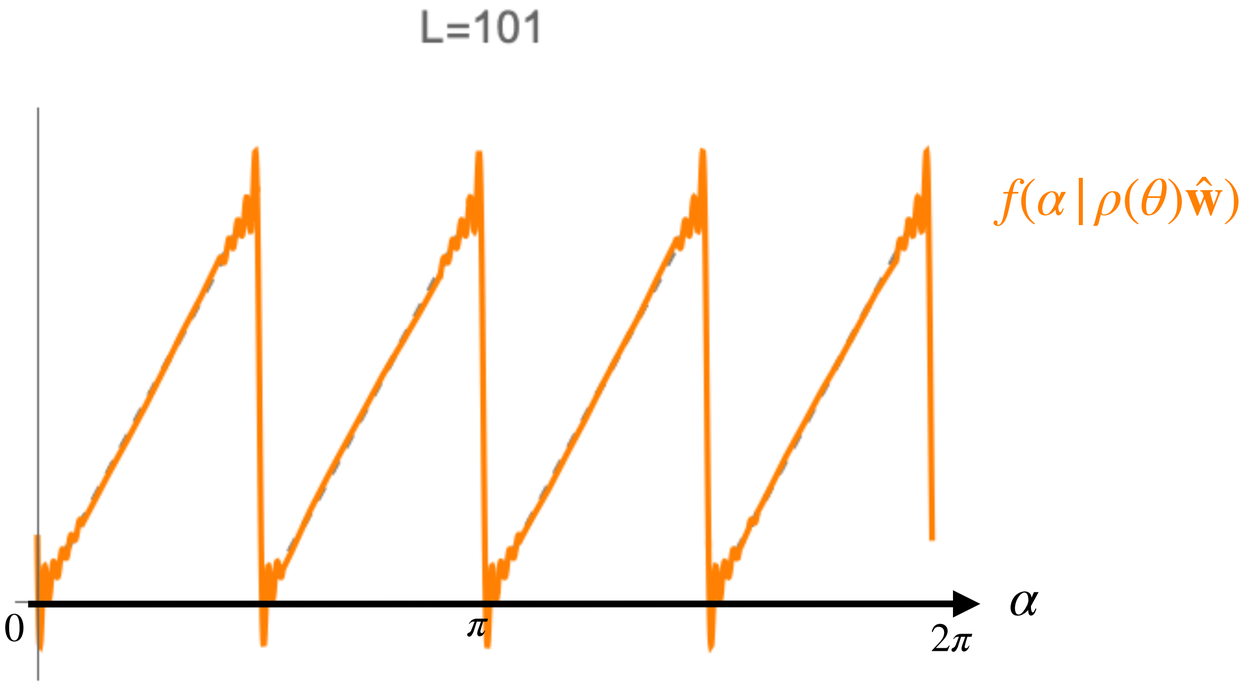
$$f(\alpha - \theta \,|\, \hat{\mathbf{w}}) = f(\alpha \,|\, \rho(\theta)\hat{\mathbf{w}})$$

Proof:
$$\begin{aligned} f(\alpha - \theta \,|\, \hat{\mathbf{w}}) &= \hat{\mathbf{w}}^\dagger Y(\alpha - \theta) \\ &= \hat{\mathbf{w}}^\dagger \rho(-\theta) Y(\alpha) \\ &= \hat{\mathbf{w}}^\dagger \rho(\theta)^\dagger Y(\alpha) \\ &= (\rho(\theta)\hat{\mathbf{w}})^\dagger Y(\alpha) \\ &= f(\alpha \,|\, \rho(\theta)\hat{\mathbf{w}}) \end{aligned}$$



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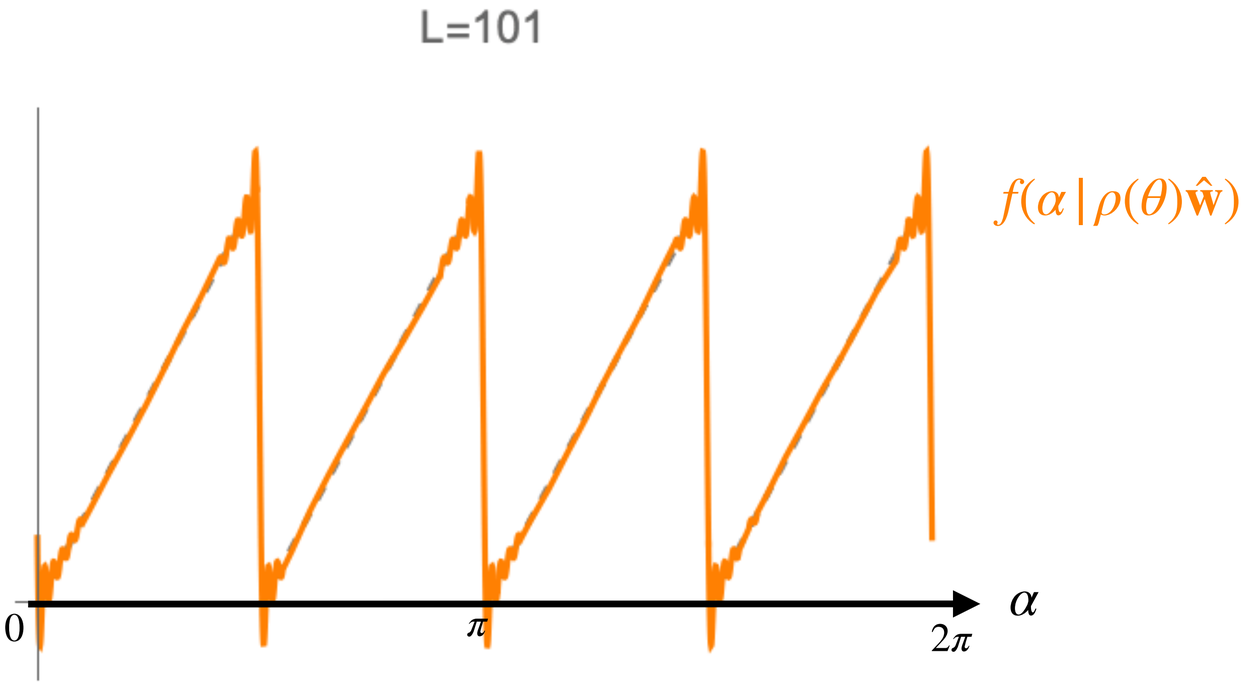
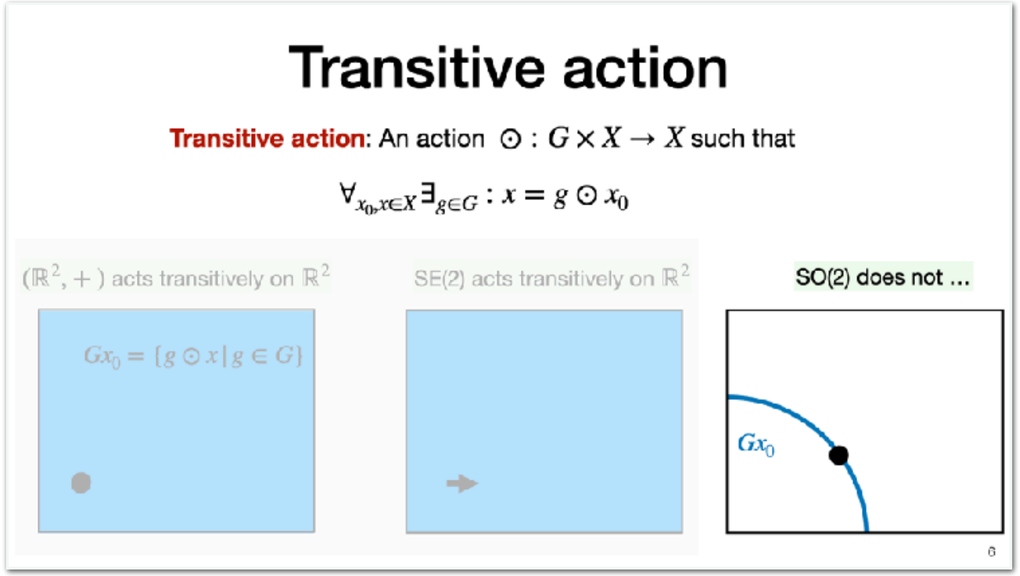


Two dimensional rotation-steerable functions

- The previous functions $\rho_l(\theta) = e^{i\,l\,\theta}$ are (irreducible) representations of $SO(2)$

- The group $SO(2)$ can also act on $\mathbb{R}^2$
  - Though not transitively…
  - It does act transitively on S^1 though

Recall lecture 1.6 (Group Theory | Homogeneous/quotient spaces)



- Use polar coordinates $\mathbb{R}^2 \ni \mathbf{x} \quad \leftrightarrow \quad (r, \alpha) \in \mathbb{R}^+ \times S^1$ to come up with a rotation-steerable basis for $\mathbb{L}_2(\mathbb{R}^2)$!

Two dimensional rotation-steerable functions

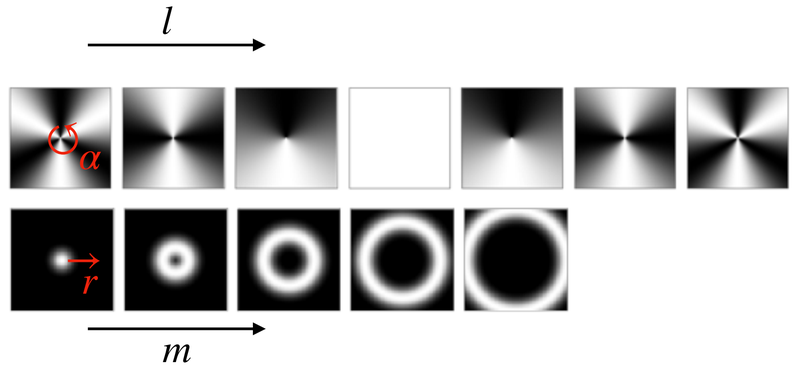
- Consider polar-separable convolution kernel:

$$k(\mathbf{x}\,|\,\mathbf{w}) = k^{\rightarrow}(r\,|\,\mathbf{w})\,k^{\circlearrowleft}(\alpha\,|\,\mathbf{w}),$$

- with $k^{\circlearrowleft}$ in an $SO(2)$ steerable basis, and $k^{\rightarrow}$ in some radial basis:

$$k^{\circlearrowleft}(\alpha\,|\,\mathbf{w}) = \sum_l \overline{w}_l Y_l(\alpha), \qquad \text{e.g., with} \qquad Y_l(\alpha) = e^{i\,l\,\alpha},$$

$$k^{\rightarrow}(r\,|\,\mathbf{w}) = \sum_m w_m \phi_m(r)$$



- Then we may as well write it as

$$\begin{aligned} k(\mathbf{x}\,|\,\mathbf{w}) &= \sum_l \sum_m w_m \overline{w}_l\, \phi_m(r)\, Y_l(\alpha) \\ &= \sum_l \sum_m \overline{w}_{ml}\, \phi_m(r)\, Y_l(\alpha) \qquad \text{(“absorb” weights)} \\ &= \sum_l \overline{\hat{w}}_l(r)\, Y_l(\alpha) \qquad \text{with radius dependent weights } \hat{w}_l(r) = \sum_m w_{ml}\, \phi_m(r) \end{aligned}$$

- Then such kernel is clearly rotation steerable!

$$k(\mathbf{R}_\theta^{-1}\mathbf{x}\,|\,\hat{\mathbf{w}}(r)) = k(\mathbf{x}\,|\,\rho(\theta)\hat{\mathbf{w}}(r))$$

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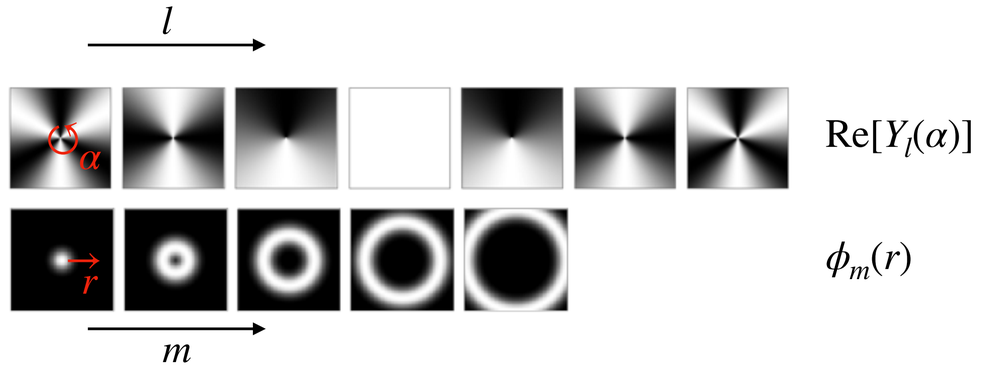

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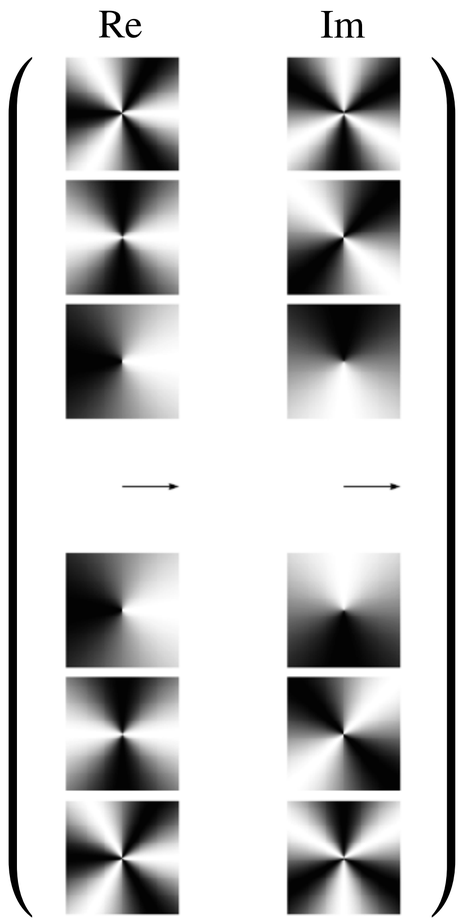
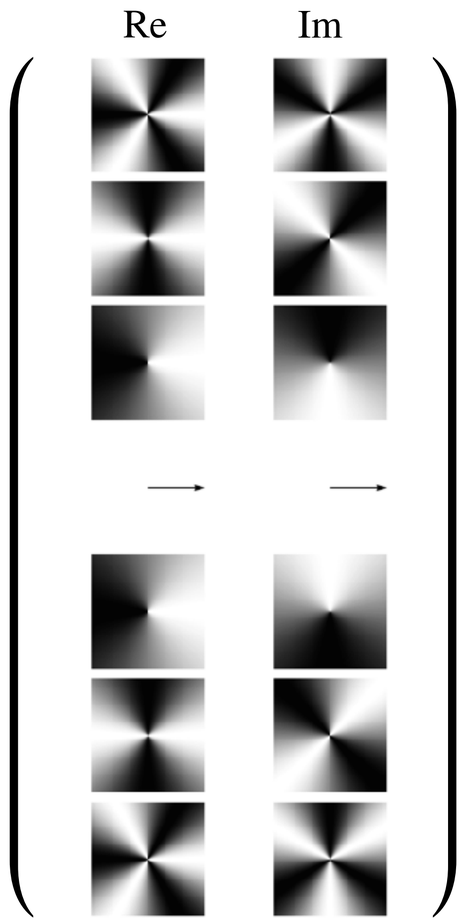
Or directly parametrize as $\hat{\mathbf{w}}(r) = \mathrm{MLP}(r\,|\,\mathbf{w})$!

Complex (irreducible) representations

$$Y(\mathbf{R}_\theta^{-1}\,\mathbf{x}) = \rho(\mathbf{R}_\theta^{-1})\, Y(\mathbf{x})$$



$$= \begin{pmatrix} e^{3\,i\theta} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{2\,i\theta} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & e^{1\,i\theta} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{-1\,i\theta} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{-2\,i\theta} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & e^{-3\,i\theta} \end{pmatrix}$$



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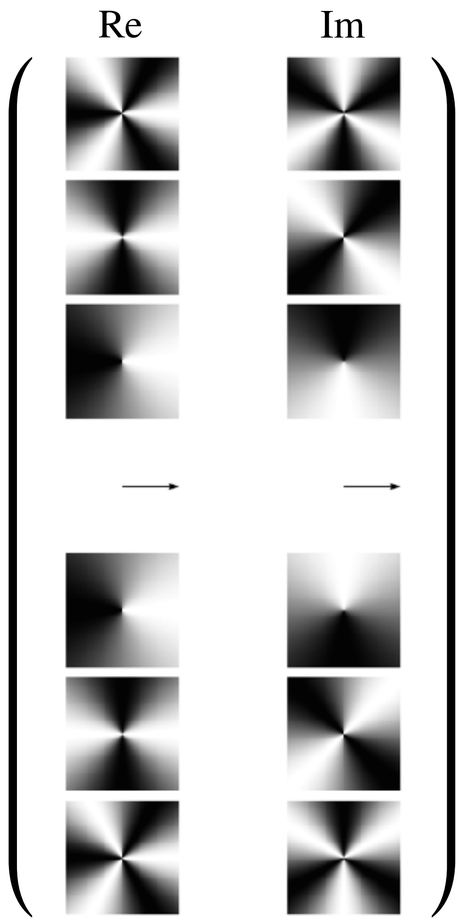

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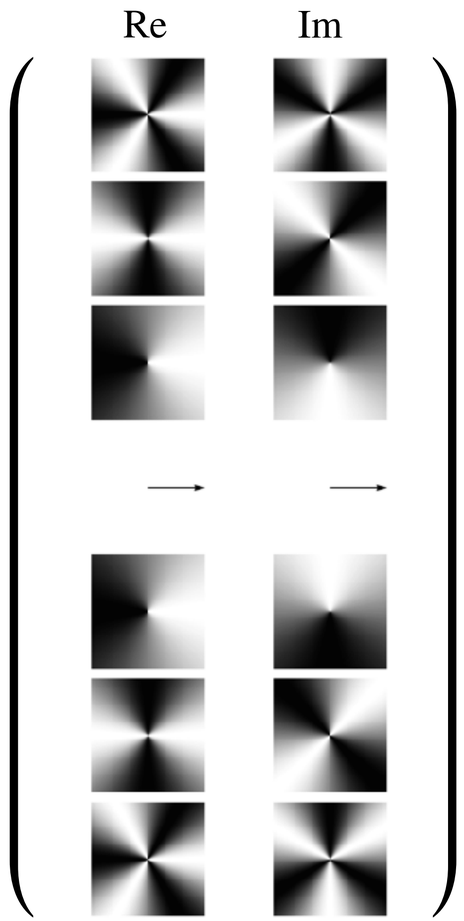
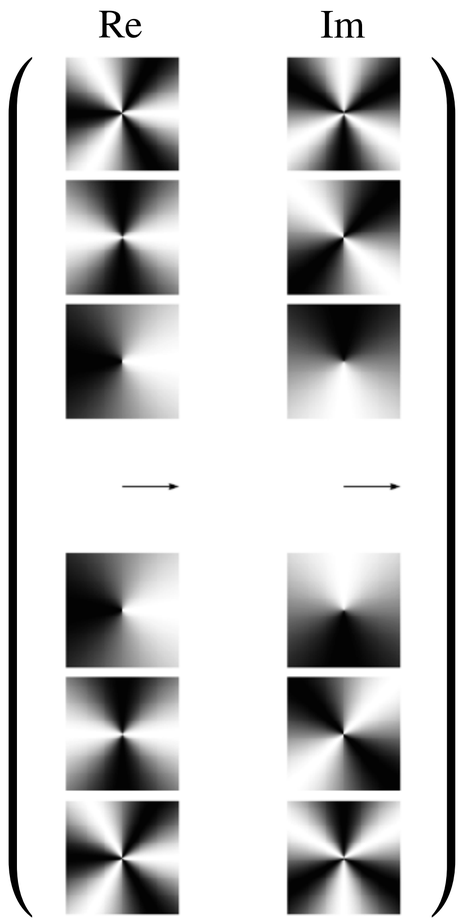


Complex (irreducible) representations

$$Y(\mathbf{R}_\theta^{-1}\,\mathbf{x}) = \rho(\mathbf{R}_\theta^{-1})\, Y(\mathbf{x})$$



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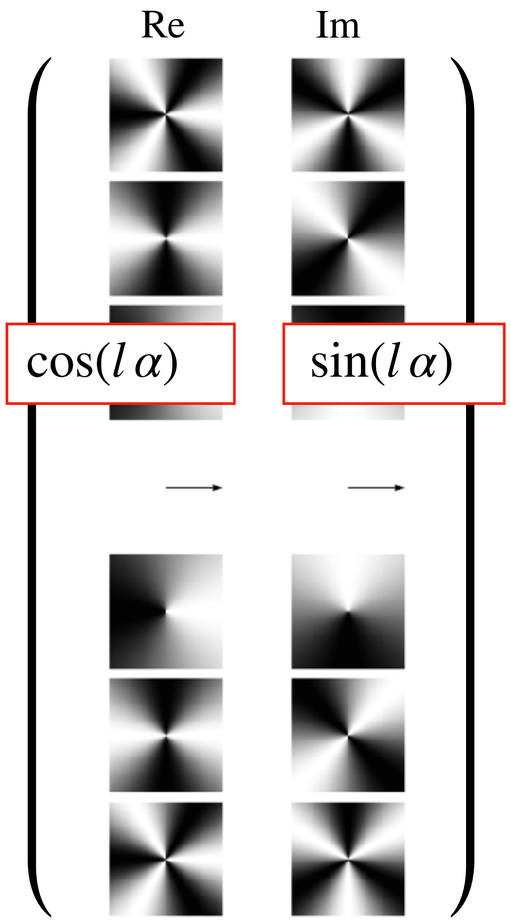
$$\begin{pmatrix}
e^{3\,i\,\theta} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & e^{2\,i\,\theta} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & e^{1\,i\,\theta} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & e^{-1\,i\,\theta} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & e^{-2\,i\,\theta} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & e^{-3\,i\,\theta}
\end{pmatrix}$$



Real (irreducible) representations

$$Y(\mathbf{R}_\theta^{-1}\,\mathbf{x}) \;=\; \rho(\mathbf{R}_\theta^{-1})\; Y(\mathbf{x})$$

$$\begin{pmatrix} \\ \\ \\ \\ \\ \\ \\ \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos\theta & \sin\theta & 0 & 0 & 0 & 0 \\ 0 & -\sin\theta & \cos\theta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cos 2\theta & \sin 2\theta & 0 & 0 \\ 0 & 0 & 0 & -\sin 2\theta & \cos 2\theta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cos 3\theta & \sin 3\theta \\ 0 & 0 & 0 & 0 & 0 & -\sin 3\theta & \cos 3\theta \end{pmatrix} \begin{pmatrix} \\ \\ \\ \\ \\ \\ \\ \end{pmatrix}$$

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$$Y(\mathbf{R}_\theta^{-1}\,\mathbf{x}) \;=\; \rho(\mathbf{R}_\theta^{-1})\; Y(\mathbf{x})$$

$$\begin{pmatrix} \\ \\ \\ \\ \\ \\ \\ \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos\theta & \sin\theta & 0 & 0 & 0 & 0 \\ 0 & -\sin\theta & \cos\theta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cos 2\theta & \sin 2\theta & 0 & 0 \\ 0 & 0 & 0 & -\sin 2\theta & \cos 2\theta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cos 3\theta & \sin 3\theta \\ 0 & 0 & 0 & 0 & 0 & -\sin 3\theta & \cos 3\theta \end{pmatrix} \begin{pmatrix} \\ \\ \\ \\ \\ \\ \\ \end{pmatrix}$$

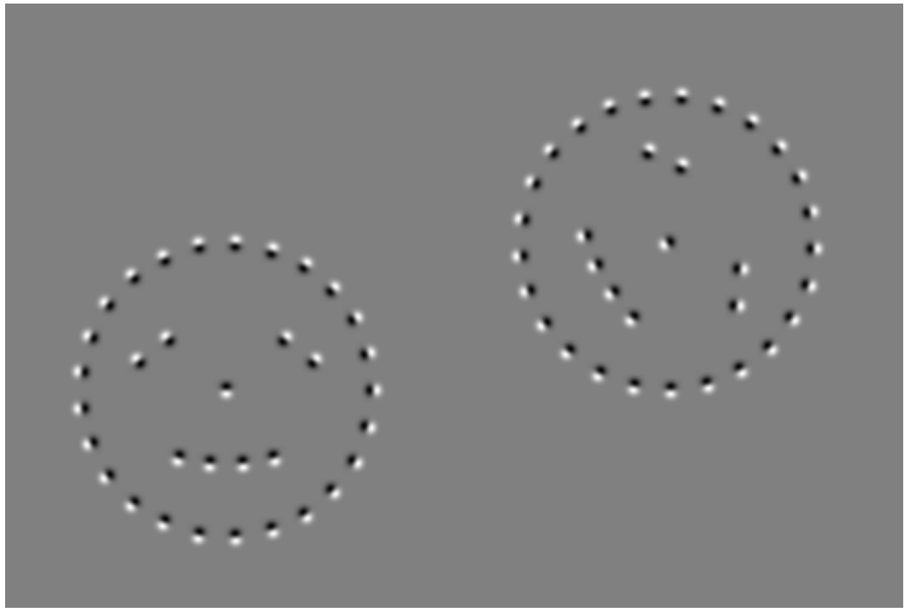
Regular group convolutions revisited

Group convolution ($G = \mathbb{R}^d \rtimes H$):

(e.g. $G = SE(2) = \mathbb{R}^2 \rtimes SO(2)$)
$X = \mathbb{R}^2$

$$(k \,\tilde{\star}\, f)(g) = (\mathscr{L}_g^{G \to \mathbb{L}_2(X)} k \,,\, f)_{\mathbb{L}_2(X)}$$

$\tilde{\star}$



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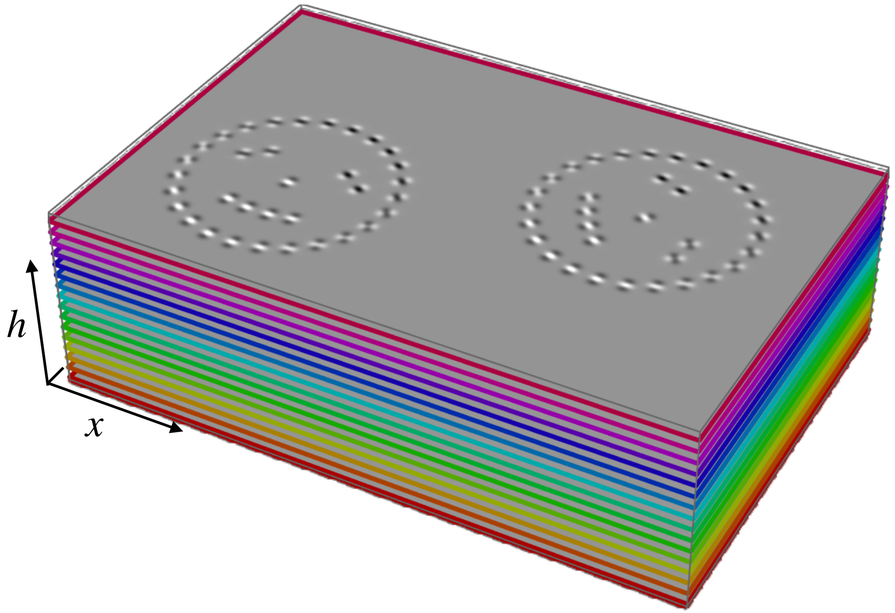

