

Advanced Topics in Equivariance: Lecture 3

Machine Learning Summer School, Indonesia 2020

Daniel Worrall



Legong Dance

This lecture: Equivariance

Grey Box Models

Convolutions

Invariance and Equivariance

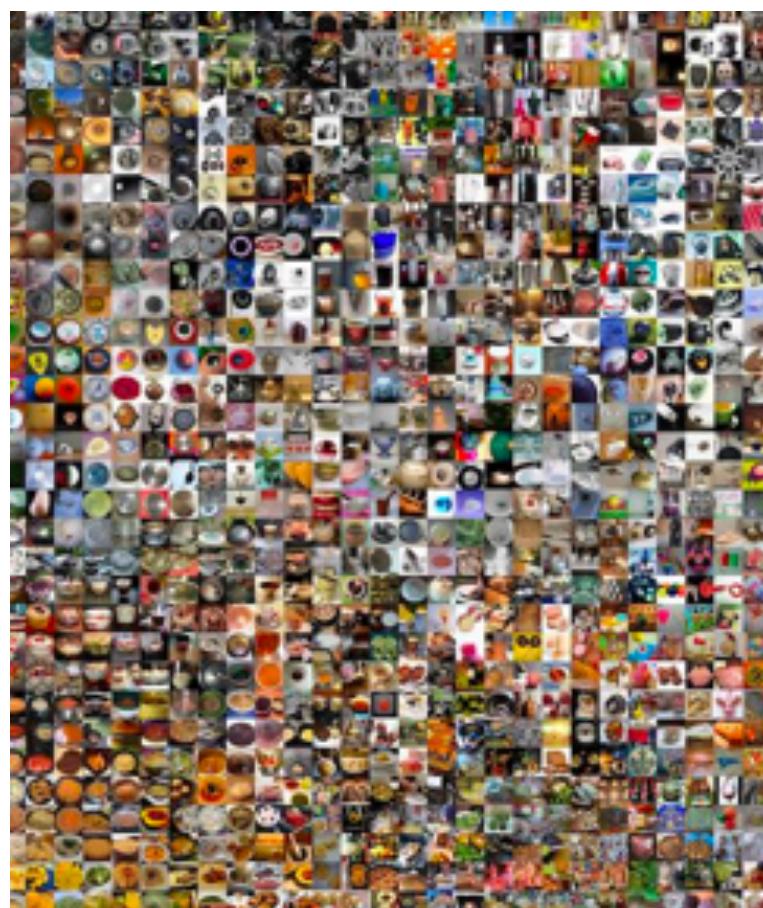
Group Theory

Convolution Generalizations

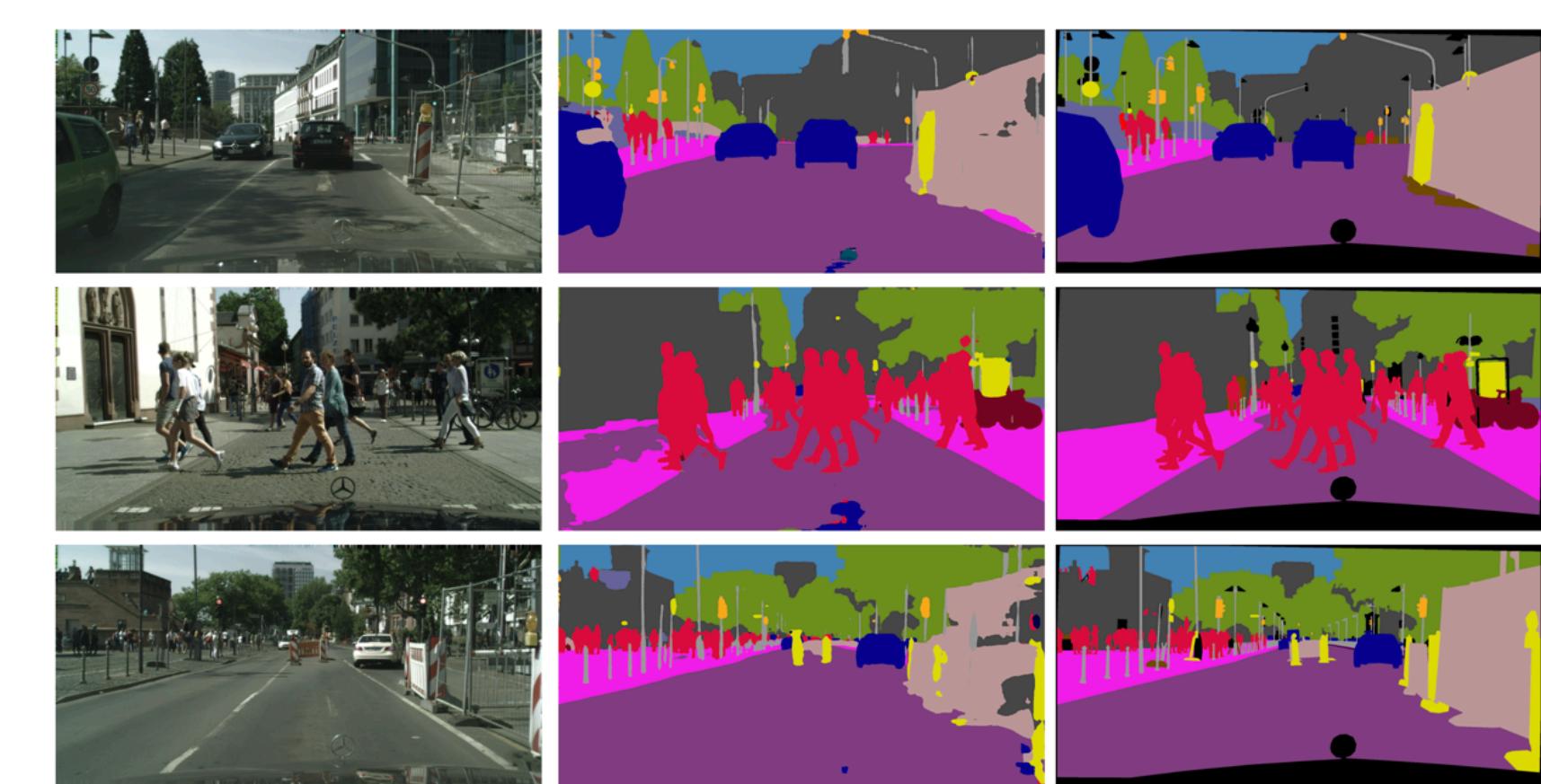
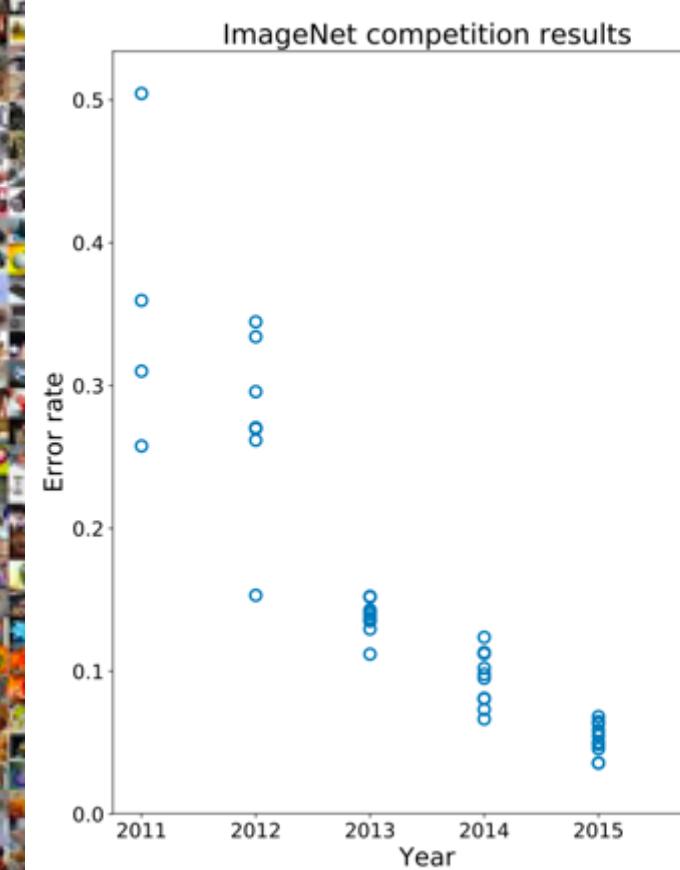
Group Convolutions, Steerable Convolutions,
Semigroup Correlation, Gauge Convolution