2D convolution kernel

2D input feature map

SE(2) output feature map

Regular group convolutions revisited

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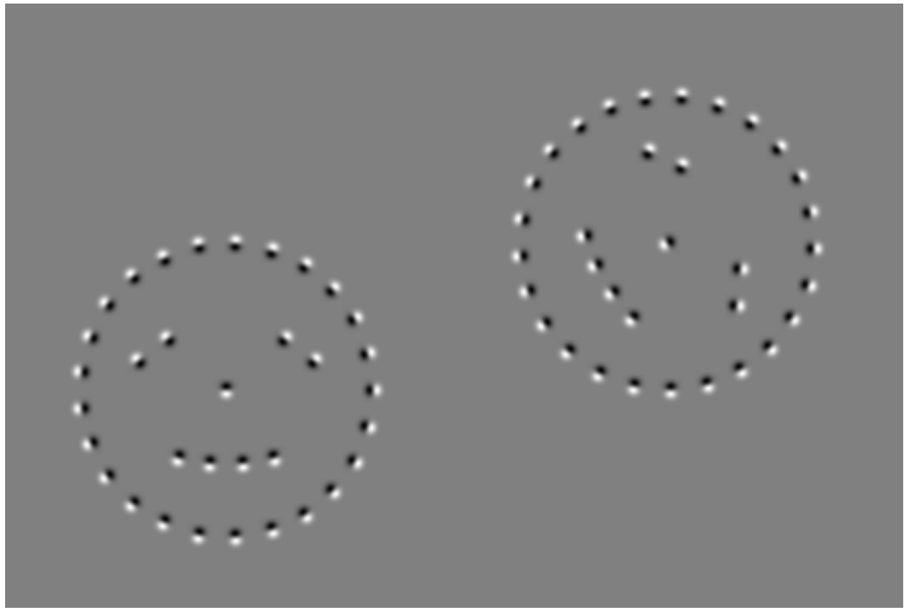
$$= \int_{\mathbb{R}^d} k(g^{-1}\mathbf{x}')f(\mathbf{x}')\mathrm{d}\mathbf{x}'$$

$\tilde{\star}$



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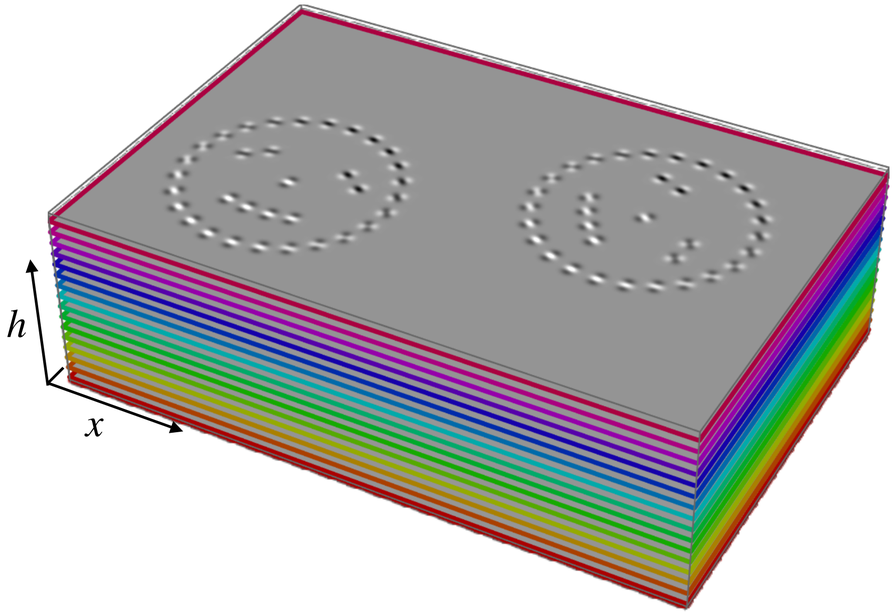

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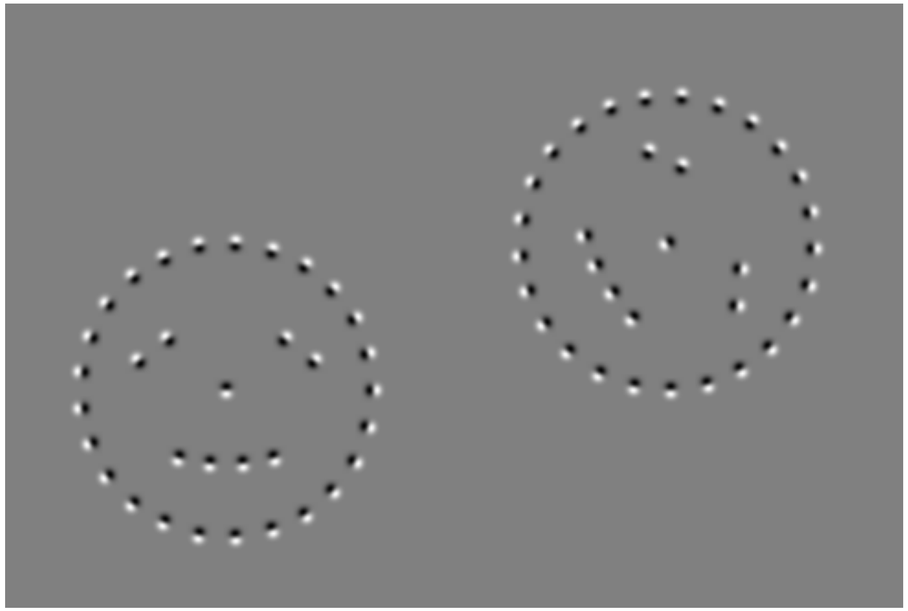

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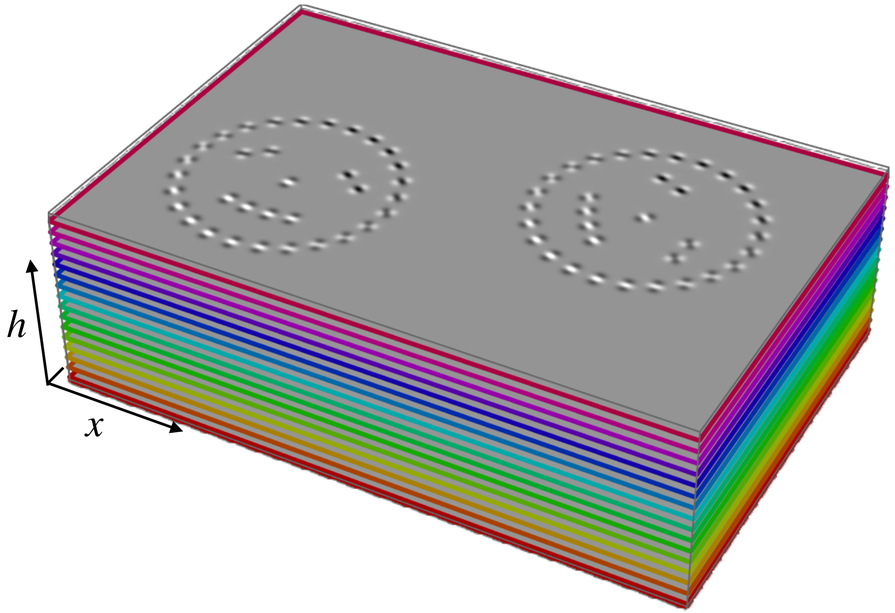

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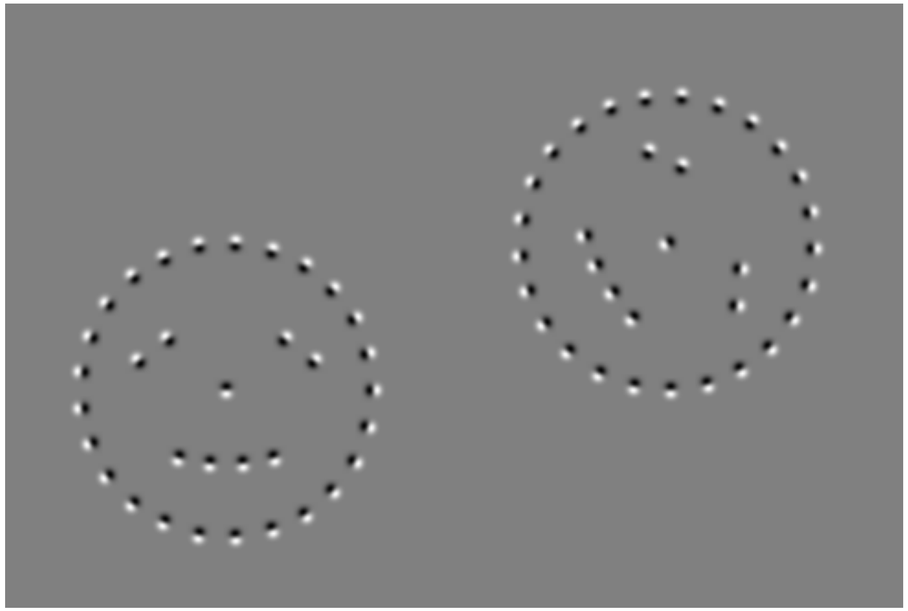
$$= \int_{\mathbb{R}^d} k(g^{-1}\mathbf{x}') f(\mathbf{x}') \mathrm{d}\mathbf{x}' = \int_{\mathbb{R}^2} k(h^{-1}(\mathbf{x}' - \mathbf{x})) f(\mathbf{x}') \mathrm{d}\mathbf{x}'$$

$\tilde{\star}$



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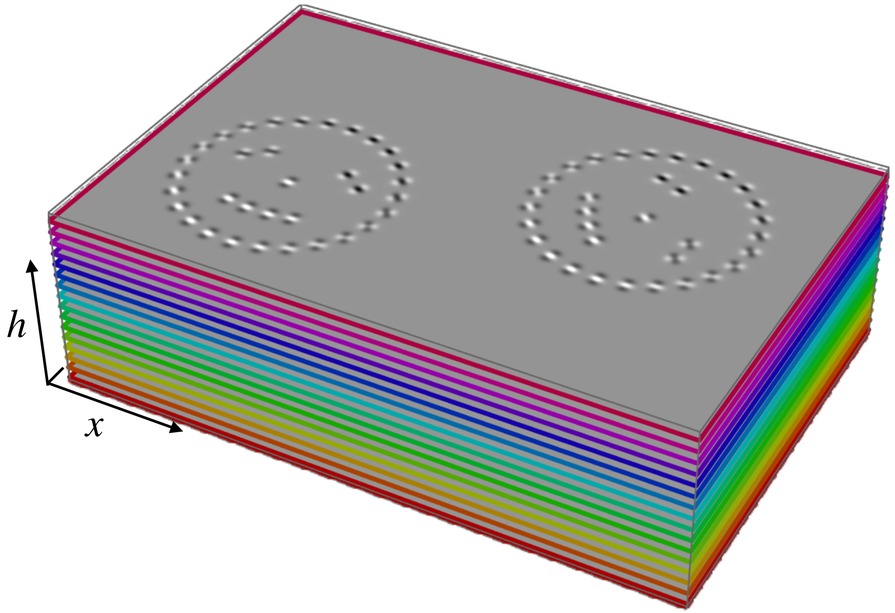

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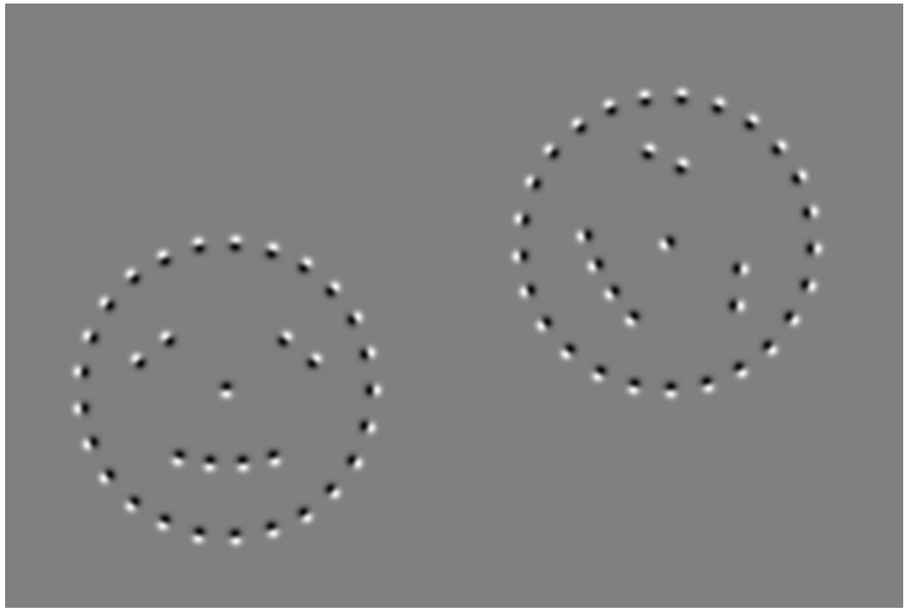
$\tilde{\star}$



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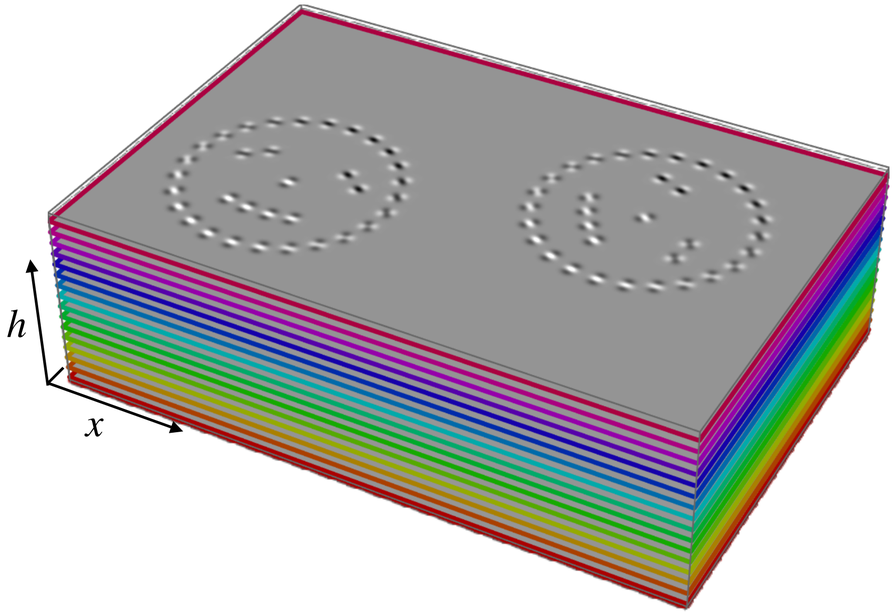

2D convolution kernel

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Regular group convolutions revisited

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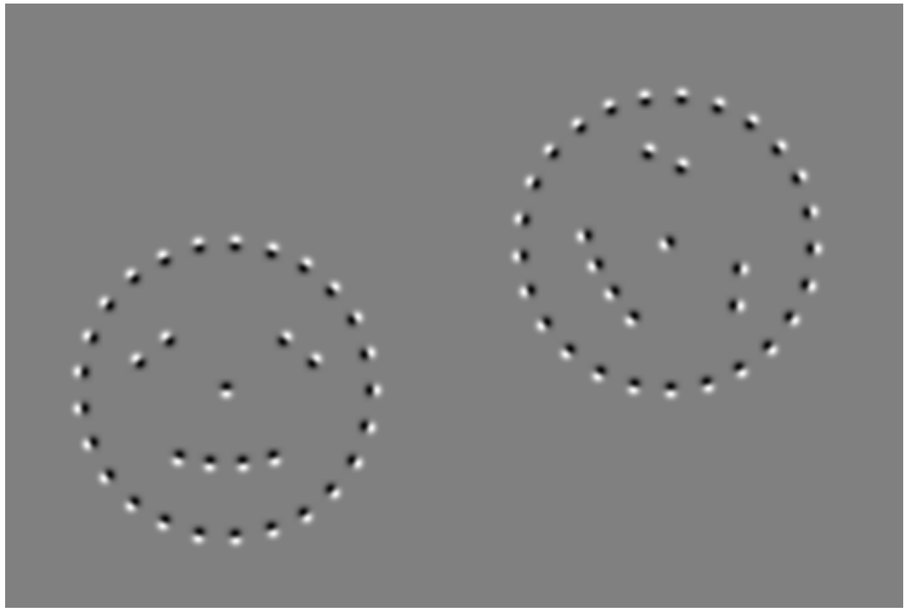
translation
"template matching"

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



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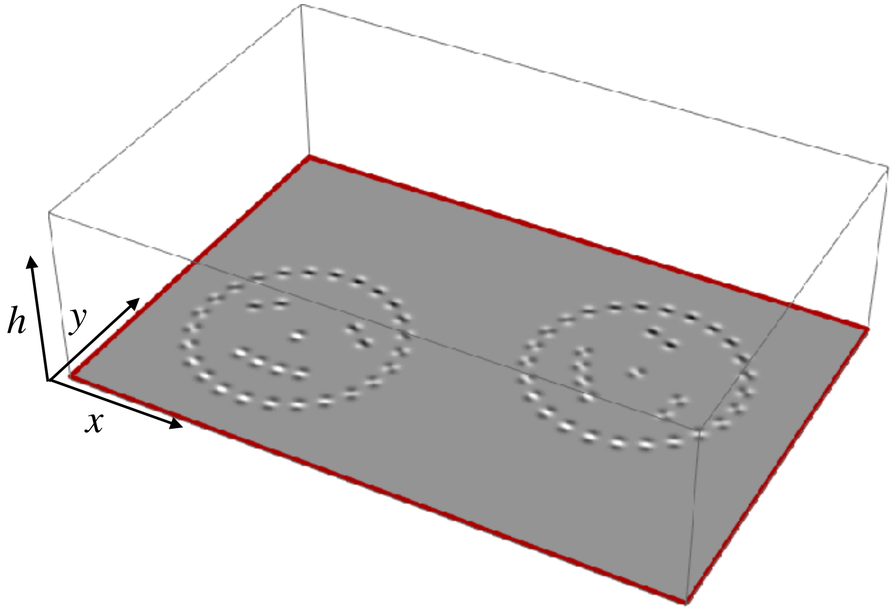

Rotated
2D convolution kernel

2D input feature map

SE(2) output feature map

Regular group convolutions revisited

Group convolution ($G = \mathbb{R}^d \rtimes H$):

(e.g. $G = SE(2) = \mathbb{R}^2 \rtimes SO(2)$)
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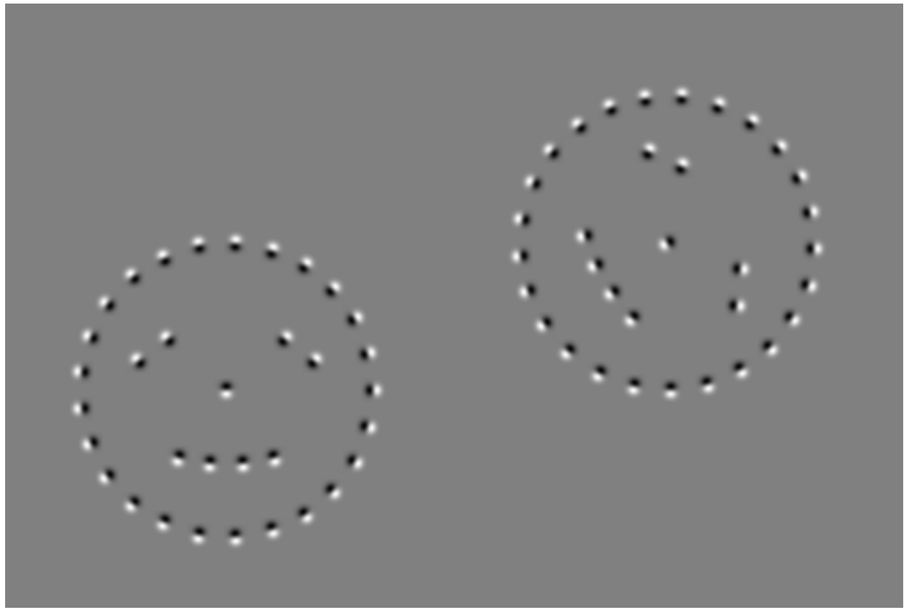
translation
"template matching"

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



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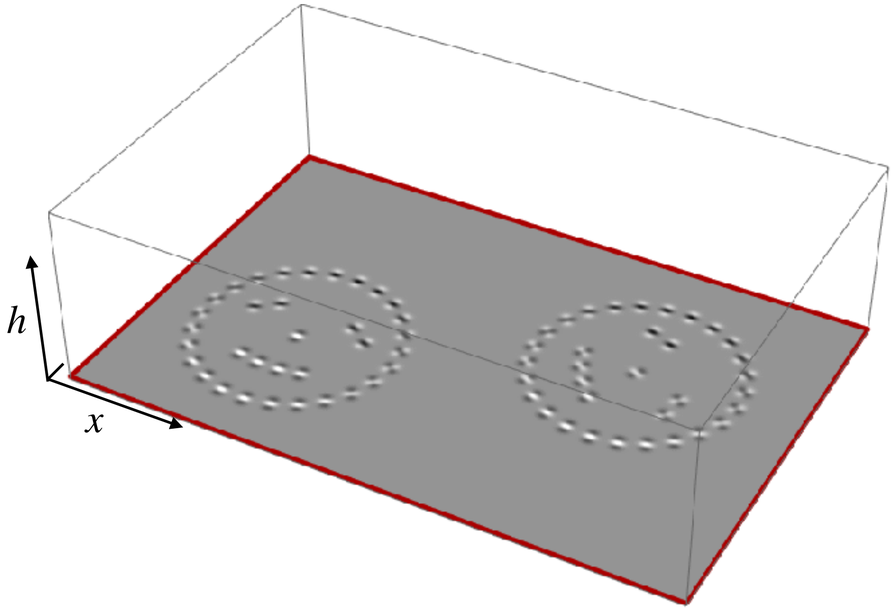

Rotated
2D convolution kernel

2D input feature map

SE(2) output feature map

Regular group convolutions revisited

Group convolution ($G = \mathbb{R}^d \rtimes H$):

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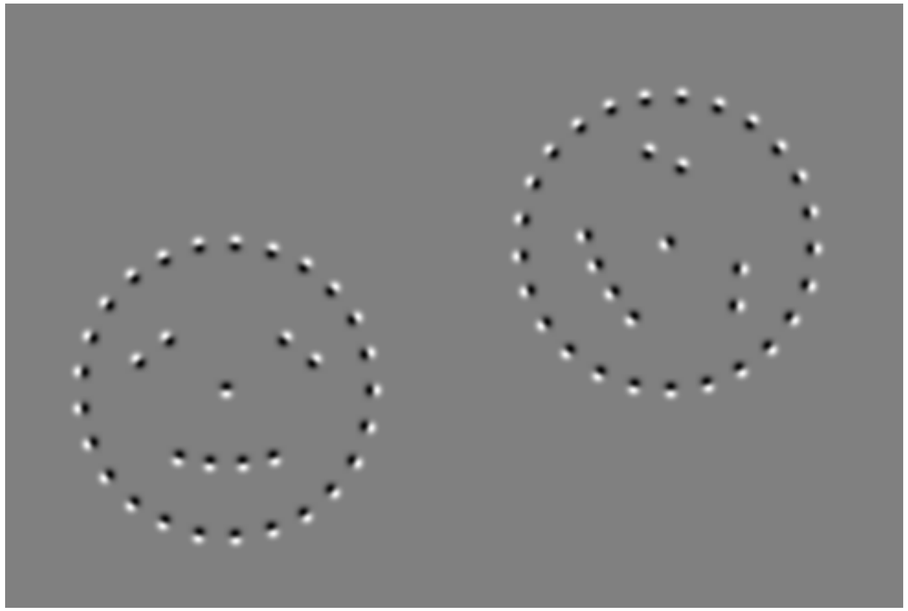
translation
"template matching"

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



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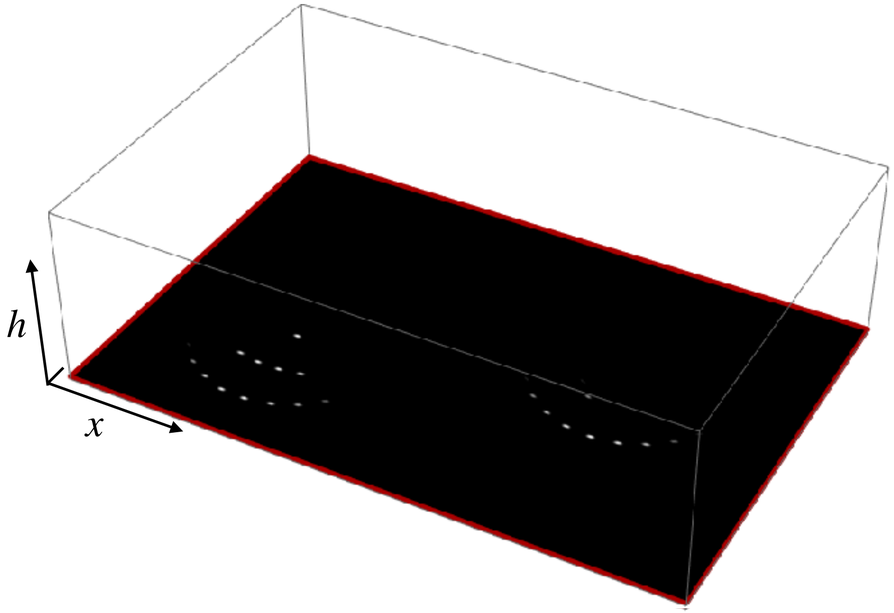

Rotated
2D convolution kernel

2D input feature map

SE(2) output feature map (after ReLU)

Regular group convolutions revisited

Group convolution ($G = \mathbb{R}^d \rtimes H$):

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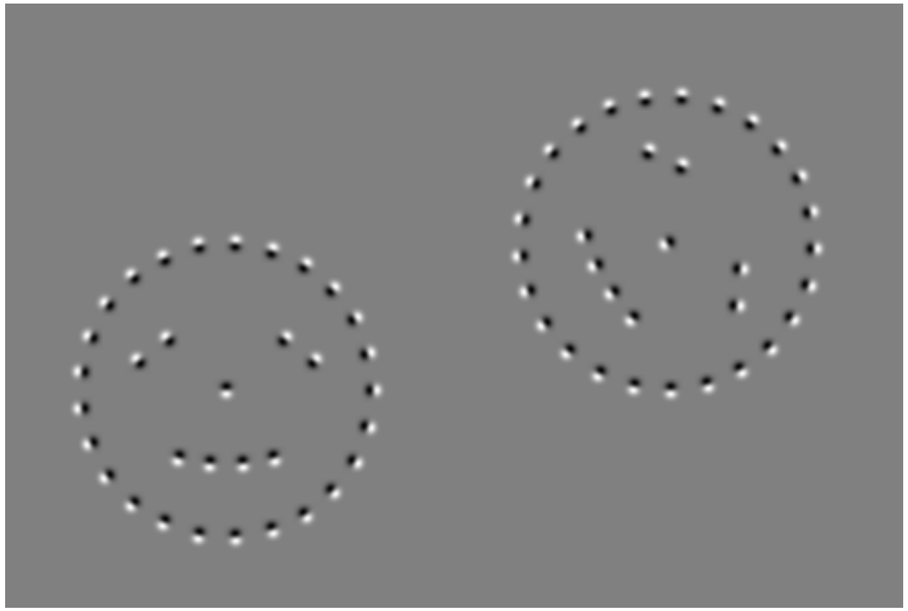
translation
"template matching"

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



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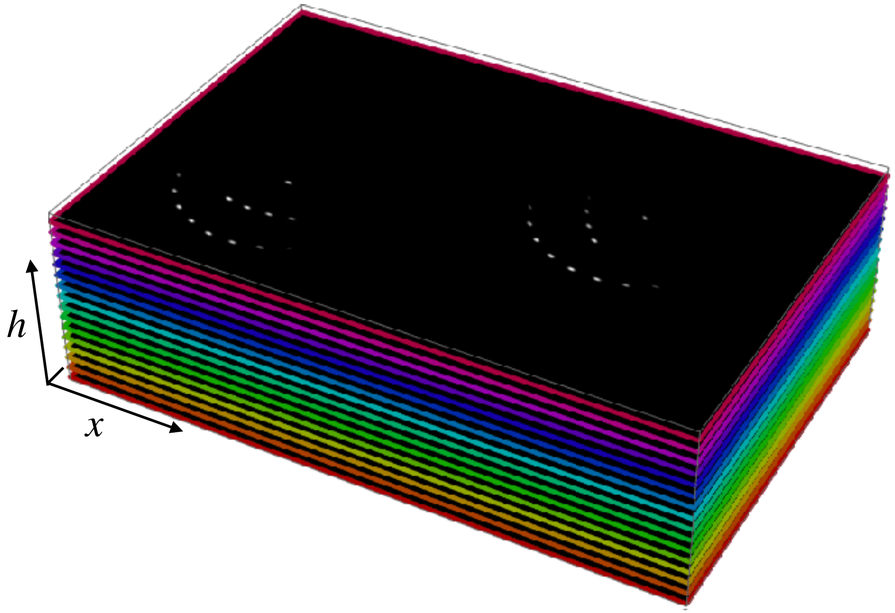

Rotated
2D convolution kernel

2D input feature map

SE(2) output feature map (after ReLU)

Lifting convolution with steerable kernel

Group convolution ($G = \mathbb{R}^d \rtimes H$):

$$(k \,\tilde{\star}\, f)(\mathbf{x}, h) = \int_{\mathbb{R}^d} k(h^{-1}(\mathbf{x}' - \mathbf{x}) \,|\, \hat{\mathbf{w}}) f(\mathbf{x}') \mathrm{d}\mathbf{x}'$$

Lifting convolution with steerable kernel

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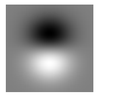
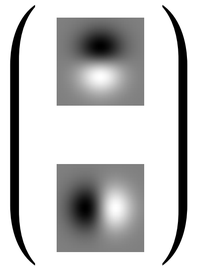
$$k(\mathbf{x} \,|\, \hat{\mathbf{w}}) = \hat{\mathbf{w}}^{\dagger} Y(\mathbf{x})$$





Lifting convolution with steerable kernel

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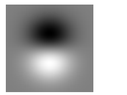
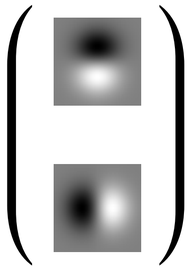
$$k(h^{-1}\,\mathbf{x} \,|\, \hat{\mathbf{w}}) = (\rho(h)\hat{\mathbf{w}})^{\dagger} \quad Y(\mathbf{x})$$





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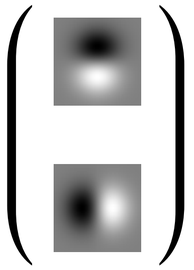
$$k(h^{-1}\,\mathbf{x} \,|\, \hat{\mathbf{w}}) = (\rho(h)\hat{\mathbf{w}})^\dagger \quad Y(\mathbf{x})$$



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$$= (\rho(h)\ \hat{\mathbf{w}})^\dagger \int_{\mathbb{R}^d} Y(\mathbf{x}' - \mathbf{x}) f(\mathbf{x}') \mathrm{d}\mathbf{x}'$$

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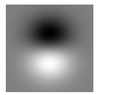
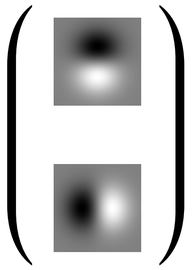
$$= (\rho(h)\ \hat{\mathbf{w}})^\dagger\ \hat{f}^Y(\mathbf{x})$$

$$k(h^{-1}\,\mathbf{x} \,|\, \hat{\mathbf{w}}) = (\rho(h)\hat{\mathbf{w}})^\dagger \quad Y(\mathbf{x})$$





Lifting convolution with steerable kernel

Group convolution ($G = \mathbb{R}^d \rtimes H$):

$$(k \tilde{\star} f)(\mathbf{x}, h) = \int_{\mathbb{R}^d} k(h^{-1}(\mathbf{x}' - \mathbf{x}) \,|\, \hat{\mathbf{w}}) f(\mathbf{x}') \mathrm{d}\mathbf{x}'$$

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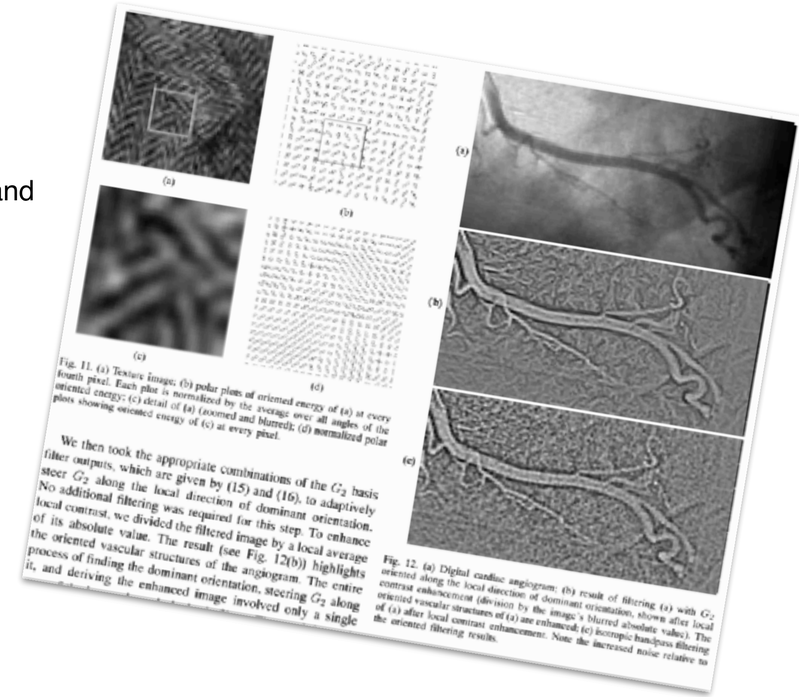

Fig. 11. (a) Texture image. (b) polar plots of oriented energy of (a) at every fourth pixel. Each plot is normalized by the average over all angles of the oriented energy; (c) detail of (a) (zoomed and blurred); (d) normalized polar plots showing oriented energy of (c) at every pixel.

We then took the appropriate combinations of the G_2 basis filter outputs, which are given by (15) and (16), to adaptively steer G_2 along the local direction of dominant orientation. No additional filtering was required for this step. To enhance local contrast, we divided the filtered image by a local average of its absolute value. The result (see Fig. 12(b)) highlights the oriented vascular structures of the angiogram. The entire process of finding the dominant orientation, steering G_2 along it, and deriving the enhanced image involved only a single

Fig. 12. (a) Digital cardiac angiogram. (b) result of filtering (a) with G_2 oriented along the local direction of dominant orientation, shown after local contrast enhancement (division by the image's blurred absolute value). The oriented vascular structures of (a) are enhanced. (c) Isotropic bandpass filtering of (a) after local contrast enhancement. Note the increased noise relative to the oriented filtering results.

Lifting convolution with steerable kernel

Group convolution ($G = \mathbb{R}^d \rtimes H$):

(e.g. $G = SE(2) = \mathbb{R}^2 \rtimes SO(2)$)
$X = \mathbb{R}^2$

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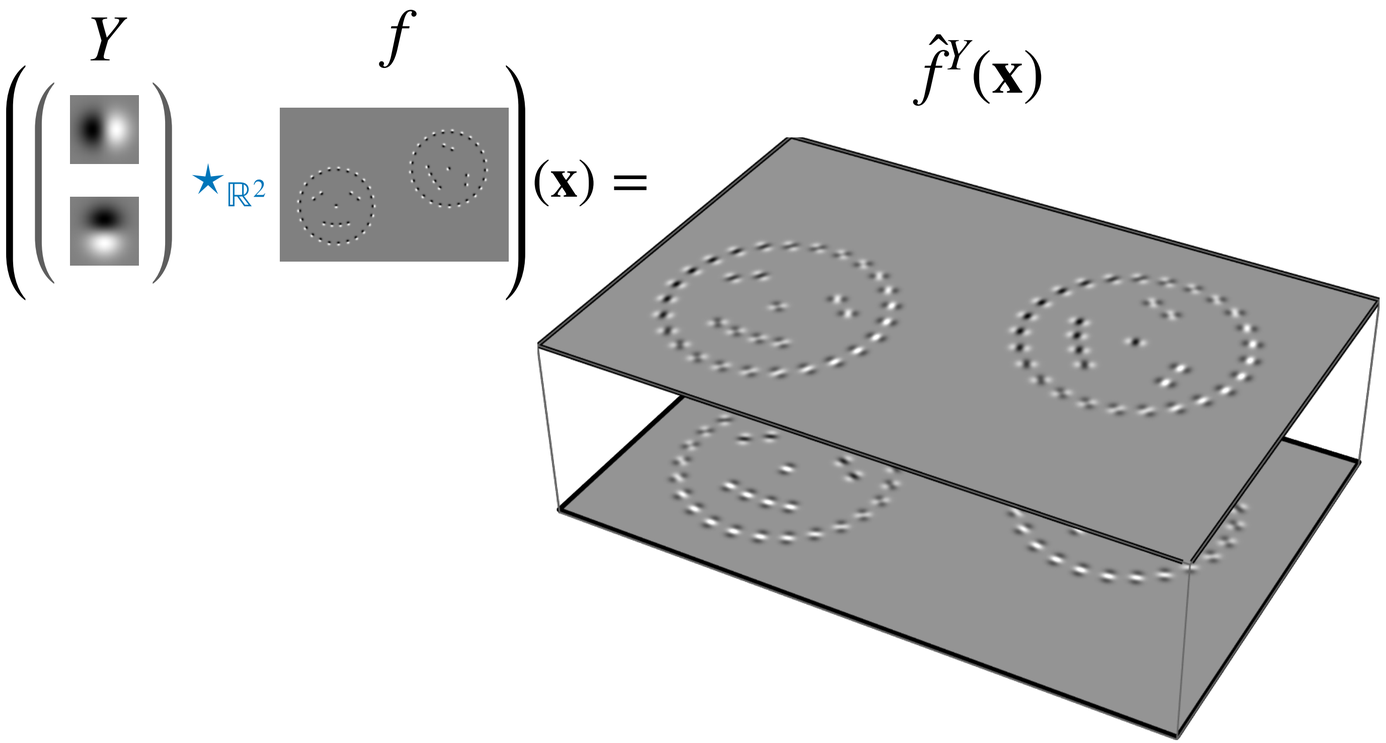

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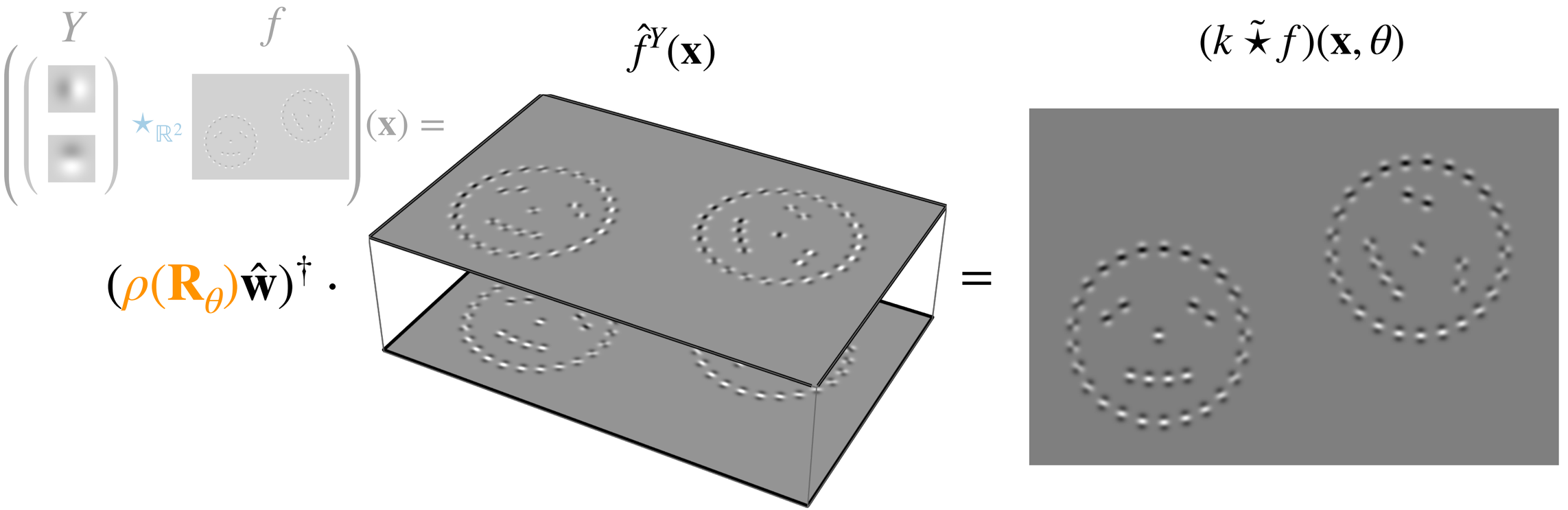

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$$= (\rho(h)\,\hat{\mathbf{w}})^\dagger \; \hat{f}^Y(\mathbf{x})$$

$$= \mathrm{tr}(\; \hat{f}^Y(\mathbf{x}) \; \hat{\mathbf{w}}^\dagger \; \rho(h^{-1}) \;)$$

$$k(h^{-1}\,\mathbf{x} \,|\, \hat{\mathbf{w}}) \;=\; (\rho(h^{-1})\hat{\mathbf{w}})^T \; Y(\mathbf{x})$$

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$\mathbf{a}^T \mathbf{b} = \mathrm{tr}(\mathbf{b}\,\mathbf{a}^T)$ and $\rho(h)^\dagger = \rho(h^{-1})$

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$$= \mathrm{tr}(\ \hat{f}^Y(\mathbf{x})\ \hat{\mathbf{w}}^\dagger\ \rho(h^{-1})\ )$$

$$= \mathrm{tr}(\ \hat{f}(\mathbf{x})\ \rho(h^{-1})\ )$$

$$= \mathcal{F}_H^{-1}[\ \hat{f}(\mathbf{x})\ ](h)$$

$$k(h^{-1}\,\mathbf{x} \,|\, \hat{\mathbf{w}}) = (\rho(h^{-1})\hat{\mathbf{w}})^T\ Y(\mathbf{x})$$

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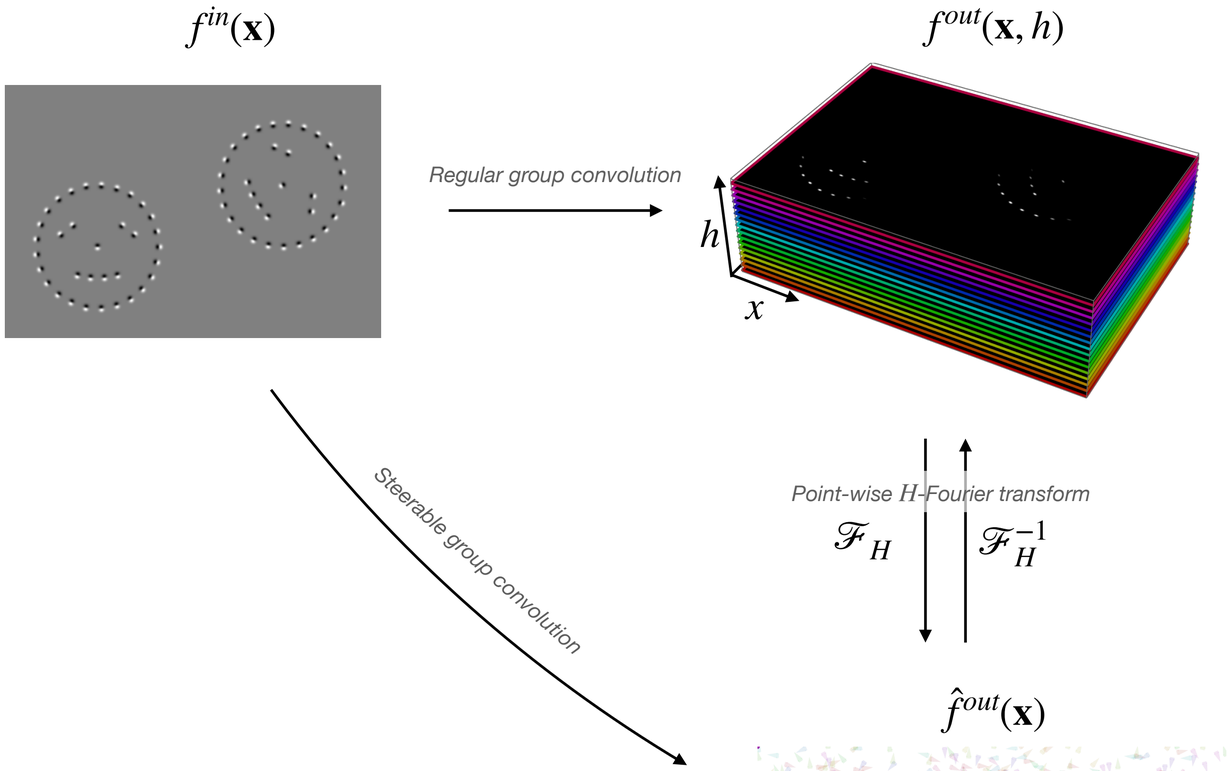
Inverse H-Fourier transform!

From regular to steerable via a Fourier transform



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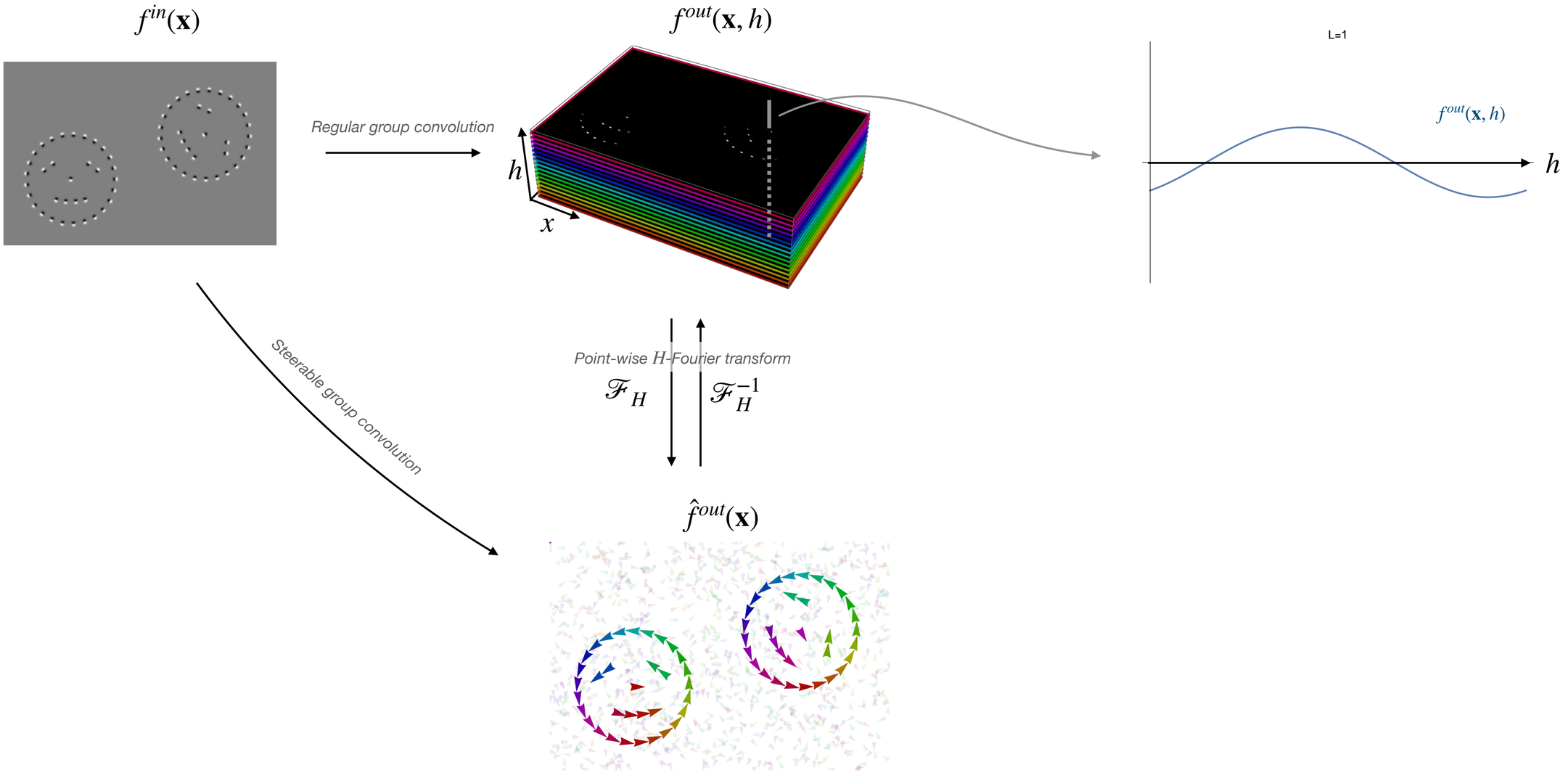

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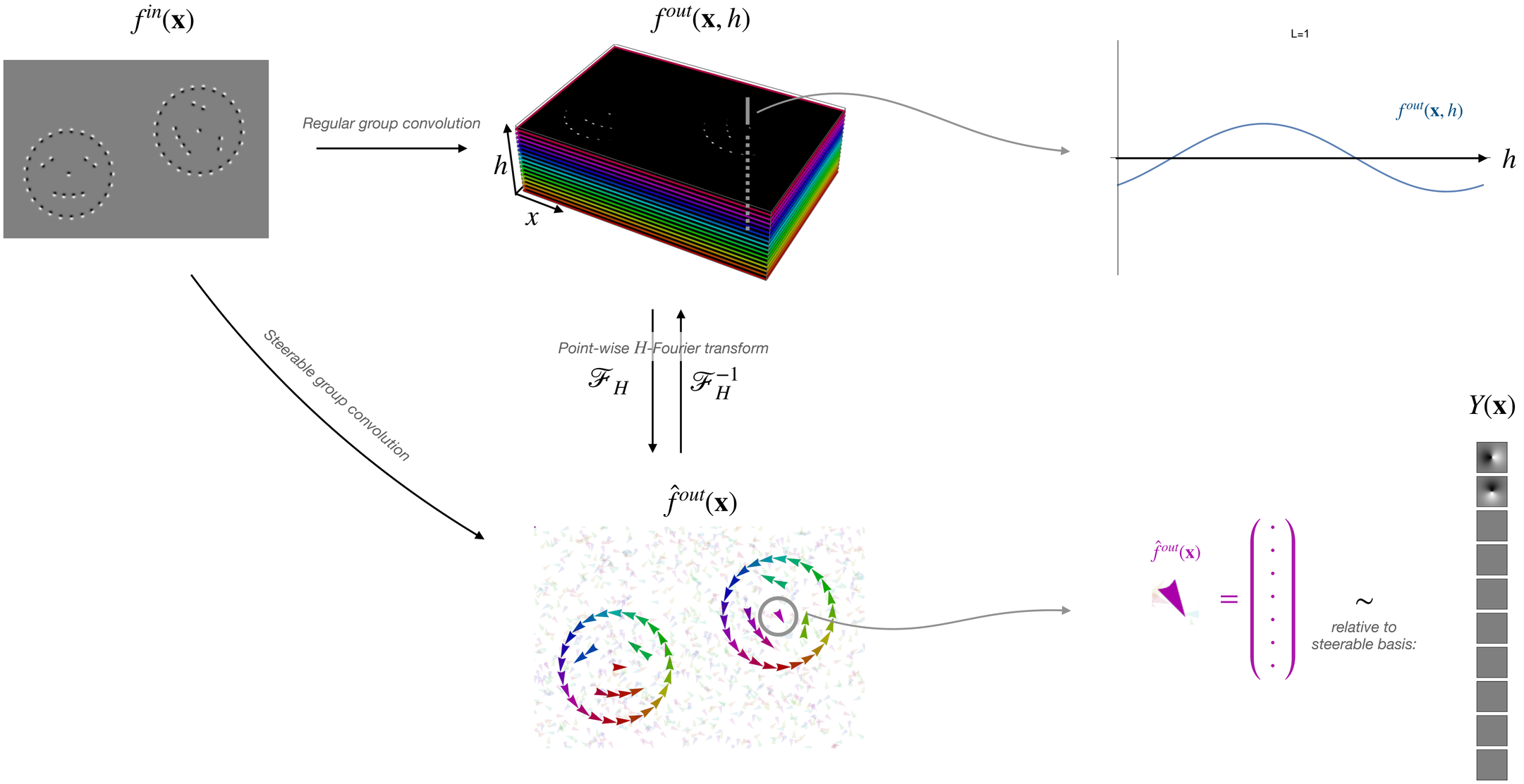

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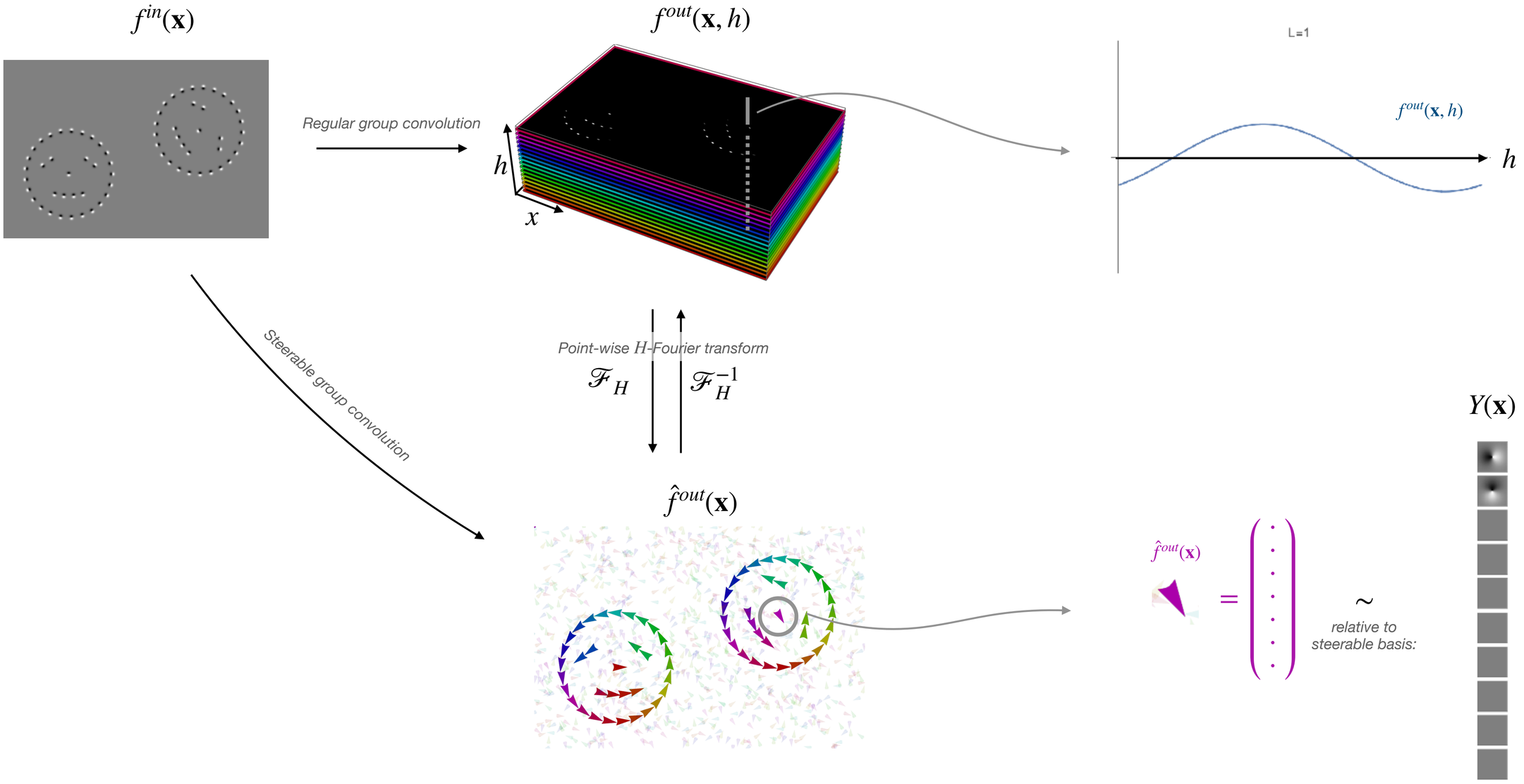


From regular to steerable via a Fourier transform

Regular group convolutions:
Domain expanded feature maps

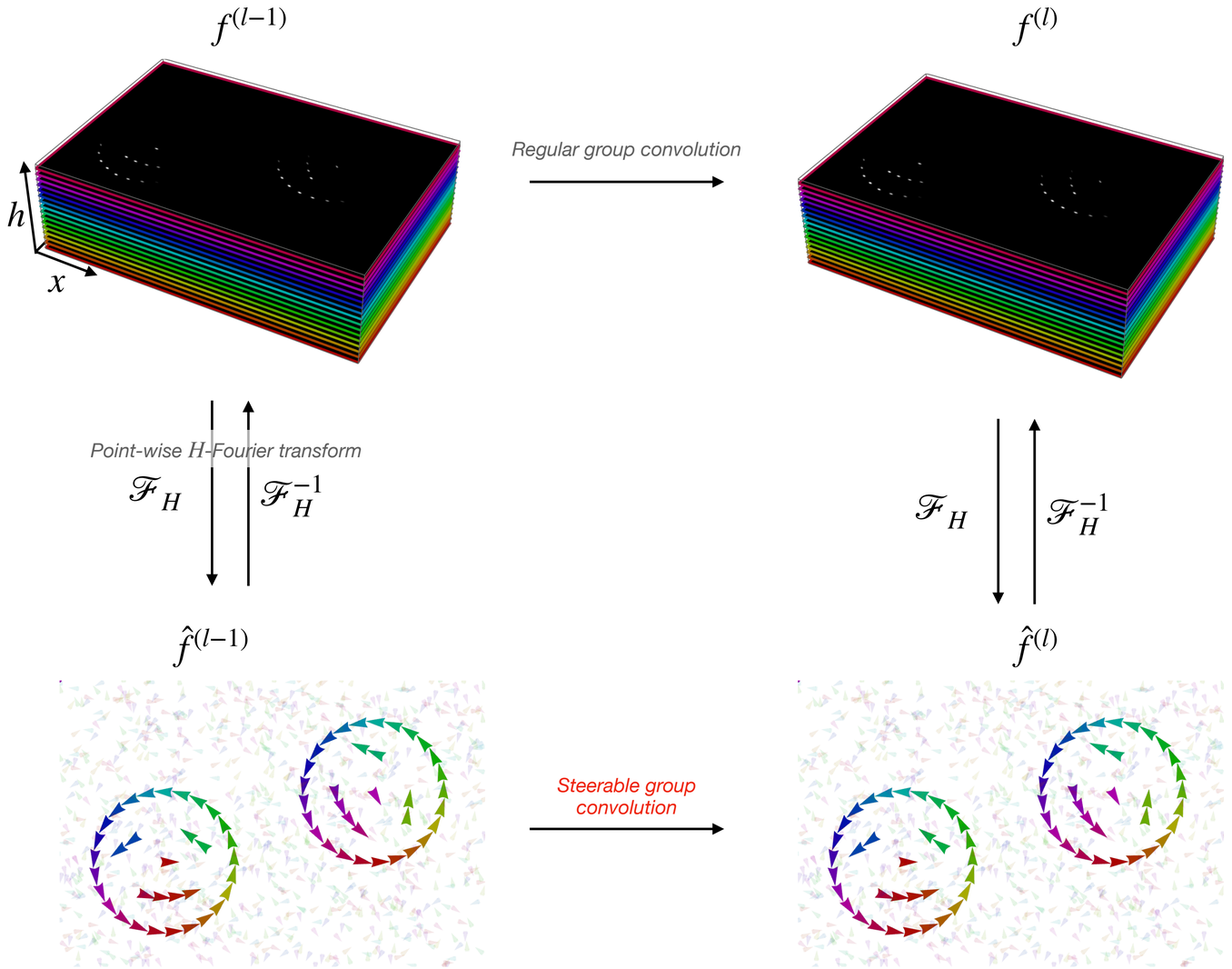
$$f^{(l)} : \mathbb{R}^d \times H \to \mathbb{R}$$

added axis

Steerable group convolutions:
Co-domain expanded feature maps (feature fields)

$$\hat{f}^{(l)} : \mathbb{R}^d \to V_H$$

vector field instead of scalar field
(vectors in V_H transform via group H representations)



1. Motivation — Equivariance → weight-sharing and generalization

2. Pattern matching using group theory — Group theory: symmetries & recognition by components
(features have “poses”)

3. Group convolutions — Template matching over groups

4. Example — Effective representation learning and generalization

5. G-convs are all you need! — Any equivariant linear layer is a group convolution

6. Steerable group convolutions — Efficient (band-limited) **grid-free** g-convs

7. Feature fields and escnn library

8. Equivariant tensor product layers

9. Equivariant graph NNs

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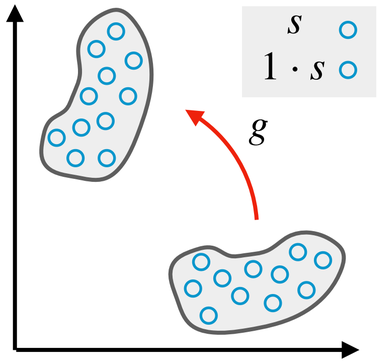
Feature field and induced representation

We call $\hat{f} : \mathbb{R}^d \to \mathbb{R}^{d_\rho}$ a feature vector field, or simply a **feature field**, if its

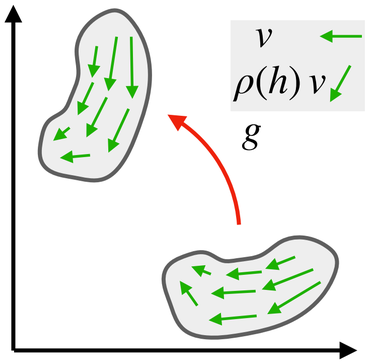
codomain	transforms via a *representation*	$\rho(h)$	of H
domain	transforms via the action	g^{-1}	of $G = (\mathbb{R}^d, +) \rtimes H$

Representation ρ defines the **type** of the field, and together with the group action of $G = (\mathbb{R}^d, +) \rtimes H$ defines the **induced representation**

$$\left(\mathrm{Ind}_H^G[\rho](\mathbf{x}, h)\,\hat{f}\right)(\mathbf{x}') := \rho(h)\,\hat{f}(h^{-1}(\mathbf{x}' - \mathbf{x}))$$



Scalar field ($\rho(h) = 1$)



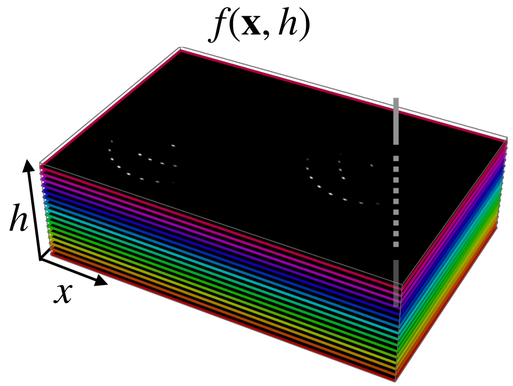
vector field

Figure adapted from: Weiler, M., & Cesa, G. (2019). General e (2)-equivariant steerable cnns. NeurIPS
See also https://github.com/QUVA-Lab/e2cnn

Feature field and induced representation

Regular G feature maps: $f(\mathbf{x}, h)$ considered so far can be considered feature fields.

$$(\mathscr{L}_g f)(\mathbf{x}', h') = f(h^{-1}(\mathbf{x}' - \mathbf{x}), h^{-1}h)$$



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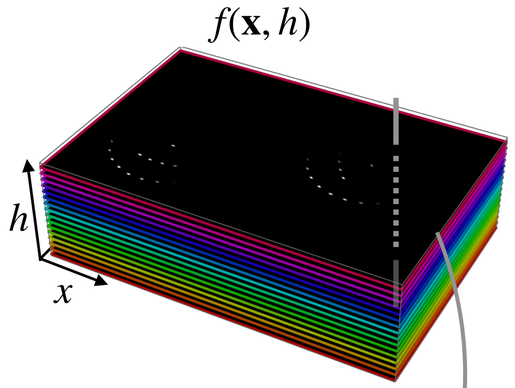

Regular H feature fields: Let $f^H(\mathbf{x}) = f(\mathbf{x}, \cdot\,)$ be the field of functions $f^H(\mathbf{x}) : H \to \mathbb{R}$ on the subgroup H, then the functions (**fibers**) transform via the regular representation $\mathscr{L}^H_h$

(recall. $\mathscr{L}^H_h f(h') = f(h^{-1}h')$)

$$(\mathscr{L}_g f)(\mathbf{x}', h') \iff \left(\mathrm{Ind}^G_H[\ \mathscr{L}^H_h\ ](\mathbf{x}, h) f^H\right)(\mathbf{x}')$$

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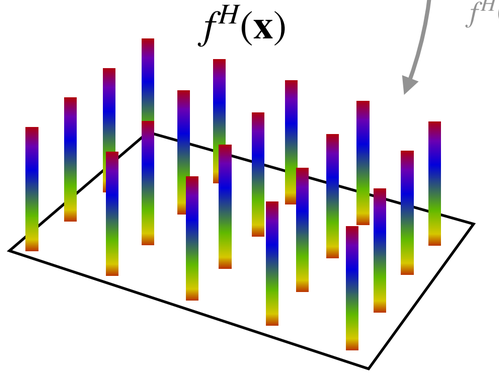

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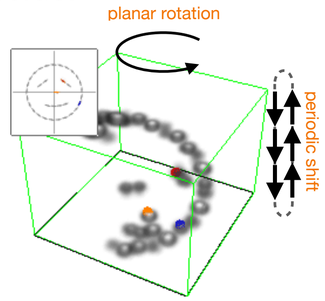

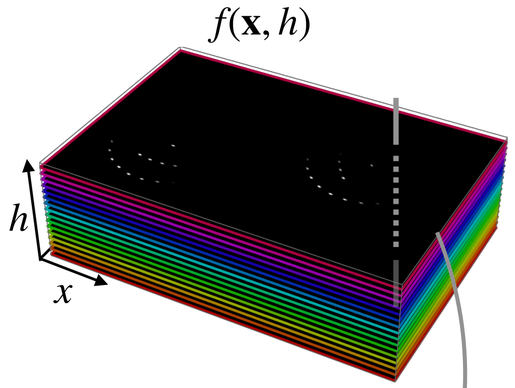

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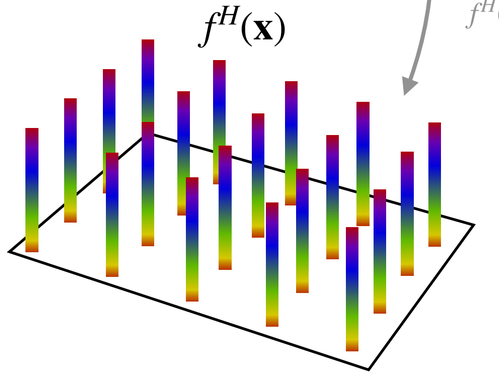

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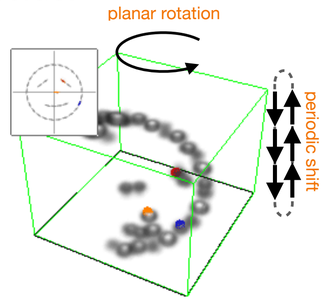

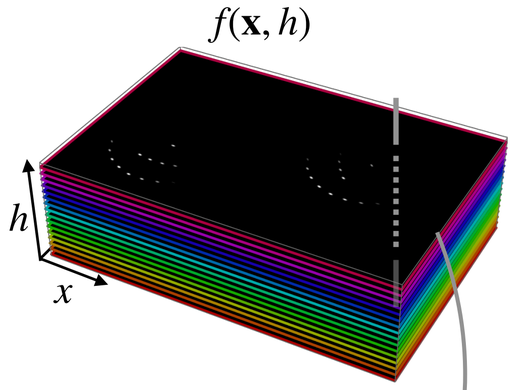

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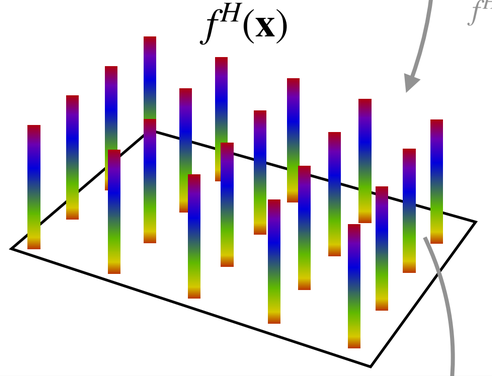
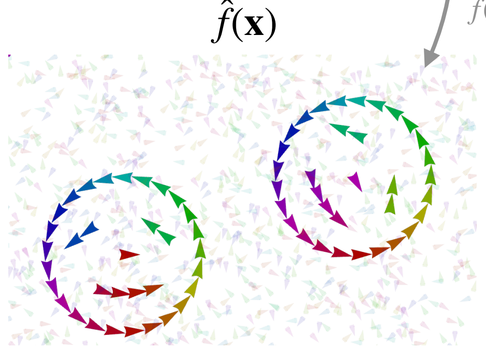


Steerable H feature fields: Since the fibers $f^H(\mathbf{x})$ are functions on H we can represent them via their Fourier coefficients $\hat{f}(\mathbf{x}) = \mathscr{F}_H[f^H(\mathbf{x})]$. These vectors of coefficients transform via irreps $\rho(h) = \oplus_l \rho_l(h)$

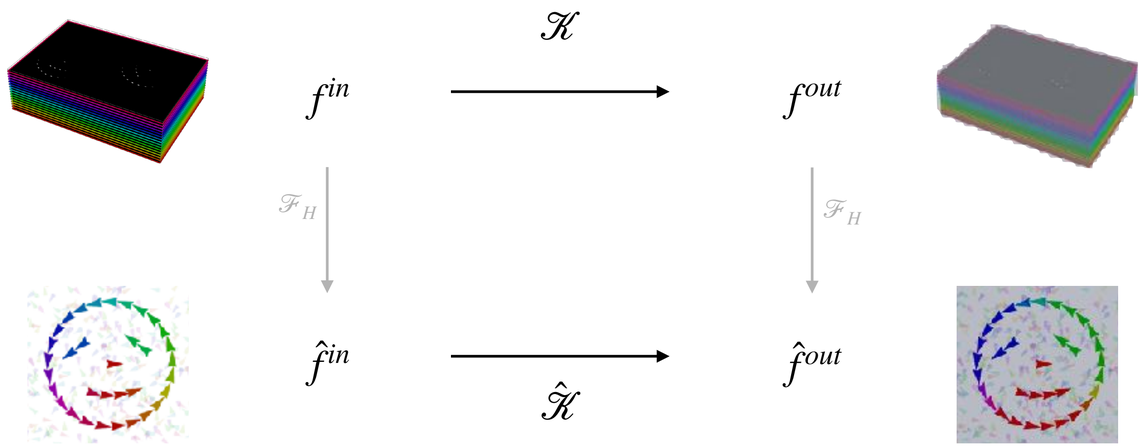
$$(\mathscr{L}_g f)(\mathbf{x}', h') \iff \left(\mathrm{Ind}^G_H[\ \mathscr{L}^H_h\ ](\mathbf{x}, h) \hat{f}\right)(\mathbf{x}') \iff \left(\mathrm{Ind}^G_H[\ \rho(h)\ ](\mathbf{x}, h) \hat{f}\right)(\mathbf{x}')$$

$\hat{f}(\mathbf{x}) = \mathscr{F}_H[f^H(\mathbf{x})]$



Steerable group convolutions

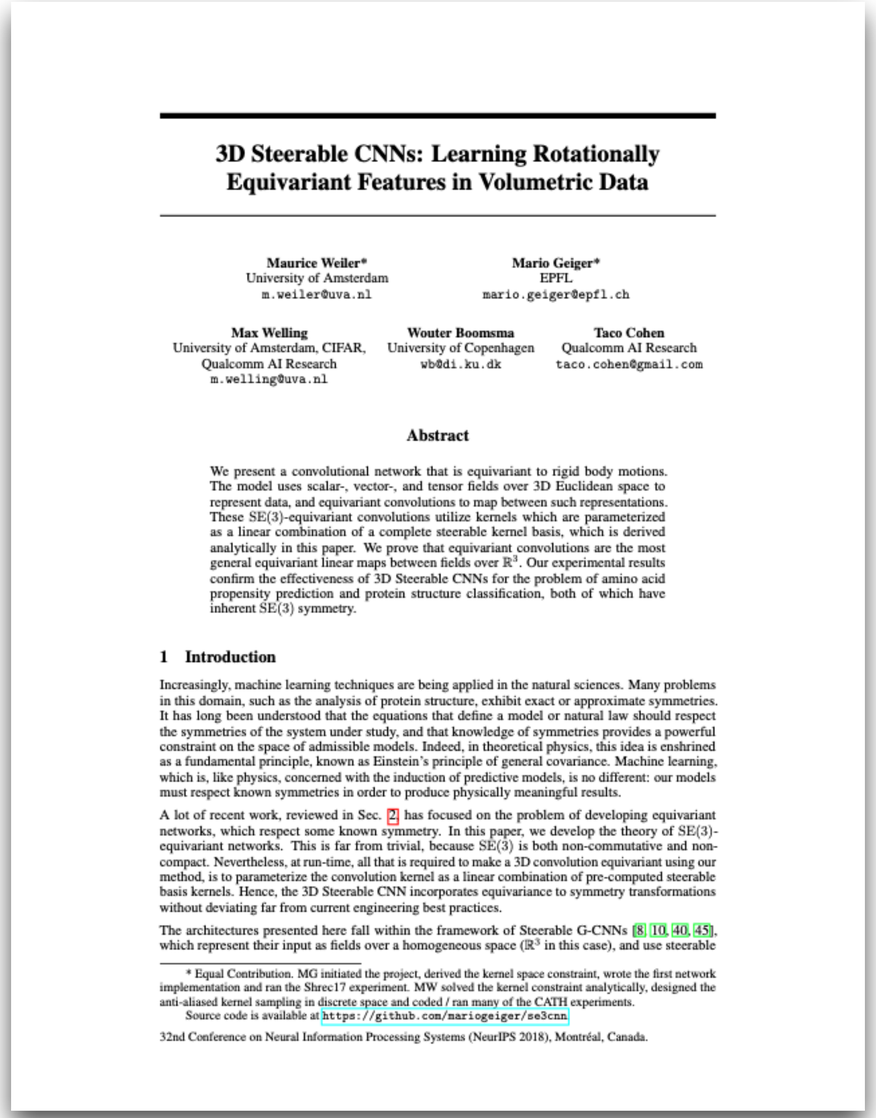
Group convolution $\mathscr{K}[f](g) = \int_G k(g^{-1}g')f(g)\mathrm{d}\mathbf{x}'\mathrm{d}g$



Normal convolution $\mathscr{K}[\hat{f}](\mathbf{x}) = \int_{\mathbb{R}^d} k(\mathbf{x}' - \mathbf{x})f(\mathbf{x}')\mathrm{d}\mathbf{x}'$

but with kernel $k : \mathbb{R}^d \to \mathbb{R}^{d_Y \times d_X}$ satisfying **constraint**

$\forall_{h\in H}\ \forall_{\mathbf{x}\in\mathbb{R}^d}$: $\quad k(g\,\mathbf{x}) = \rho_Y(h)k(\mathbf{x})\rho_X(h^{-1})$



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

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Abstract

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

1 Introduction

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

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

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

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

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

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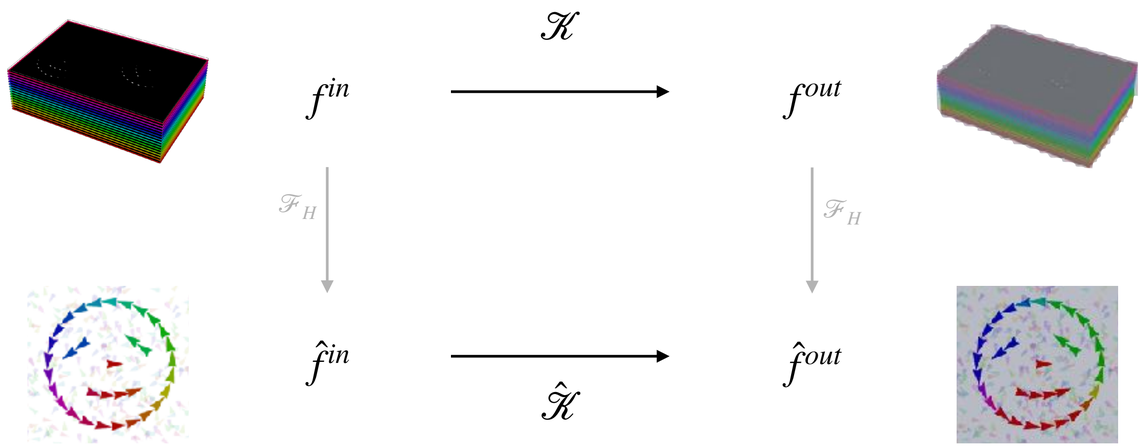

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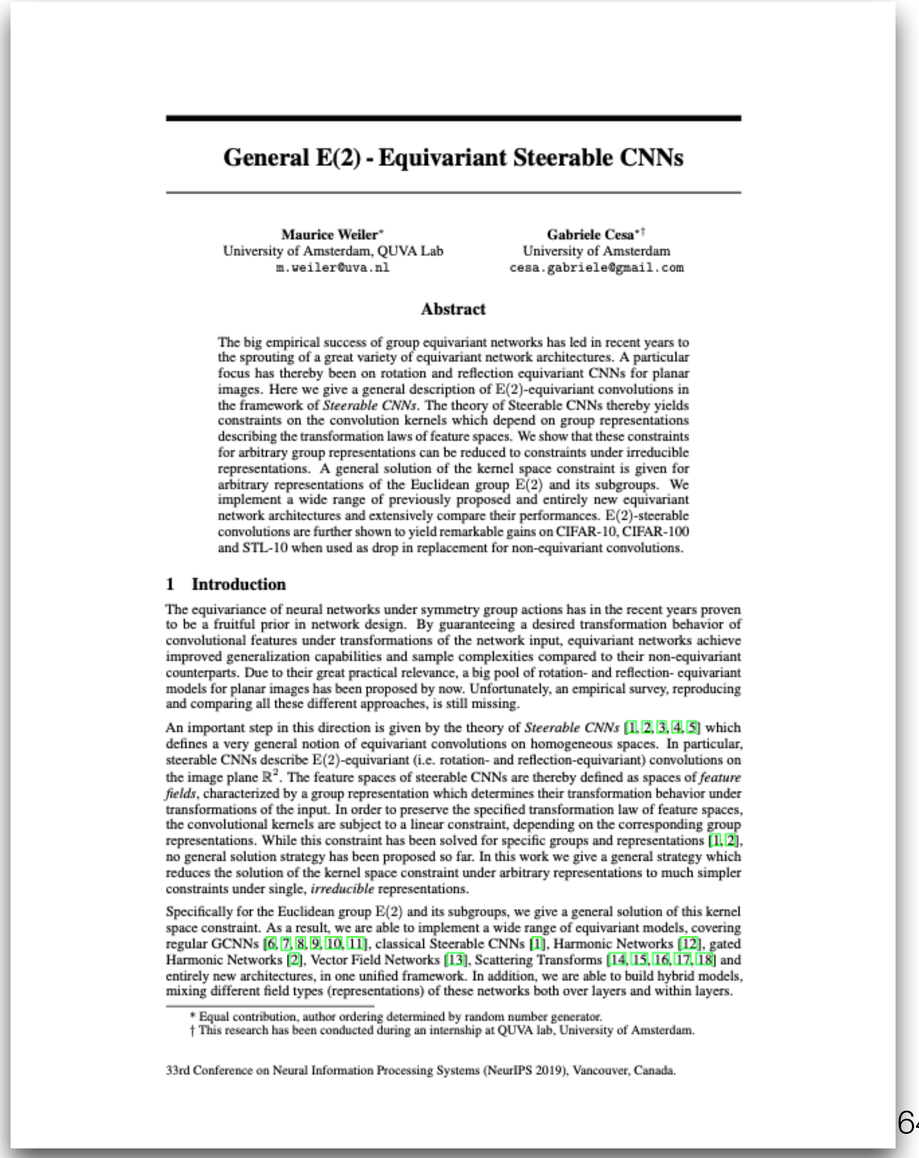

General E(2) - Equivariant Steerable CNNs

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Gabriele Cesa*†
University of Amsterdam
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Abstract

The big empirical success of group equivariant networks has led in recent years to the sprouting of a great variety of equivariant network architectures. A particular focus has thereby been on rotation and reflection equivariant CNNs for planar images. Here we give a general description of E(2)-equivariant convolutions in the framework of *Steerable CNNs*. The theory of Steerable CNNs thereby yields constraints on the convolution kernels which depend on group representations describing the transformation laws of feature spaces. We show that these constraints for arbitrary group representations can be reduced to constraints under irreducible representations. A general solution of the kernel space constraint is given for arbitrary representations of the Euclidean group E(2) and its subgroups. We implement a wide range of previously proposed and entirely new equivariant network architectures and extensively compare their performances. E(2)-steerable convolutions are further shown to yield remarkable gains on CIFAR-10, CIFAR-100 and STL-10 when used as drop in replacement for non-equivariant convolutions.

1 Introduction

The equivariance of neural networks under symmetry group actions has in the recent years proven to be a fruitful prior in network design. By guaranteeing a desired transformation behavior of convolutional features under transformations of the network input, equivariant networks achieve improved generalization capabilities and sample complexities compared to their non-equivariant counterparts. Due to their great practical relevance, a big pool of rotation- and reflection- equivariant models for planar images has been proposed by now. Unfortunately, an empirical survey, reproducing and comparing all these different approaches, is still missing.

An important step in this direction is given by the theory of *Steerable CNNs* [1, 2, 3, 4, 5] which defines a very general notion of equivariant convolutions on homogeneous spaces. In particular, steerable CNNs describe E(2)-equivariant (i.e. rotation- and reflection-equivariant) convolutions on the image plane $\mathbb{R}^2$. The feature spaces of steerable CNNs are thereby defined as spaces of *feature fields*, characterized by a group representation which determines their transformation behavior under transformations of the input. In order to preserve the specified transformation law of feature spaces, the convolutional kernels are subject to a linear constraint, depending on the corresponding group representations. While this constraint has been solved for specific groups and representations [1, 2], no general solution strategy has been proposed so far. In this work we give a general strategy which reduces the solution of the kernel space constraint under arbitrary representations to much simpler constraints under single, *irreducible* representations.

Specifically for the Euclidean group E(2) and its subgroups, we give a general solution of this kernel space constraint. As a result, we are able to implement a wide range of equivariant models, covering regular GCNNs [6, 7, 8, 9, 10, 11], classical Steerable CNNs [1], Harmonic Networks [12], gated Harmonic Networks [2], Vector Field Networks [13], Scattering Transforms [14, 15, 16, 17, 18] and entirely new architectures, in one unified framework. In addition, we are able to build hybrid models, mixing different field types (representations) of these networks both over layers and within layers.

* Equal contribution, author ordering determined by random number generator.
† This research has been conducted during an internship at QUVA lab, University of Amsterdam.

33rd Conference on Neural Information Processing Systems (NeurIPS 2019), Vancouver, Canada.

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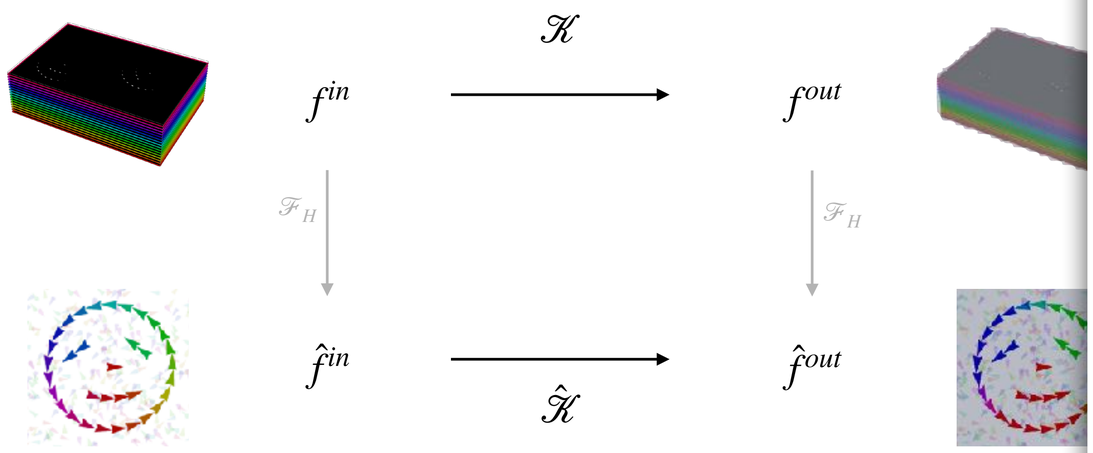

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Equivariance is becoming an increasingly popular design choice to build data efficient neural networks by exploiting prior knowledge about the symmetries of the problem at hand. Euclidean steerable CNNs are one of the most common classes of equivariant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

1 INTRODUCTION

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

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

up convolutions

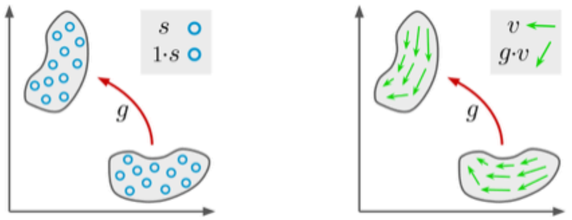
E(n)-Equivariant Steerable CNNs

Documentation | **Paper ICLR 22** | **Paper NeurIPS 19** | **e2cnn library** | **e2cnn experiments** | **Thesis**

escnn is a PyTorch extension for equivariant deep learning. *escnn* is the successor of the e2cnn library, which only supported planar isometries.

Equivariant neural networks guarantee a specified transformation behavior of their feature spaces under transformations of their input. For instance, classical convolutional neural networks (*CNNs*) are by design equivariant to translations of their input. This means that a translation of an image leads to a corresponding translation of the network's feature maps. This package provides implementations of neural network modules which are equivariant under all *isometries* E(2) of the image plane $\mathbb{R}^2$ and all *isometries* E(3) of the 3D space $\mathbb{R}^3$, that is, under *translations*, *rotations* and *reflections* (and can, potentially, be extended to all isometries E(n) of $\mathbb{R}^n$). In contrast to conventional CNNs, E(n)-equivariant models are guaranteed to generalize over such transformations, and are therefore more data efficient.

The feature spaces of E(n)-Equivariant Steerable CNNs are defined as spaces of *feature fields*, being characterized by their transformation law under rotations and reflections. Typical examples are scalar fields (e.g. gray-scale images or temperature fields) or vector fields (e.g. optical flow or electromagnetic fields).



scalar field

vector field

Instead of a number of channels, the user has to specify the field *types* and their *multiplicities* in order to define a feature space. Given a specified input- and output feature space, our `R2conv` and `R3conv` modules instantiate

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The feature
characteriz
gray-scale

Instead of a
feature spa

Getting Started

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

```
from escnn import gspaces                                    #  1
from escnn import nn                                         #  2
import torch                                                 #  3
                                                             #  4
r2_act = gspaces.rot2dOnR2(N=8)                              #  5
feat_type_in  = nn.FieldType(r2_act,  3*[r2_act.trivial_repr])   #  6
feat_type_out = nn.FieldType(r2_act, 10*[r2_act.regular_repr])   #  7
                                                             #  8
conv = nn.R2Conv(feat_type_in, feat_type_out, kernel_size=5)     #  9
relu = nn.ReLU(feat_type_out)                                # 10
                                                             # 11
x = torch.randn(16, 3, 32, 32)                               # 12
x = feat_type_in(x)                                          # 13
                                                             # 14
y = relu(conv(x))                                            # 15
```

Line 5 specifies the symmetry group action on the image plane $\mathbb{R}^2$ under which the network should be equivariant. We choose the *cyclic group* C_8, which describes discrete rotations by multiples of 2π/8. Line 6 specifies the input feature field types. The three color channels of an RGB image are thereby to be identified as three independent scalar fields, which transform under the *trivial representation* of C_8. Similarly, the output feature space is in line 7 specified to consist of 10 feature fields which transform under the *regular representation* of C_8. The C_8-equivariant convolution is then instantiated by passing the input and output type as well as the kernel size to the constructor (line 9). Line 10 instantiates an equivariant ReLU nonlinearity which will operate on the output field and is therefore passed the output field type.

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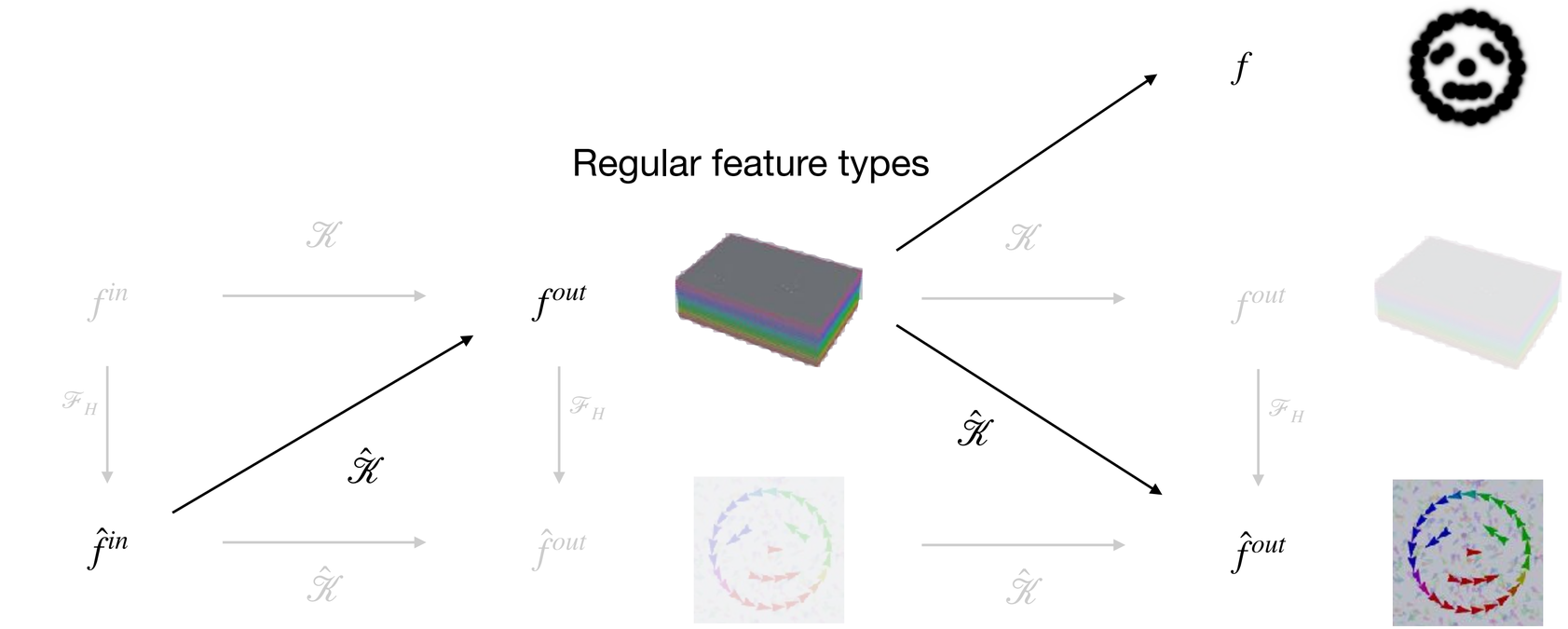
Type-0 field usual 2D feature map
(e.g. for segmentation)



Steerable (irrep) feature types

Type-1 vector fields
(e.g. force/velocity vectors)

1. Motivation — Equivariance → weight-sharing and generalization

2. Pattern matching using group theory — Group theory: symmetries & recognition by components
(features have “poses”)

3. Group convolutions — Template matching over groups

4. Example — Effective representation learning and generalization

5. G-convs are all you need! — Any equivariant linear layer is a group convolution

6. Steerable group convolutions — Efficient (band-limited) **grid-free** g-convs

7. Feature fields and escnn library — Flexible framework for equivariant layers

8. Equivariant tensor product layers

9. Equivariant graph NNs

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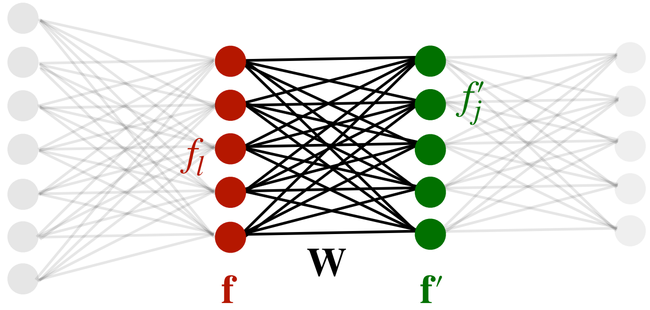
8. Equivariant tensor product layers

9. Equivariant graph NNs

Equivariant MLP



$$\mathbf{f} \quad \mapsto \quad \mathbf{f}' = \mathbf{W}(\mathbf{x}_b - \mathbf{x}_a)\,\mathbf{f} \quad \mapsto \quad \mathbf{f}'' = \sigma(\,\mathbf{f}'\,)$$

linear layer activation

(Repeat L times)

Linear layer (matrix-vector multiplication)

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$$f'_j = \sum_l w_l^j\, f_l$$

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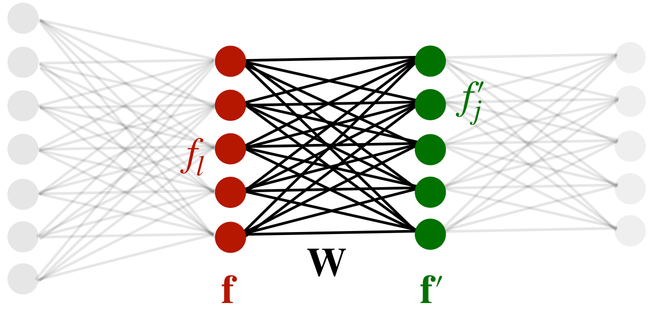

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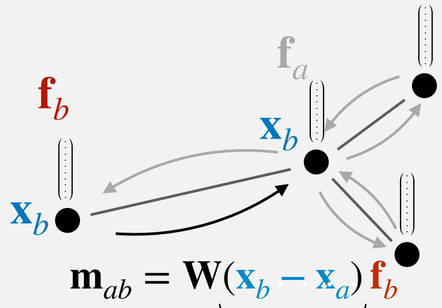
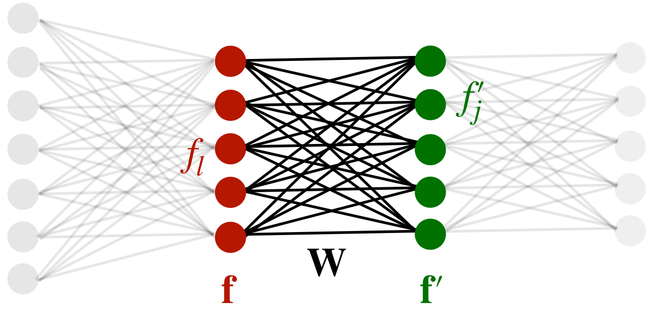
Conditional linear layer (weight matrix depends on $\mathbf{x}_b - \mathbf{x}_a$)

$$\mathbf{f}' = \mathbf{W}(\mathbf{x}_b - \mathbf{x}_a)\,\mathbf{f} \qquad f'_j = \sum_l w_l^j(\mathbf{x}_b - \mathbf{x}_a)\, f_l$$

Convolutional message passing



Equivariant MLP



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Let $\mathbf{W} : \mathbb{R}^3 \to \mathbb{R}^{C' \times C}$ a matrix valued function (conv-kernel)

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- Matrix-valued weights $\mathbf{W}_J$ with elements w_{Jl}^j

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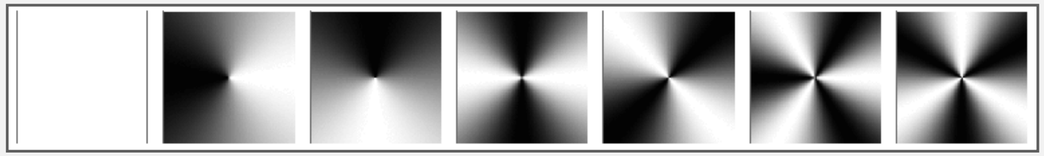

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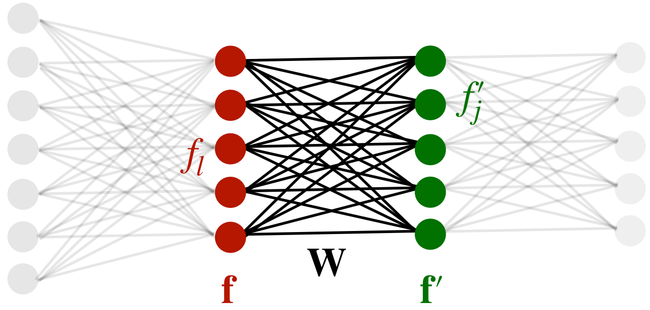

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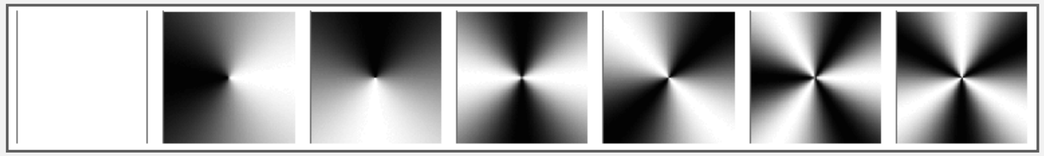

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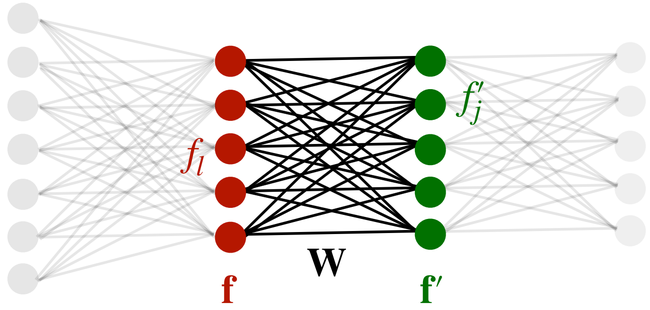

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Conditional linear layer

$$\mathbf{f}' = \mathbf{W}(\mathbf{x}_b - \mathbf{x}_a)\,\mathbf{f}$$

$$f'_j = \sum_l w^j_l(\mathbf{x}_b - \mathbf{x}_a)\,f_l$$

Conditional linear layers are tensor products!!!

$$\mathbf{f}' = \mathbf{W}(\mathbf{x}_b - \mathbf{x}_a)\,\mathbf{f} \quad \Leftrightarrow \quad \mathbf{f}' = \mathbf{f} \otimes^{\mathbf{w}} Y_J(\mathbf{x}_b - \mathbf{x}_a)$$

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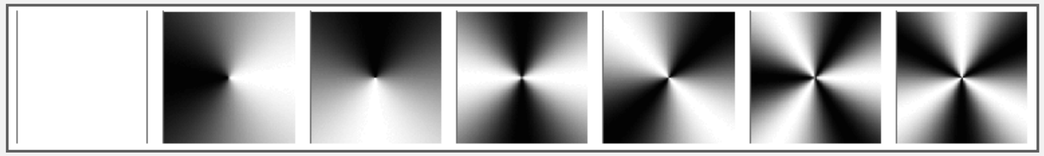

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2. Pattern matching using group theory — Group theory: symmetries & recognition by components
(features have “poses”)

3. Group convolutions — Template matching over groups

4. Example — Effective representation learning and generalization

5. G-convs are all you need! — Any equivariant linear layer is a group convolution

6. Steerable group convolutions — Efficient (band-limited) **grid-free** g-convs

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Neural Message Passing for Quantum Chemistry

Justin Gilmer [1] **Samuel S. Schoenholz** [1] **Patrick F. Riley** [2] **Oriol Vinyals** [3] **George E. Dahl** [1]

Abstract

Supervised learning on molecules has incredible potential to be useful in chemistry, drug discovery, and materials science. Luckily, several promising and closely related neural network models invariant to molecular symmetries have already been described in the literature. These models learn a message passing algorithm and aggregation procedure to compute a function of their entire input graph. At this point, the next step is to find a particularly effective variant of this general approach and apply it to chemical prediction benchmarks until we either solve them or reach the limits of the approach. In this paper, we reformulate existing models into a single common framework we call Message Passing Neural Networks (MPNNs) and explore additional novel variations within this framework. Using MPNNs we demonstrate state of the art results on an important molecular property prediction benchmark; these results are strong enough that we believe future work should focus on datasets with larger molecules or more accurate ground truth labels.

1. Introduction

The past decade has seen remarkable success in the use of deep neural networks to understand and translate natural language (Wu et al., 2016), generate and decode complex audio signals (Hinton et al., 2012), and infer features from real-world images and videos (Krizhevsky et al., 2012). Although chemists have applied machine learning to many problems over the years, predicting the properties of molecules and materials using machine learning (and especially deep learning) is still in its infancy. To date, most research applying machine learning to chemistry tasks (Hansen et al., 2015; Huang & von Lilienfeld, 2016; Rupp et al., 2012; Rogers & Hahn, 2010; Montavon et al., 2012; Behler & Parrinello, 2007; Schoenholz et al., 2016) has revolved around feature engineering. While neural networks have been applied in a variety of situations (Merkwirth & Lengauer, 2005; Micheli, 2009; Lusci et al., 2013; Duvenaud et al., 2015), they have yet to become widely adopted. This situation is reminiscent of the state of image models before the broad adoption of convolutional neural networks and is due, in part, to a dearth of empirical evidence that neural architectures with the appropriate inductive bias can be successful in this domain.

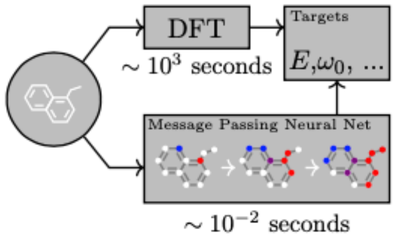

Figure 1. A Message Passing Neural Network predicts quantum properties of an organic molecule by modeling a computationally expensive DFT calculation.

Recently, large scale quantum chemistry calculation and molecular dynamics simulations coupled with advances in high throughput experiments have begun to generate data at an unprecedented rate. Most classical techniques do not make effective use of the larger amounts of data that are now available. The time is ripe to apply more powerful and flexible machine learning methods to these problems, assuming we can find models with suitable inductive biases. The symmetries of atomic systems suggest neural networks that operate on graph structured data and are invariant to graph isomorphism might also be appropriate for molecules. Sufficiently successful models could someday help automate challenging chemical search problems in drug discovery or materials science.

In this paper, our goal is to demonstrate effective machine learning models for chemical prediction problems

[1]Google Brain [2]Google [3]Google DeepMind. Correspondence to: Justin Gilmer <gilmer@google.com>, George E. Dahl <gdahl@google.com>.

Proceedings of the 34th International Conference on Machine Learning, Sydney, Australia, PMLR 70, 2017.

The Message Passing Framework

Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$

- nodes $v_i \in \mathcal{V}$ with node feature $\mathbf{f}_i \in \mathbb{R}^{C_v}$
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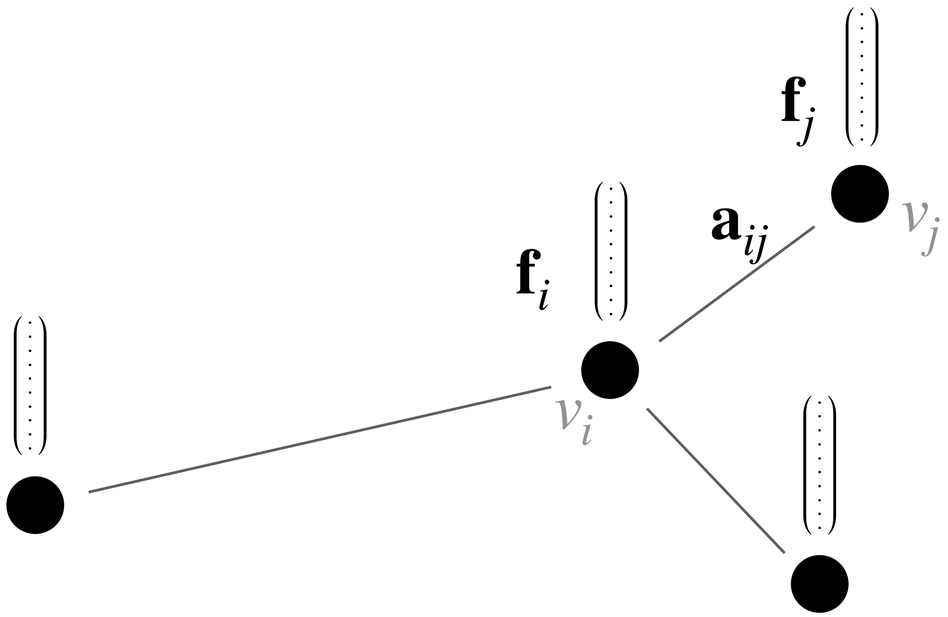

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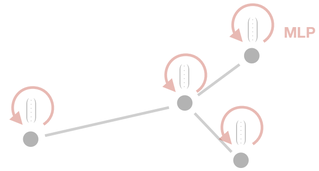
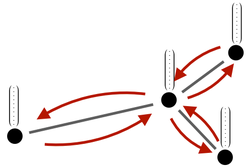
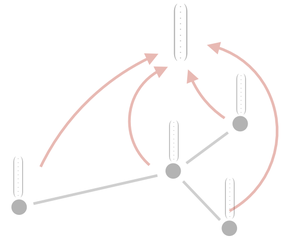


node-wise transformations

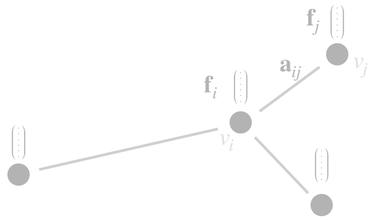


message passing



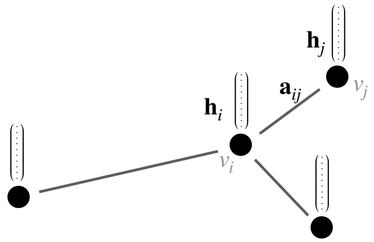
permutation invariant aggregation

MLP



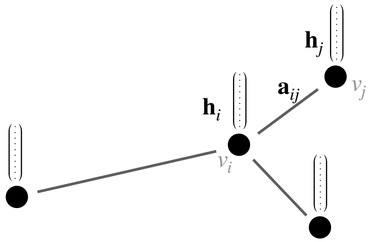
Input graph

node embedding



Initial node embeddings

interaction layers



Final node embeddings

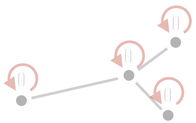
pooling

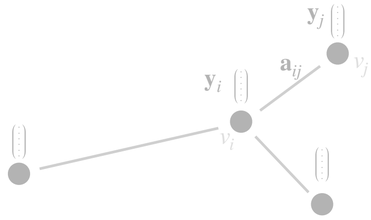
Graph embedding

read-out (prediction)

Graph-level prediction

read-out (prediction)





Node-level predictions

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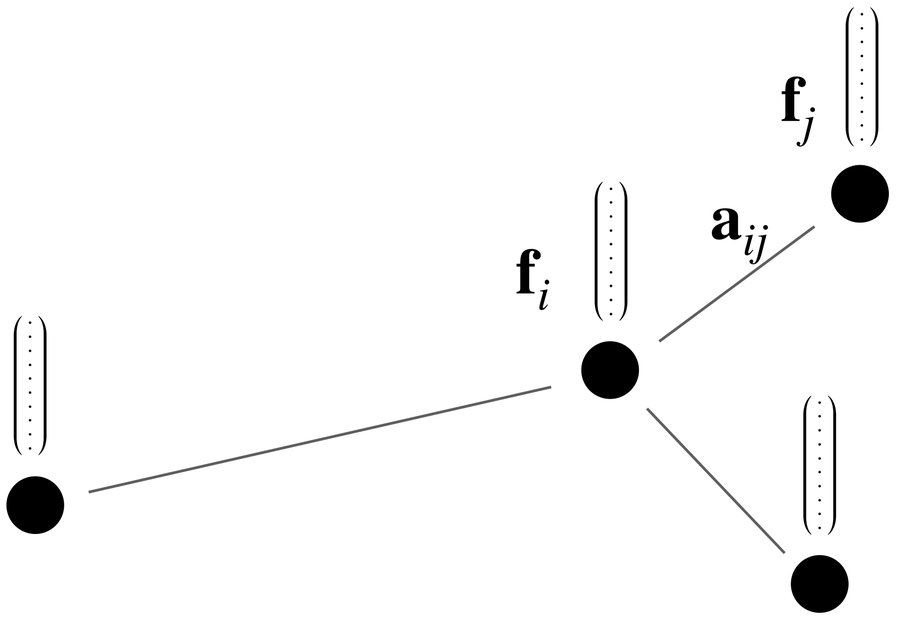

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Message passing layer:

- Messages

$$\mathbf{m}_{ij} = \phi_m(\mathbf{f}_i, \mathbf{f}_j, \mathbf{a}_{ij})$$

- Aggregate + node updates

$$\mathbf{f}'_i = \phi_f(\mathbf{f}_i, \sum_{j \in \mathcal{N}(i)} \mathbf{m}_{ij})$$

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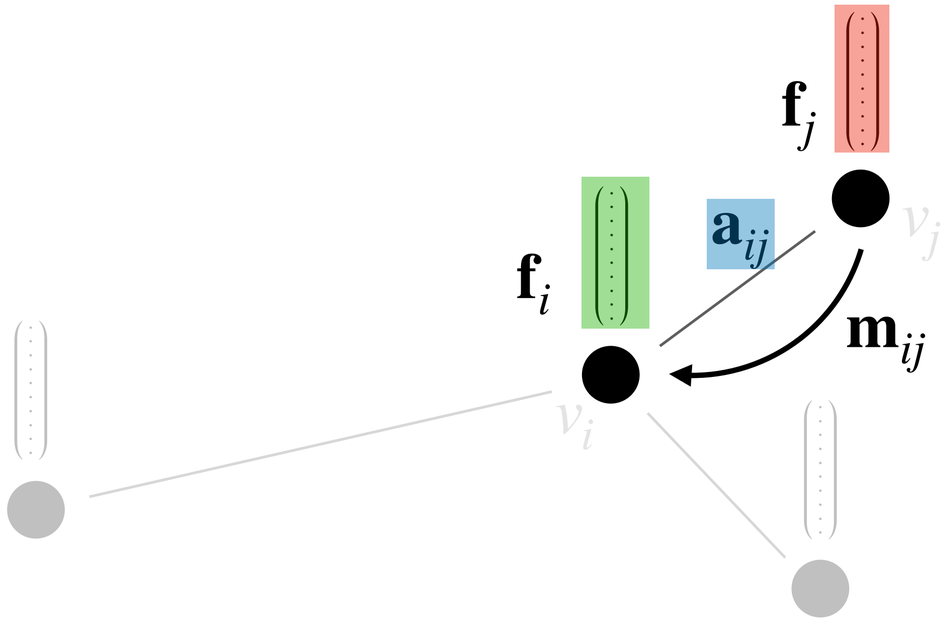

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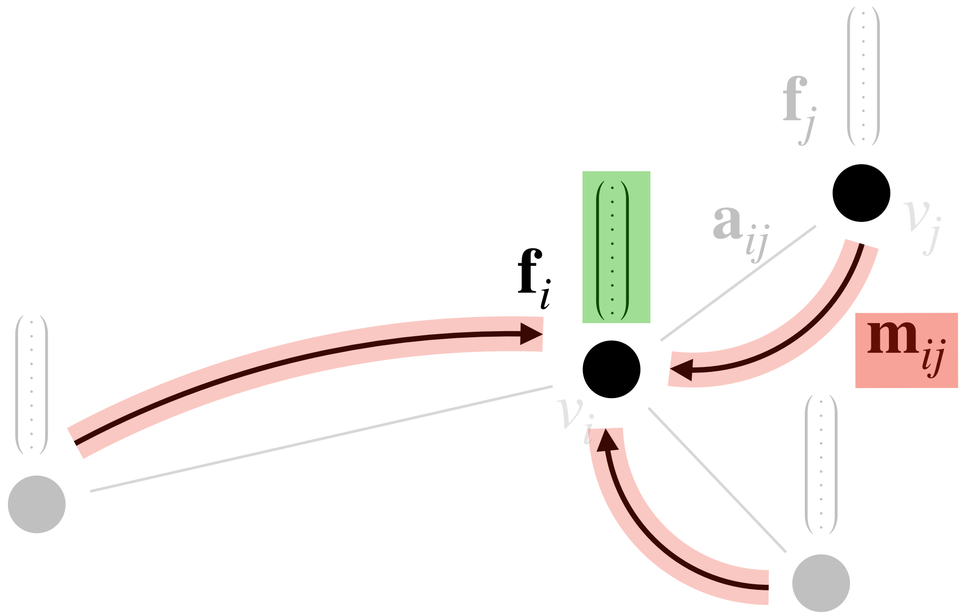

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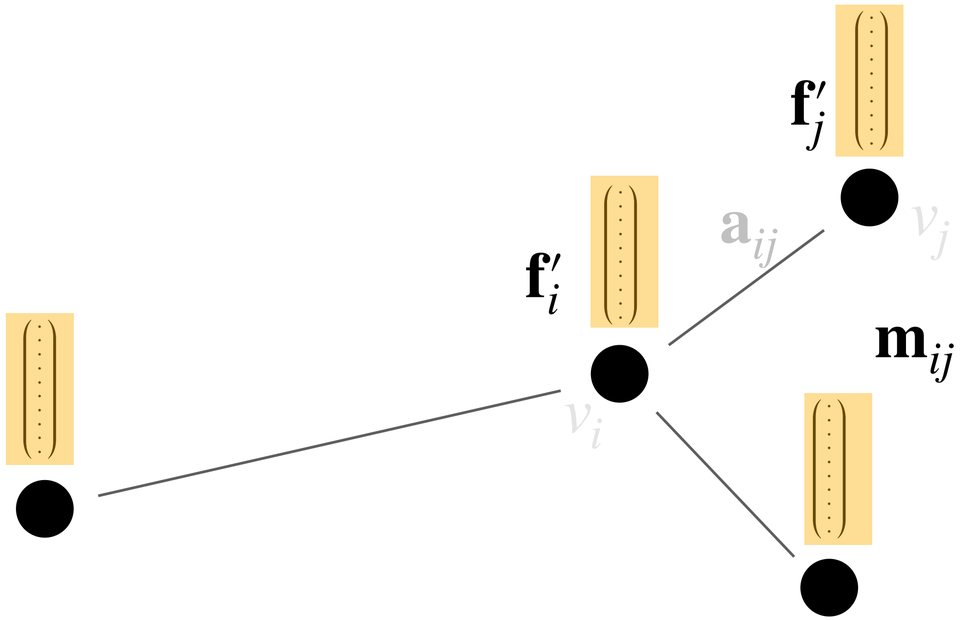

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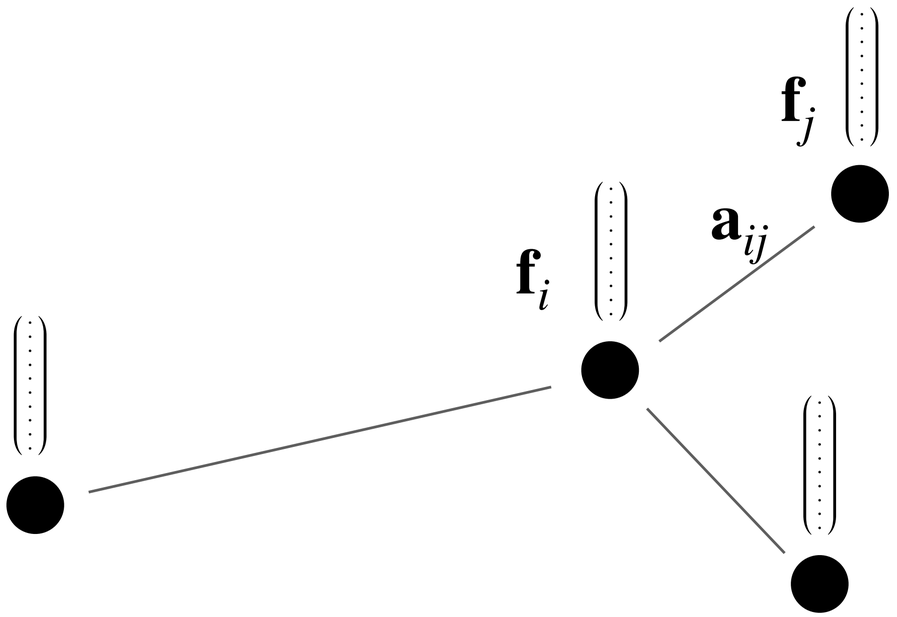

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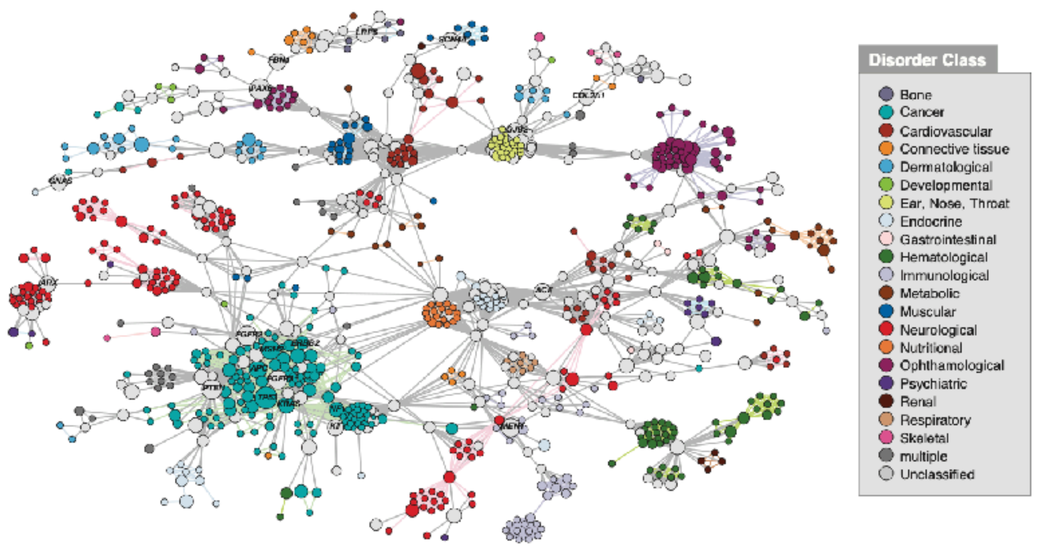
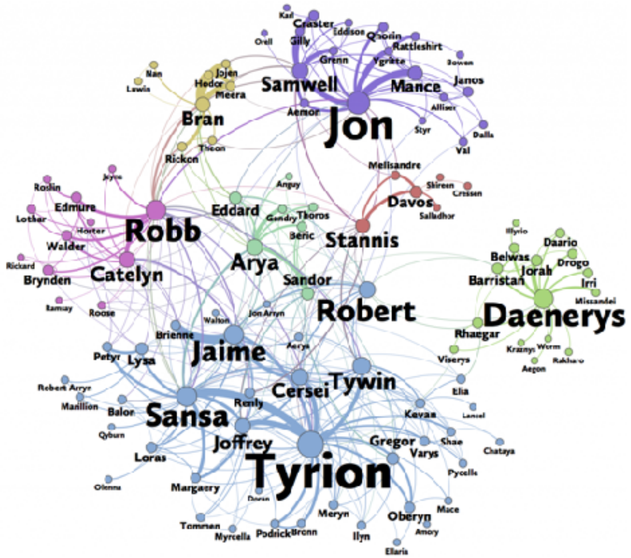
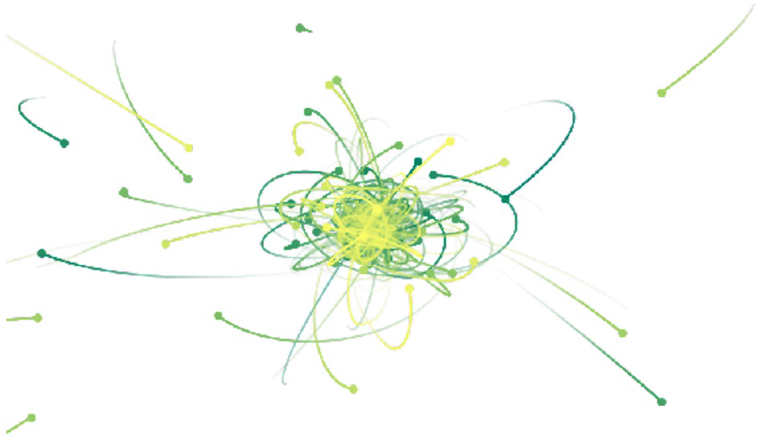


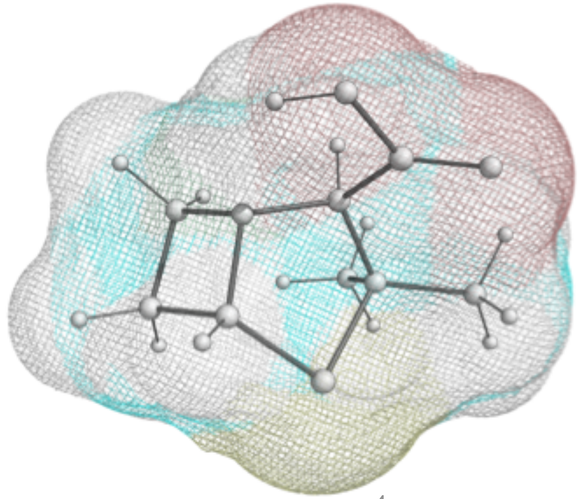
Gene/Protein interaction graphs[1]



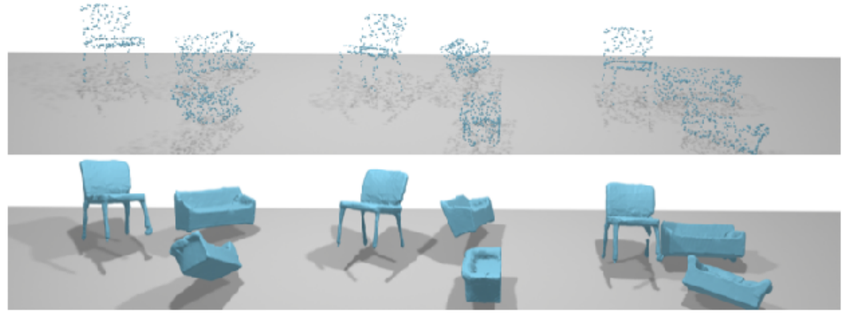
Social network graph[2]



Physical system[3]



Molecule[4]



Point cloud/shapes[5]

Figures from: [1]Goh, K. I., Cusick, M. E., Valle, D., Childs, B., Vidal, M., & Barabási, A. L. (2007). The human disease network. Proceedings of the National Academy of Sciences, 104(21), 8685-8690.

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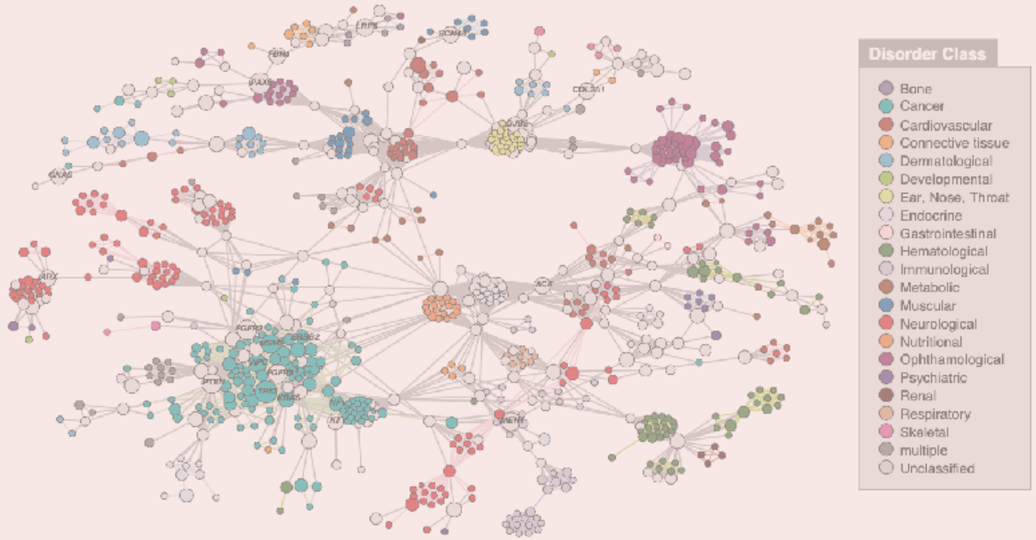
General graphs



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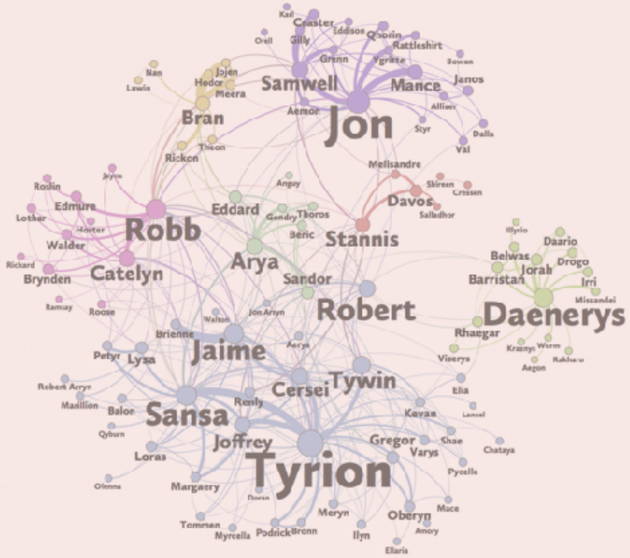
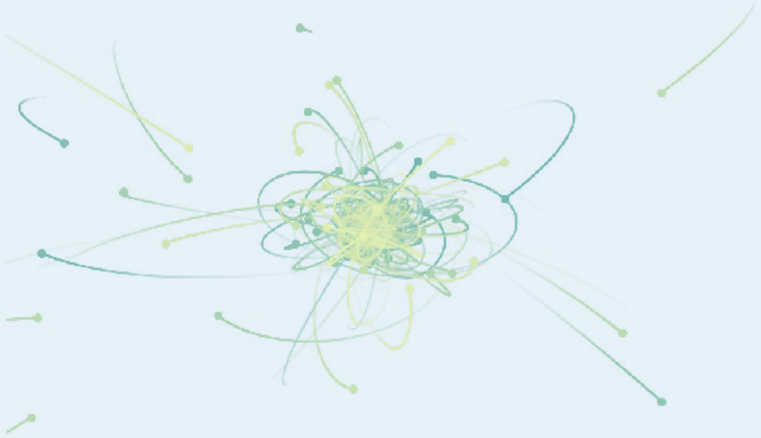


Social network graph[2]

Geometric graphs

(nodes correspond to points in a manifold)



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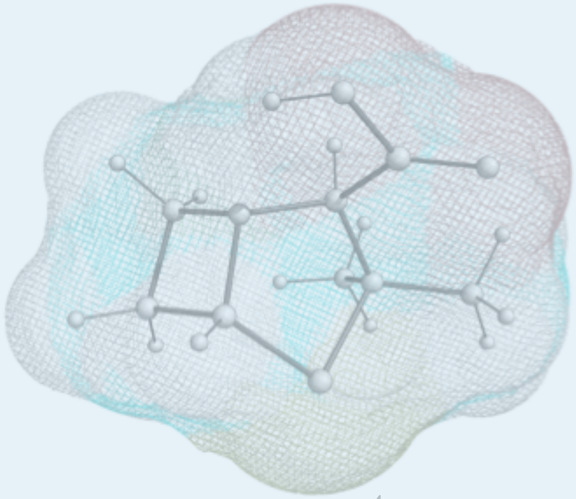

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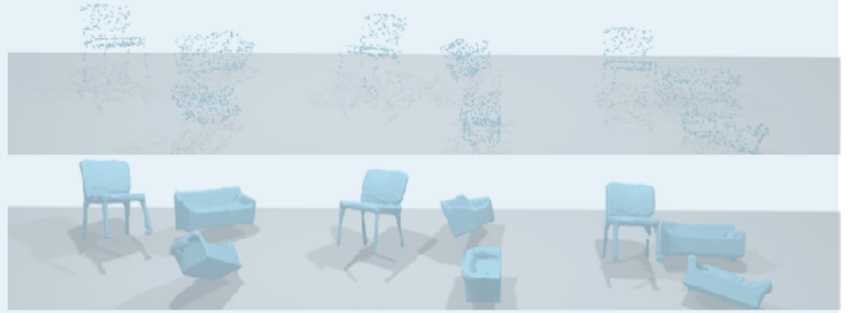

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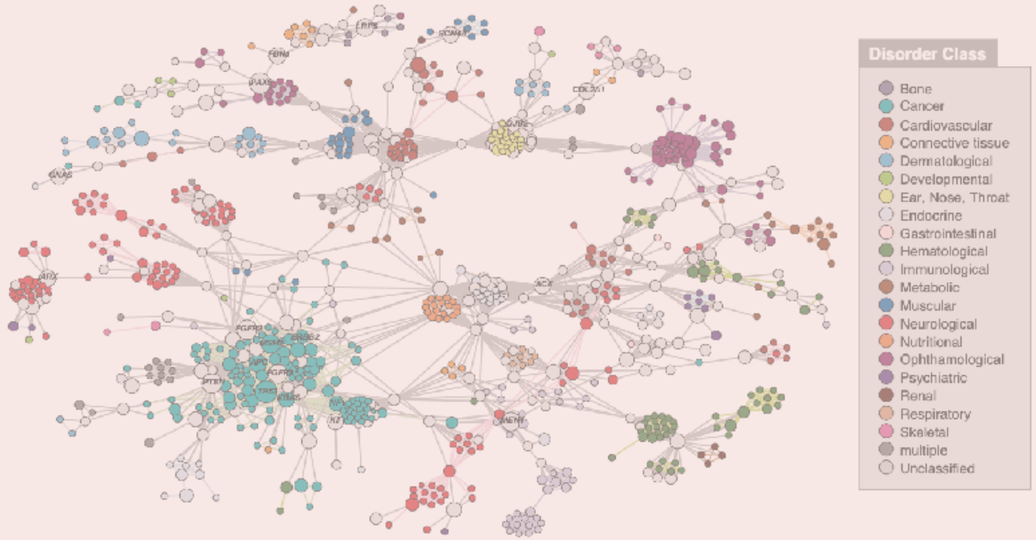

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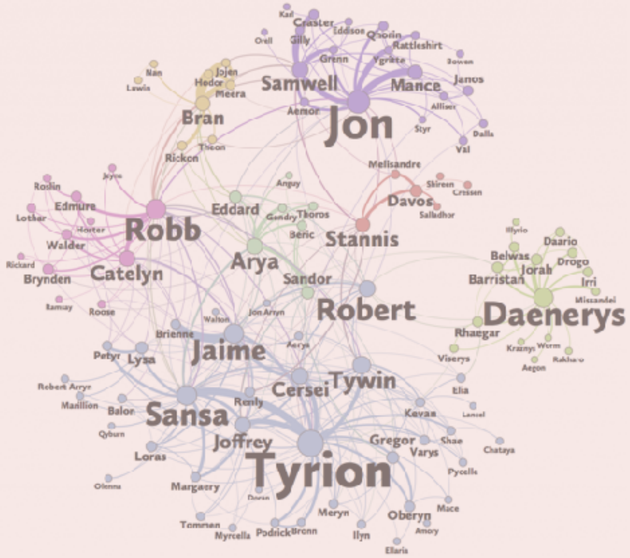


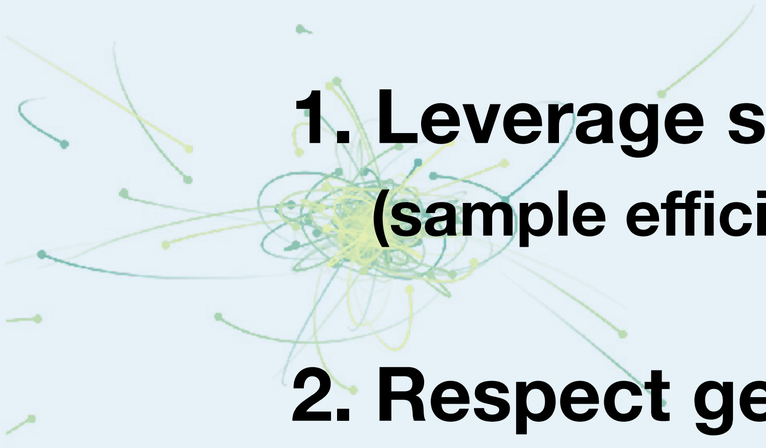
Social network graph[2]

Geometric graphs
(nodes correspond to points in a manifold)

1. Leverage symmetries

(sample efficiency, model complexity, generalizability)

2. Respect geometrical/physical constraints



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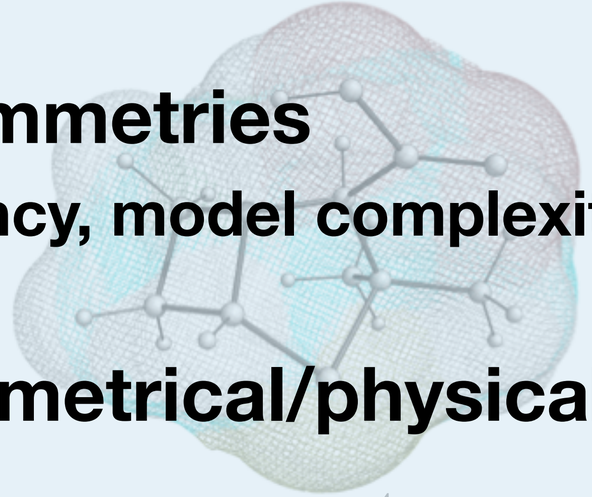

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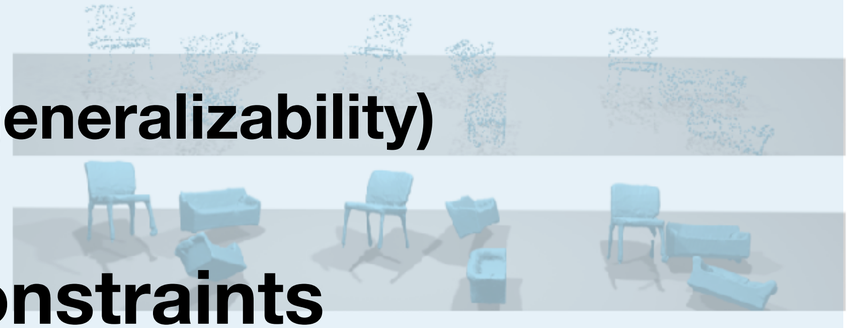

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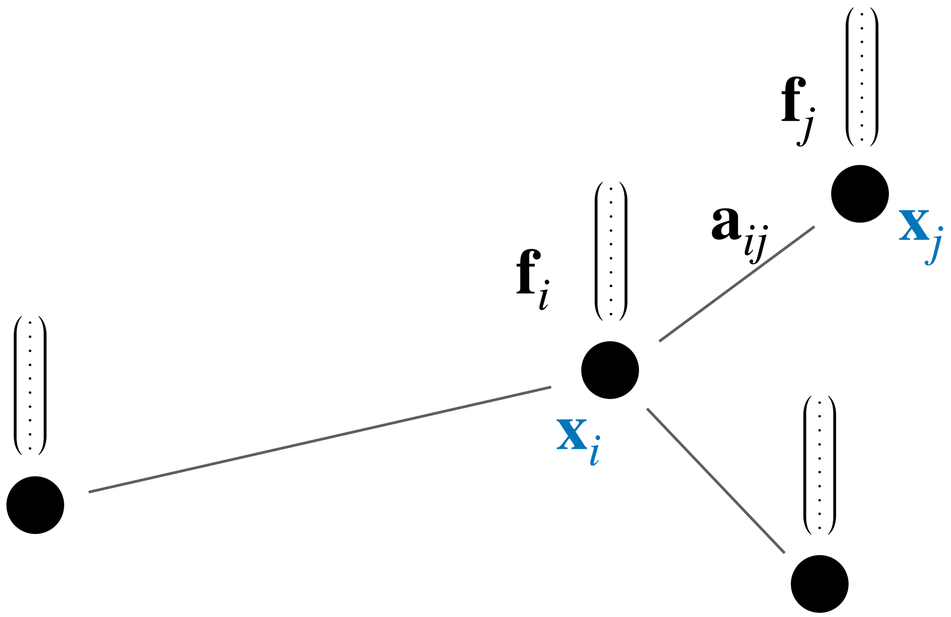
The *Geometric* Message Passing Framework

Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$

- nodes $v_i \in \mathcal{V}$ with node feature $\mathbf{f}_i \in \mathbb{R}^{C_v}$ and position $x_i \in X$
- edges $e_{ij} \in \mathcal{E}$ with edge attribute $\mathbf{a}_{ij} \in \mathbb{R}^{C_e}$



Goal: iteratively update node features to obtain useful hidden representations $\mathbf{h} \in \mathbb{R}^{C_h}$

Message passing layer:

- Messages

$$\mathbf{m}_{ij} = \phi_m(\mathbf{f}_i, \mathbf{f}_j, \mathbf{a}_{ij})$$

- Aggregate + node updates

$$\mathbf{f}'_i = \phi_f(\mathbf{f}_i, \sum_{j \in \mathcal{N}(i)} \mathbf{m}_{ij})$$

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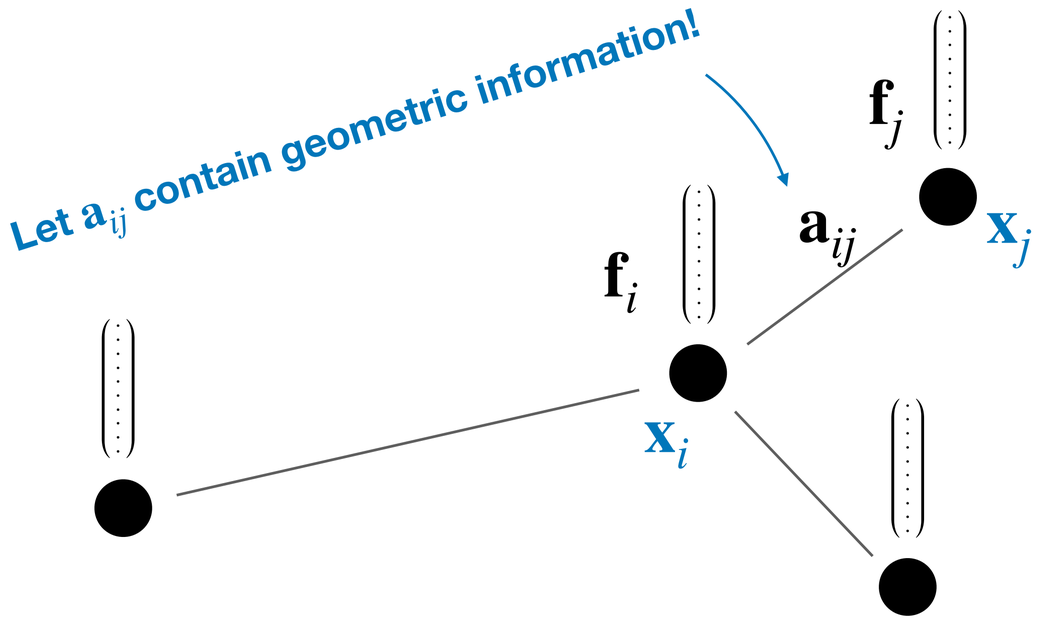

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$$\mathbf{m}_{ij} = \phi_m(\mathbf{f}_i, \mathbf{f}_j, \mathbf{a}_{ij})$$

"Condition" messages on geometry

- Aggregate + node updates

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$(X = \mathbb{R}^d)$ $\mathbf{m}_{ij} = \phi_m(\mathbf{f}_i, \mathbf{f}_j, \mathbf{x}_j - \mathbf{x}_i)$

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Only equivariant to translations…

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Full $E(3)$ equivariance, but a bit restrictive…

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Full $E(3)$ equivariance, but a bit restrictive…

$(X = G)$ $\mathbf{m}_{ij} = \phi_m(\mathbf{f}_i, \mathbf{f}_j, g_j^{-1} g_i)$

Solution 1: Lift to the group!

The *Geometric* Message Passing Framework

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$(X = \mathbb{R}^d)$ $\hat{\mathbf{m}}_{ij} = \hat{\phi}_m(\hat{\mathbf{f}}_i, \hat{\mathbf{f}}_j, Y(\mathbf{x}_j - \mathbf{x}_i))$

Solution 2: work with steerable feature fields!

The *Geometric* Message Passing Framework

Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
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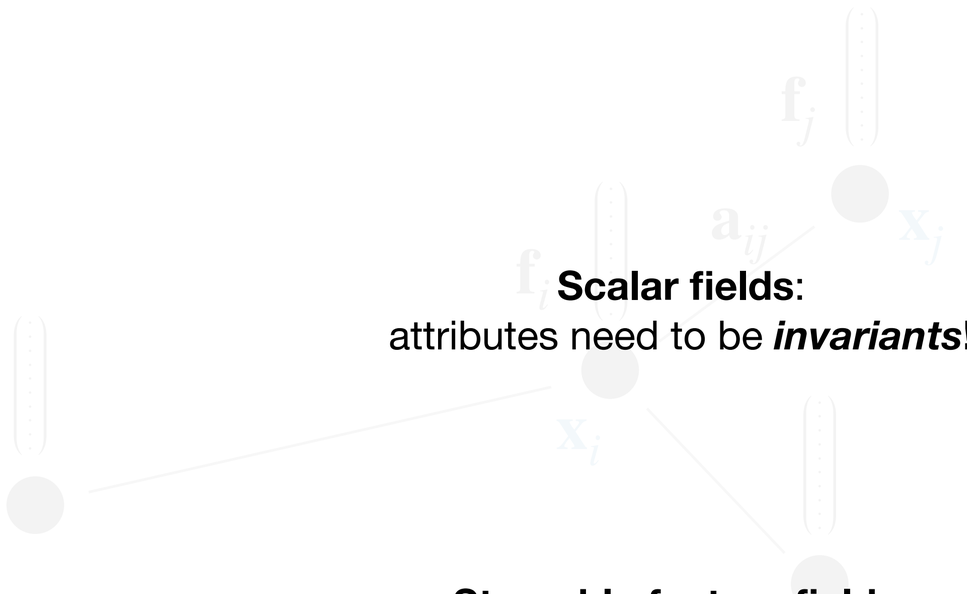

Scalar fields:
attributes need to be ***invariants***!

Steerable feature fields:
attributes can be ***covariants***!

Message passing layer:

- Messages

$$\begin{cases} (X = \mathbb{R}^d) & \mathbf{m}_{ij} = \phi_m(\mathbf{f}_i, \mathbf{f}_j, \mathbf{x}_j - \mathbf{x}_i) \\ (X = \mathbb{R}^d) & \mathbf{m}_{ij} = \phi_m(\mathbf{f}_i, \mathbf{f}_j, \|\mathbf{x}_j - \mathbf{x}_i\|) \\ (X = G) & \mathbf{m}_{ij} = \phi_m(\mathbf{f}_i, \mathbf{f}_j, g_j^{-1} g_i) \end{cases}$$

Only equivariant to translations…

Full $E(3)$ equivariance, but a bit restrictive…

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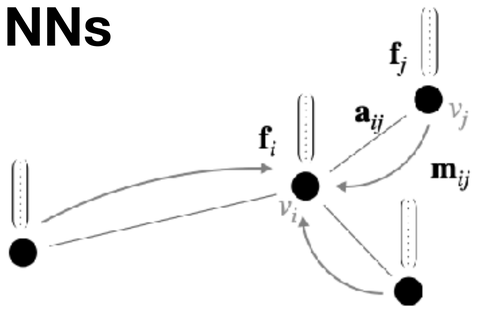
Solution 2: work with steerable feature fields!

Linear vs non-linear (group) convolutions

Message passing NNs

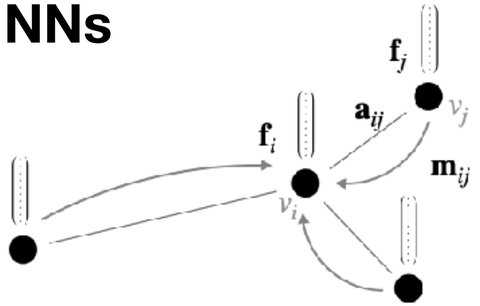


Compute messages: $\mathbf{m}_{ij} = \phi_m(\mathbf{f}_i, \mathbf{f}_j, \mathbf{a}_{ij})$

Aggregate and update: $\mathbf{f}_i' = \phi_f\left(\mathbf{f}_i, \sum_{j \in \mathcal{N}(i)} \mathbf{m}_{ij}\right)$

Linear vs non-linear (group) convolutions

Message passing NNs



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Classic point convolutions

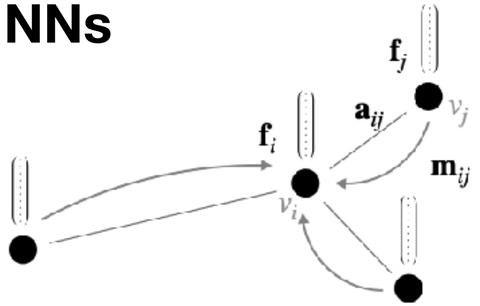
(Lecture 1.7: regular g-convs on homogeneous spaces)

$$\mathbf{m}_{ij} = \mathbf{W}(\|\mathbf{x}_j - \mathbf{x}_i\|)\mathbf{f}_j$$

$$\mathbf{m}_{ij} = \mathbf{W}(g_i^{-1} g_j)\mathbf{f}_j$$

Linear vs non-linear (group) convolutions

Message passing NNs



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Steerable G-CNNs

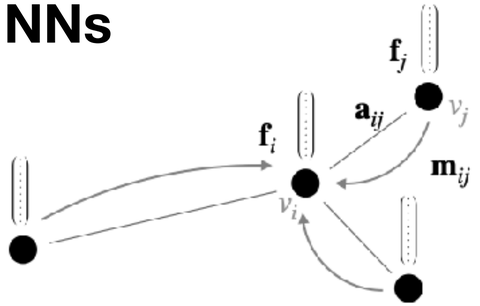
(Lecture 2: steerable g-convs)

$$\mathbf{m}_{ij} = \mathbf{W}_{\hat{\mathbf{a}}_{ij}}(\|\mathbf{x}_j - \mathbf{x}_i\|)\hat{\mathbf{f}}_j$$

$$:= \hat{\mathbf{f}}_j \otimes_{cg}^{\mathbf{W}(\|\mathbf{x}_j - \mathbf{x}_i\|)} \hat{\mathbf{a}}_{ij}$$

Linear vs non-linear (group) convolutions

Message passing NNs



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$\mathcal{F}_H$

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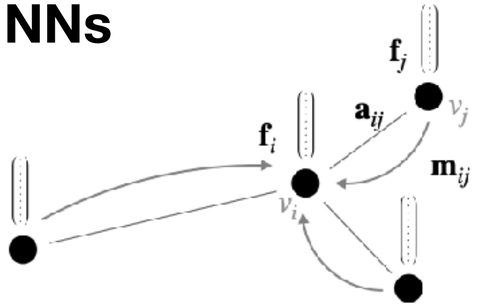

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Classic point convolutions

(Lecture 1.7: regular g-convs on homogeneous spaces)

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$$\mathbf{m}_{ij} = \mathbf{W}(g_i^{-1} g_j)\mathbf{f}_j$$

$\mathcal{F}_H$

Steerable G-CNNs

(Lecture 2: steerable g-convs)

$$\mathbf{m}_{ij} = \mathbf{W}_{\hat{\mathbf{a}}_{ij}}(\|\mathbf{x}_j - \mathbf{x}_i\|)\hat{\mathbf{f}}_j$$

$$:= \hat{\mathbf{f}}_j \otimes_{cg}^{\mathbf{W}(\|\mathbf{x}_j - \mathbf{x}_i\|)} \hat{\mathbf{a}}_{ij}$$

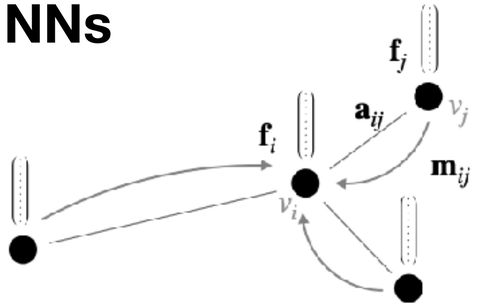
Invariant Message Passing NNs

(Lecture 3)

$$\mathbf{m}_{ij} = \mathrm{MLP}(\mathbf{f}_i, \mathbf{f}_j, \|\mathbf{x}_j - \mathbf{x}_i\|)$$

Linear vs non-linear (group) convolutions

Message passing NNs



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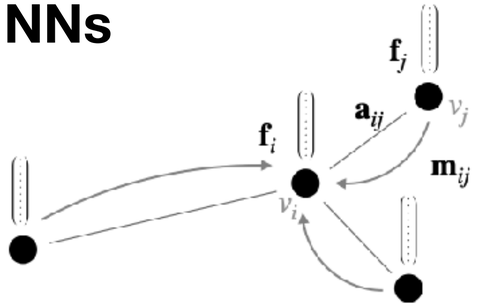

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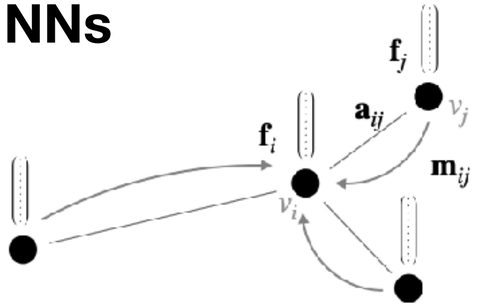

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Non-linear "convolution"

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GEOMETRIC AND PHYSICAL QUANTITIES IMPROVE E(3) EQUIVARIANT MESSAGE PASSING

Anonymous authors
Paper under double-blind review

ABSTRACT

Including covariant information, such as position, force, velocity or spin is important in many tasks in computational physics and chemistry. We introduce Steerable E(3) Equivariant Graph Neural Networks (SEGNNs) that generalise equivariant graph networks, such that node and edge attributes are not restricted to invariant scalars, but can contain covariant information, such as vectors or tensors. This model, composed of steerable MLPs, is able to incorporate geometric and physical information in both the message and update functions. Through the definition of steerable node attributes, the MLPs provide a new class of activation functions for general use with steerable feature fields. We discuss ours and related work through the lens of *equivariant non-linear convolutions*, which further allows us to pin-point the successful components of SEGNNs: *non-linear* message aggregation improves upon classic *linear* (steerable) point convolutions; *steerable messages* improve upon recent equivariant graph networks that send invariant messages. We demonstrate the effectiveness of our method on several tasks in computational physics and chemistry and provide extensive ablation studies.

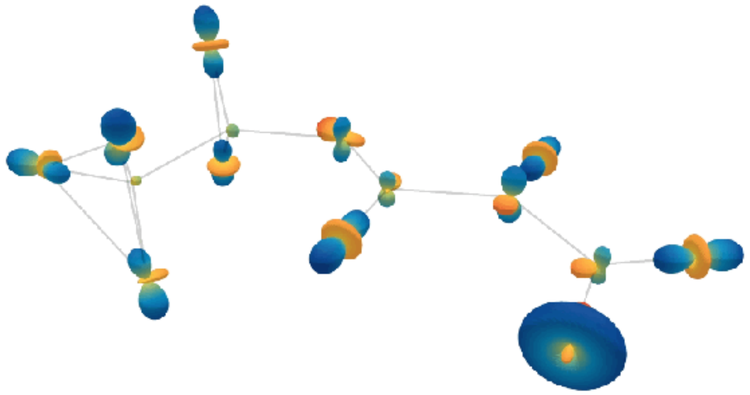
1 INTRODUCTION

The success of Convolutional Neural Networks (CNNs) (LeCun et al., 1998; 2015; Schmidhuber, 2015; Krizhevsky et al., 2012) is a key factor for the rise of deep learning, attributed to their capability of exploiting translation symmetries, hereby introducing a strong inductive bias. Recent work has shown that designing CNNs to exploit additional symmetries via group convolutions has even further increased their performance (Cohen & Welling, 2016; 2017; Worrall et al., 2017; Cohen et al., 2018; Kondor & Trivedi, 2018; Weiler et al., 2018; Bekkers et al., 2018; Bekkers, 2019; Weiler & Cesa, 2019). Graph neural networks (GNNs) and CNNs are closely related to each other via their aggregation of local information. More precisely, CNNs can be formulated as message passing layers (Gilmer et al., 2017) based on a sum aggregation of messages that are obtained by relative position-dependent *linear* transformations of neighbouring node features. The power of message passing layers is, however, that node features are transformed and propagated in a highly *non-linear* manner. Equivariant GNNs have been proposed before as either PointConv-type (Wu et al., 2019; Kristof et al., 2017) implementations of steerable (Thomas et al., 2018; Anderson et al., 2019; Fuchs et al., 2020) or regular group convolutions (Finzi et al., 2020). The most important component in these methods are the convolution layers. Although powerful, such layers only (pseudo[1]) linearly transform the graphs and non-linearity is only obtained via point-wise activations.

In this paper, we propose non-linear E(3) *equivariant message passing* layers using the same principles that underlie steerable group convolutions, and view them as *non-linear group convolutions*. Central to our method is the use of steerable vectors and their equivariant transformations to represent and process node features; we present the underlying mathematics of both in Sec. 2 and illustrate it in Fig. 1 on a molecular graph. As a consequence, information at nodes and edges can now be rotationally invariant (scalar) or covariant (vector, tensor). In steerable message passing frameworks, the Clebsch-Gordan (CG) tensor product is used to steer the update and message functions by geometric information such as relative orientation (pose). Through a notion of steerable node attributes we provide a new class of equivariant activation functions for general use with steerable

[1]Methods such as SE(3)-transformers (Fuchs et al., 2020) and Cormorant (Anderson et al., 2019) include an input-dependent attention component that augments the convolutions.

Task: Molecular property prediction



Property

	Task Units	Cutoff radius	α bohr^3	$\Delta\varepsilon$ meV	$\varepsilon_{\mathrm{HOMO}}$ meV	$\varepsilon_{\mathrm{LUMO}}$ meV	μ D	C_ν cal/mol K	Time [s]
Isotropic (fully connected graph)	(S)EGNN ($l_f = 0, l_a = 0$)	-	.091	53	34	28	.042	.043	0.016
Isotropic (local)	(S)EGNN ($l_f = 0, l_a = 0$)	2Å	.24	98	60	60	.34	.077	0.014
Anisotropic (local)	SEGNN ($l_f = 1, l_a = 2$)	2Å	.074	48	27	25	.031	.035	0.048
	SEGNN ($l_f = 2, l_a = 3$)	2Å	.060	42	24	21	.023	.031	0.097

(Steerable) G-CNNs allow for local connectivity (Scales to large proteins!!!)

isotropic convs require full connectivity in order to infer the geometry

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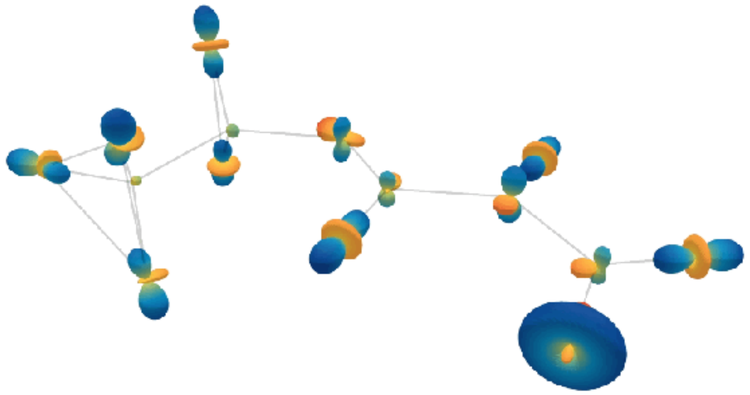

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Task: Trajectory prediction N-body problem

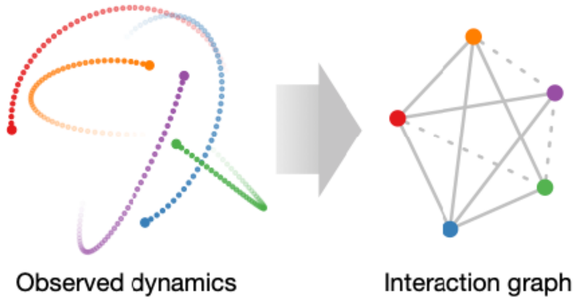


*Figure from Kipf et al 2018

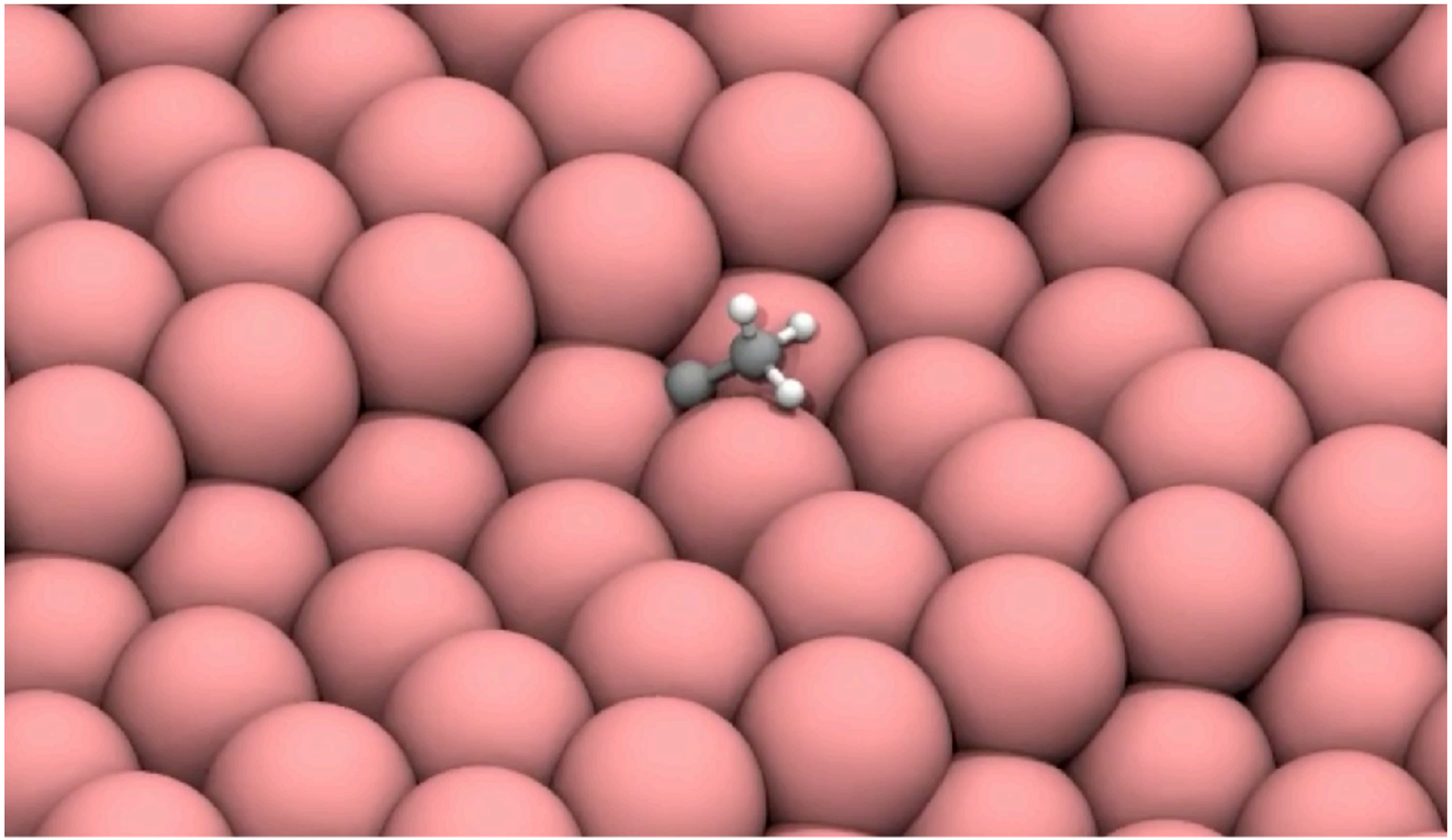
	Method	MSE	Time [s]
G-CNNs	Linear	.0819	.0001
	SE(3)-Tr. (Fuchs et al., 2020)	.0244	.0742
	TFN (Thomas et al., 2018)	.0155	.0182
	NMP (Gilmer et al., 2017)	.0107	.0017
	Radial Field (Köhler et al., 2019)	.0104	.0019
Isotropic "non-linear CNNs"	EGNN (Satorras et al., 2021)	.0070± .00022	.0029
"non-linear G-CNNs"	$\text{SE}_{\text{linear}}$ $(l_f = 2, l_a = 2)$	.0116± .00021	.064
	$\text{SE}_{\text{non-linear}}$ $(l_f = 1, l_a = 1)$	.0060± .00019	.031
	SEGNN_{G} $(l_f = 1, l_a = 1)$	.0056± .00025	.025
	$\text{SEGNN}_{\text{G+P}}$ $(l_f = 1, l_a = 1)$	.0043± .00015	.026

G-CNNs outperform CNNs with isotropic kernels

"Non-linear convolutions" outperform linear convolutions

Steerable methods for computational chemistry

Brandstetter, Hesselink, van der Pol, Bekkers, Welling **Geometric and Physical Quantities Improve E(3) Equivariant Message Passing** - arXiv:2110.02905



Video: Open Catalyst Project

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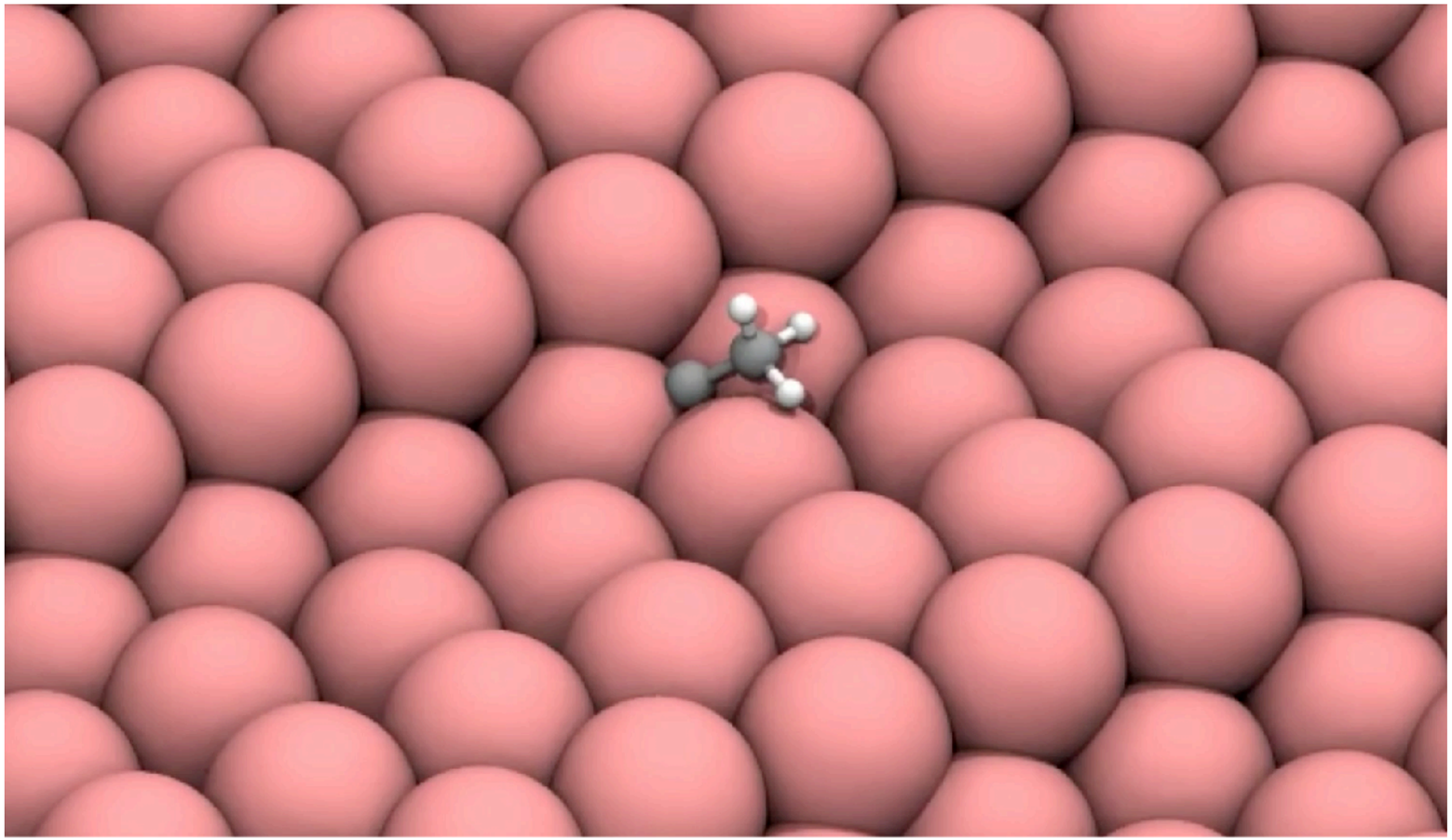

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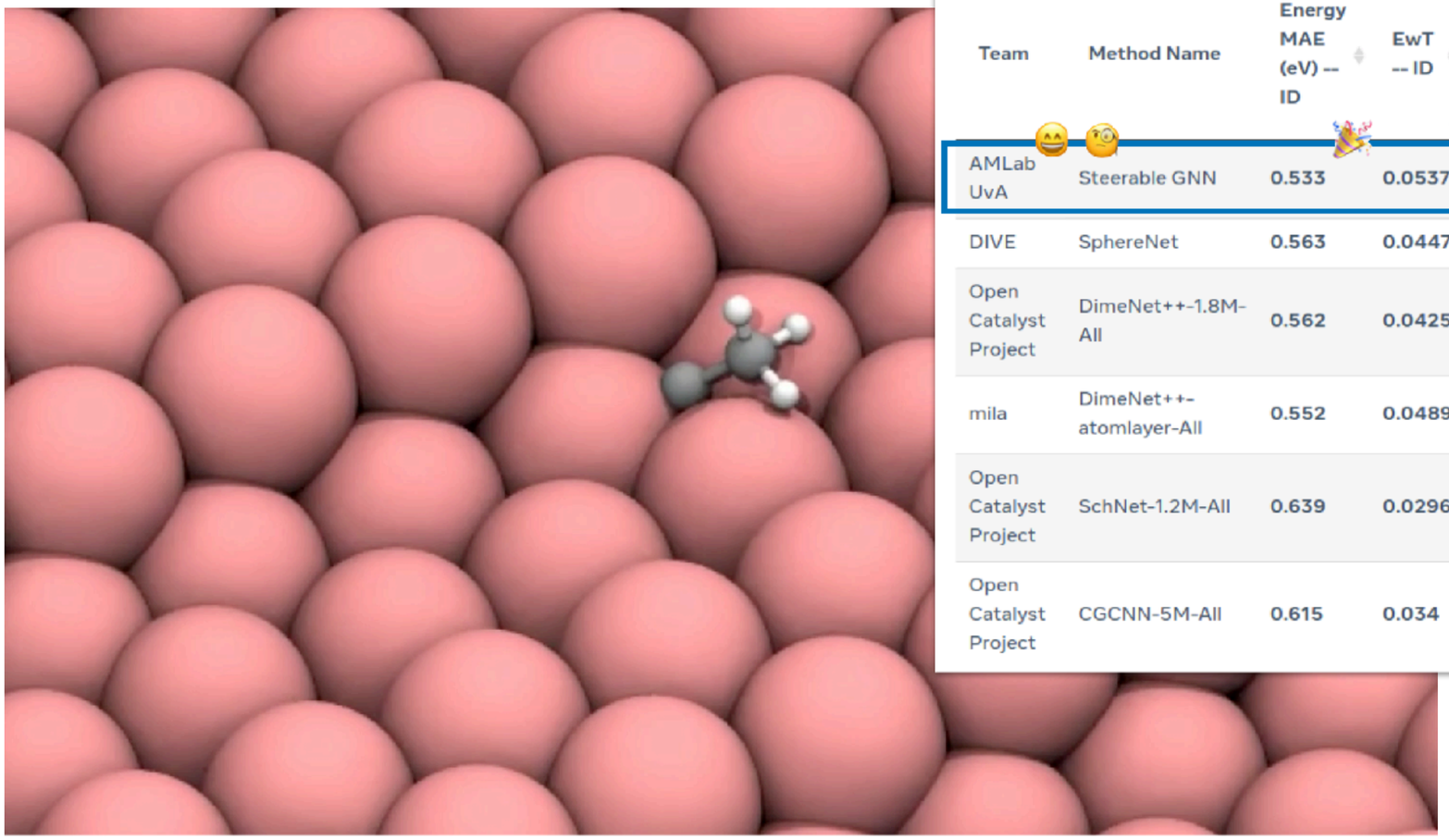

Team	Method Name	Energy MAE (eV) -- ID	EwT -- ID	Energy MAE (eV) -- OOD Ads	EwT -- OOD Ads	Energy MAE (eV) -- OOD Cat	EwT -- OOD Cat	Energy MAE (eV) -- OOD Both	EwT -- OOD Both	Submitted
AMLab UvA	Steerable GNN	0.533	0.0537	0.692	0.0246	0.537	0.0492	0.679	0.0263	2021/06/12
DIVE	SphereNet	0.563	0.0447	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

Table 2: Performance comparison on the QM9 dataset. M
Error (MAE) between model predictions and ground truth

			Task	α	$\Delta\varepsilon$	$\varepsilon_{\text{HOMO}}$	$\varepsilon_{\text{LUMO}}$	μ	C_ν
			Units	bohr^3	meV	meV	meV	D	cal/mol
non-linear		no geometry	NMP	.092	69	43	38	.030	.040
	regular	$\mathbb{R}^3$	SchNet *	.235	63	41	34	.033	.033
pseudo-linear	steerable	$\mathbb{R}^3$	Cormorant	.085	61	34	38	.038	.026
	steerable	$SE(3)$	L1Net	.088	68	46	35	.043	.031
	regular	G	LieConv	.084	49	30	25	.032	.038
	steerable	$SE(3)$	TFN	.223	58	40	38	.064	.101
pseudo-linear	steerable	$SE(3)$	SE(3)-Tr.	.142	53	35	33	.051	.054
non-linear	regular	$\mathbb{R}^3 \times S^2 \times \mathbb{R}^+$	DimeNet++ *	**.043**	**32**	24	19	.029	.023
non-linear	regular	$\mathbb{R}^3 \times S^2 \times \mathbb{R}^+$	SphereNet *	.046	**32**	**23**	**18**	.026	**.021**
non-linear	reguleerable?	$SE(3)$	PaiNN *	.045	45	27	20	**.012**	.024
non-linear	regular	$\mathbb{R}^3$	EGNN	.071	48	29	25	.029	.031
non-linear	steerable	$SE(3)$	SEGNN (Ours)	.060	42	24	21	.023	.031

Table 2: Comparison on QM9.

1. Motivation — Equivariance → weight-sharing and generalization

2. Pattern matching using group theory — Group theory: symmetries & recognition by components
(features have “poses”)

3. Group convolutions — Template matching over groups

4. Example — Effective representation learning and generalization

5. G-convs are all you need! — Any equivariant linear layer is a group convolution

6. Steerable group convolutions — Efficient (band-limited) **grid-free** g-convs

7. Feature fields and escnn library — Flexible framework for equivariant layers

8. Equivariant tensor product layers — Conv layers ↔ TPs with coordinate embeddings
(Clebsch-Gordan: equivariant TP)

9. Equivariant graph NNs — Equivariant MP via geometry conditioned layers

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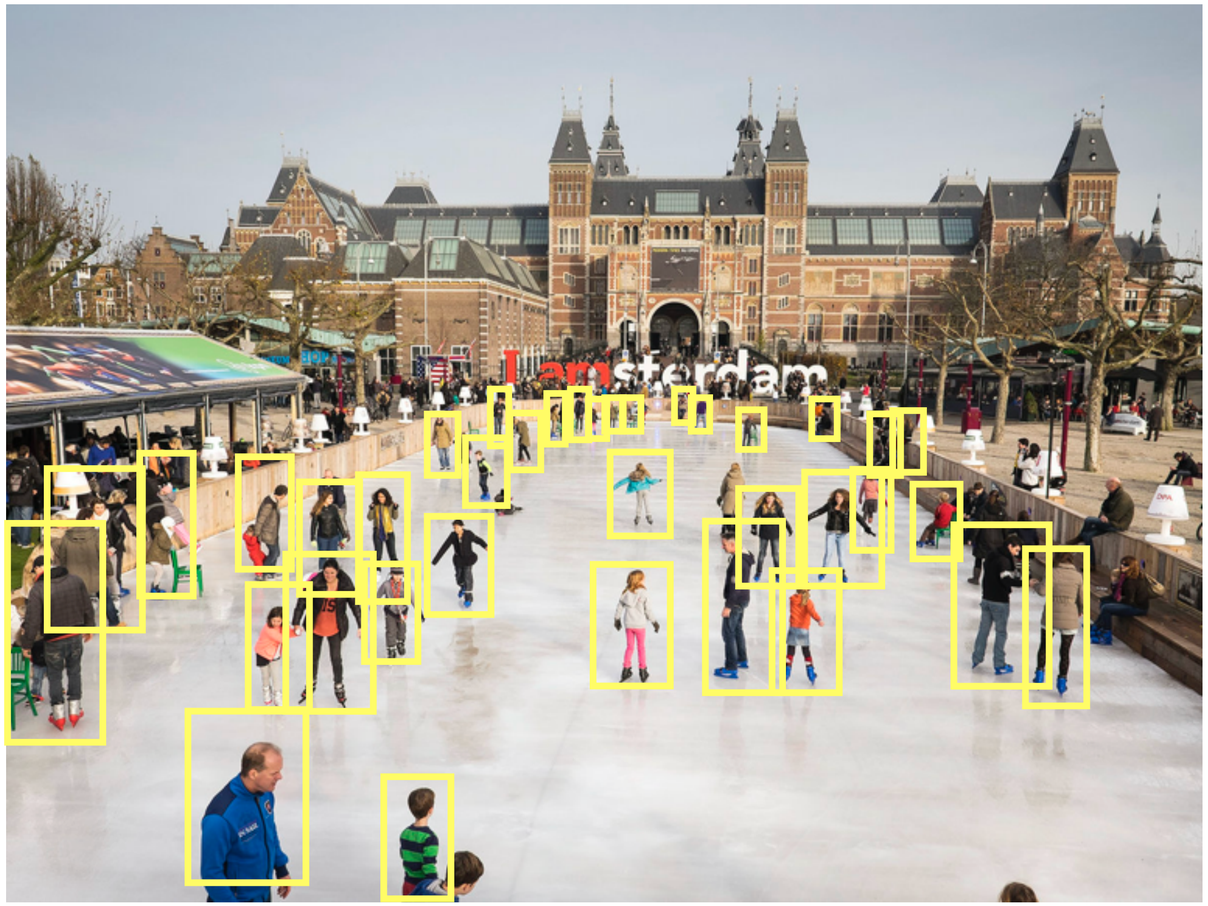
Conclusion

Geometric guarantees (equivariance)



Importance of equivariance:

- No information is lost when the input is transformed

- Guaranteed stability to (local + global) transformations

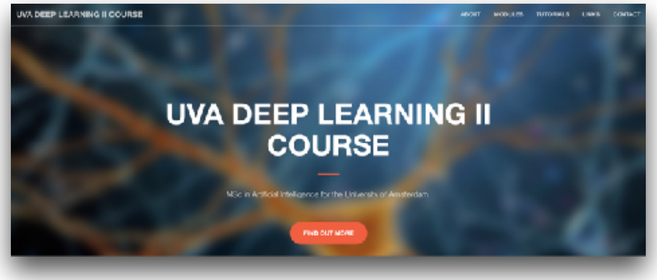
Group convolutions:

- Equivariance beyond translations
- Geometric guarantees
- Increased weight sharing

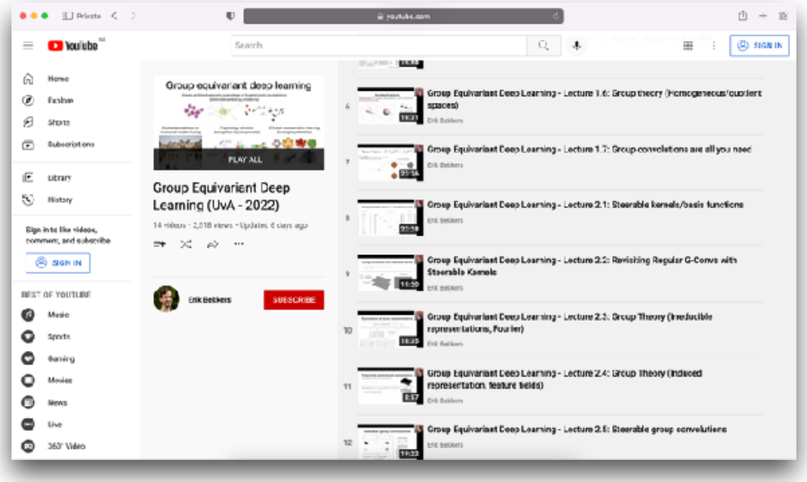
} + **performance**
+ **generalization**

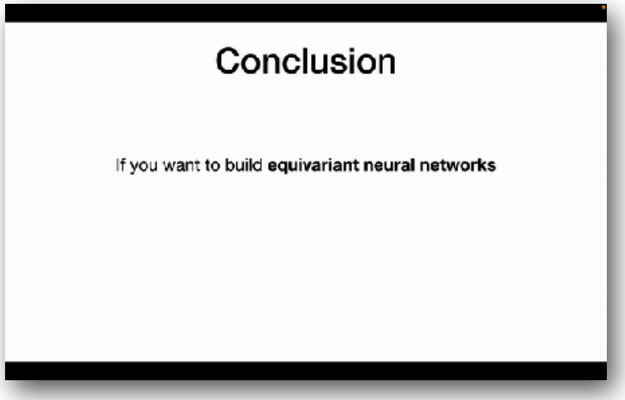
G-CNNs are not only relevant for invariant problems but for any type of structured data!

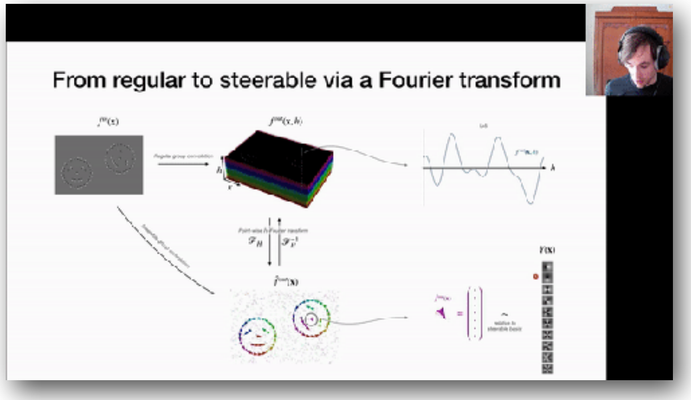
UvA course on group equivariant deep learning (https://uvagedl.github.io)



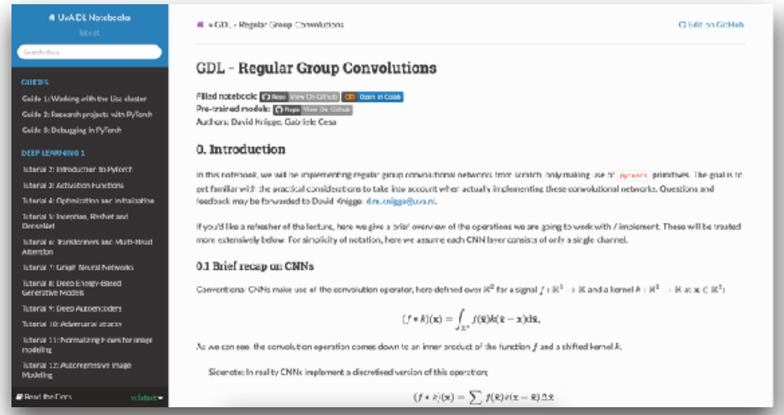
Youtube playlist

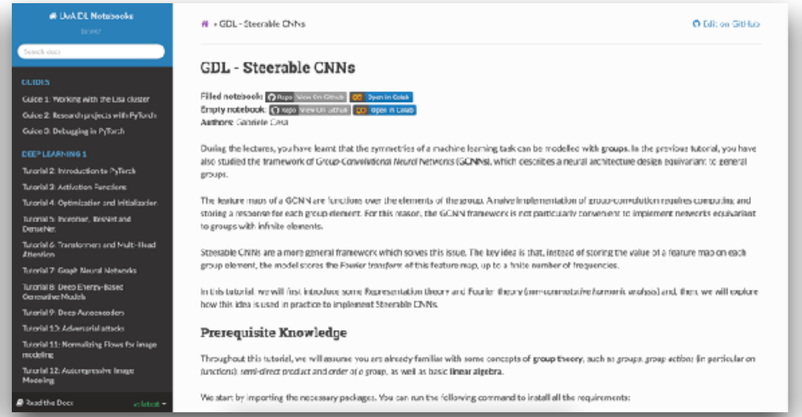


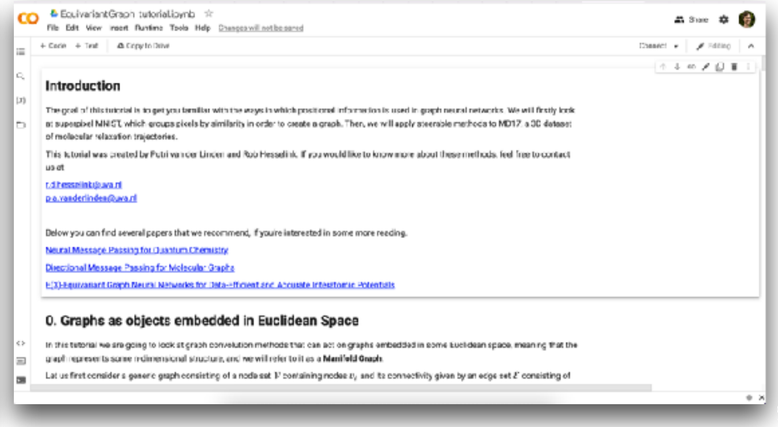




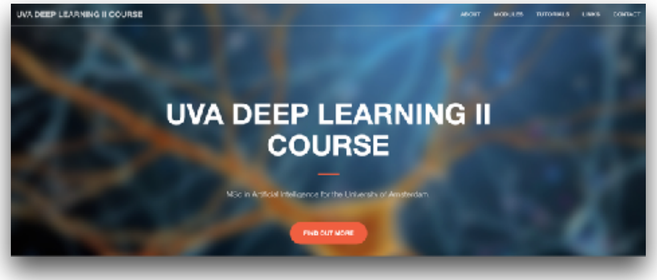
Tutorial notebooks



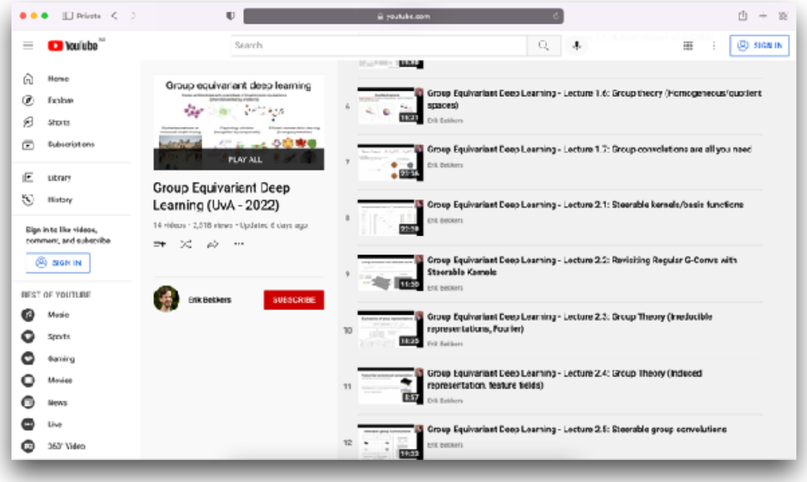


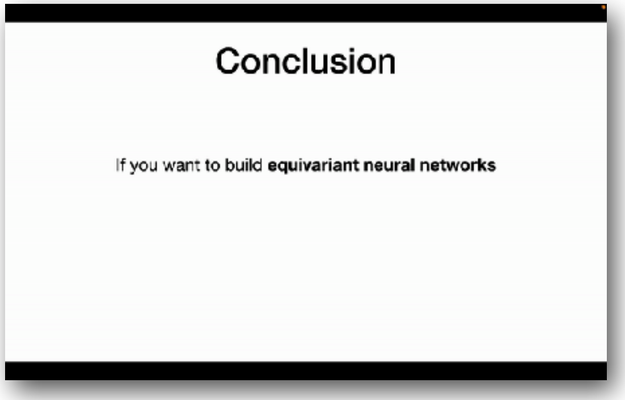


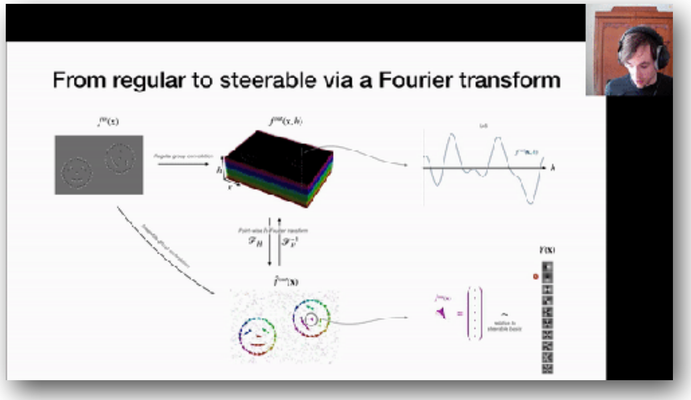
UvA course on group equivariant deep learning (https://uvagedl.github.io)



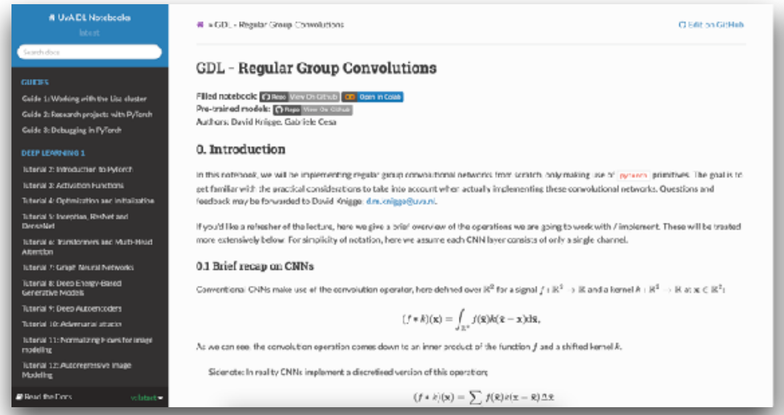
Youtube playlist

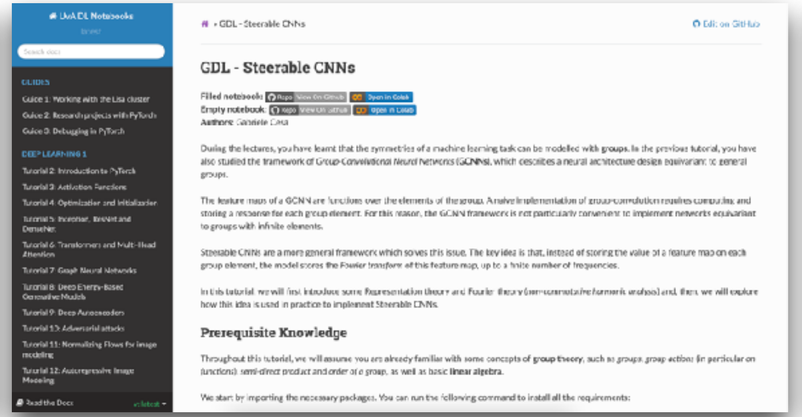


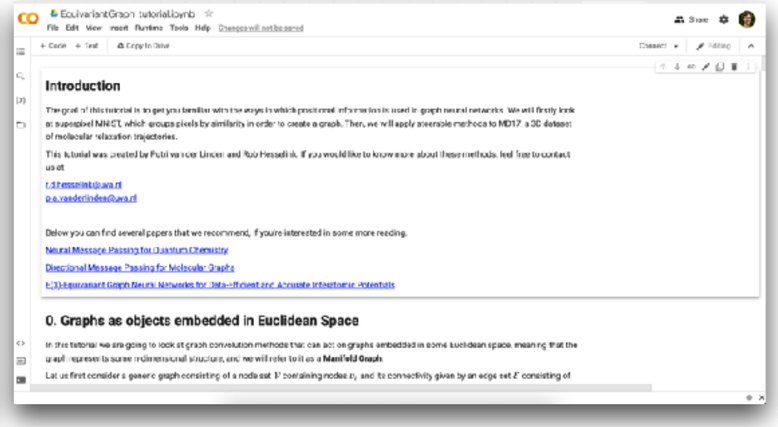




Tutorial notebooks







Thank you for listening!