CNNs are responsible for many successes



ImageNet [figure from Wikipedia]

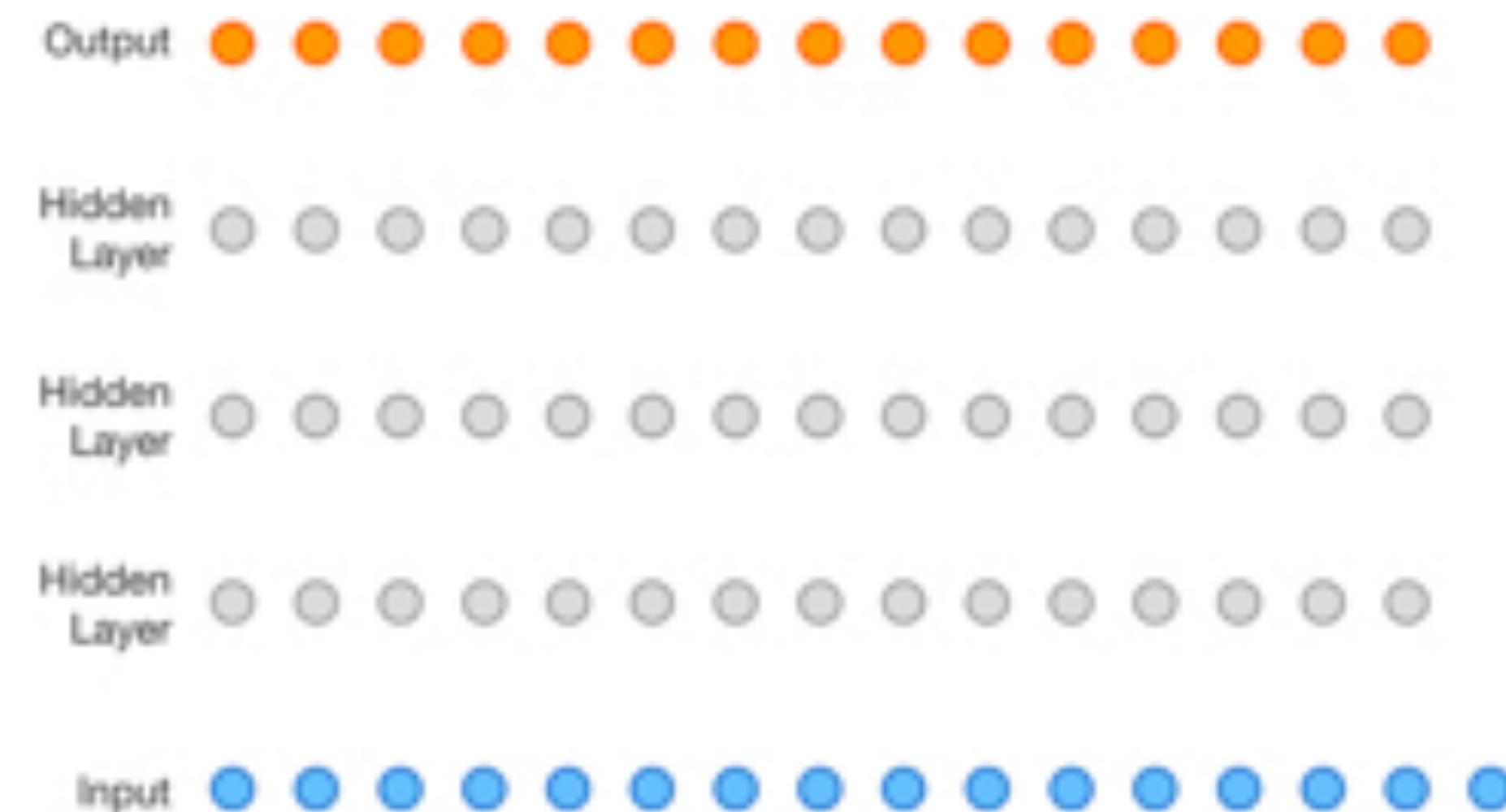


(a) Input

(c) DRN-C-26

(d) Ground truth

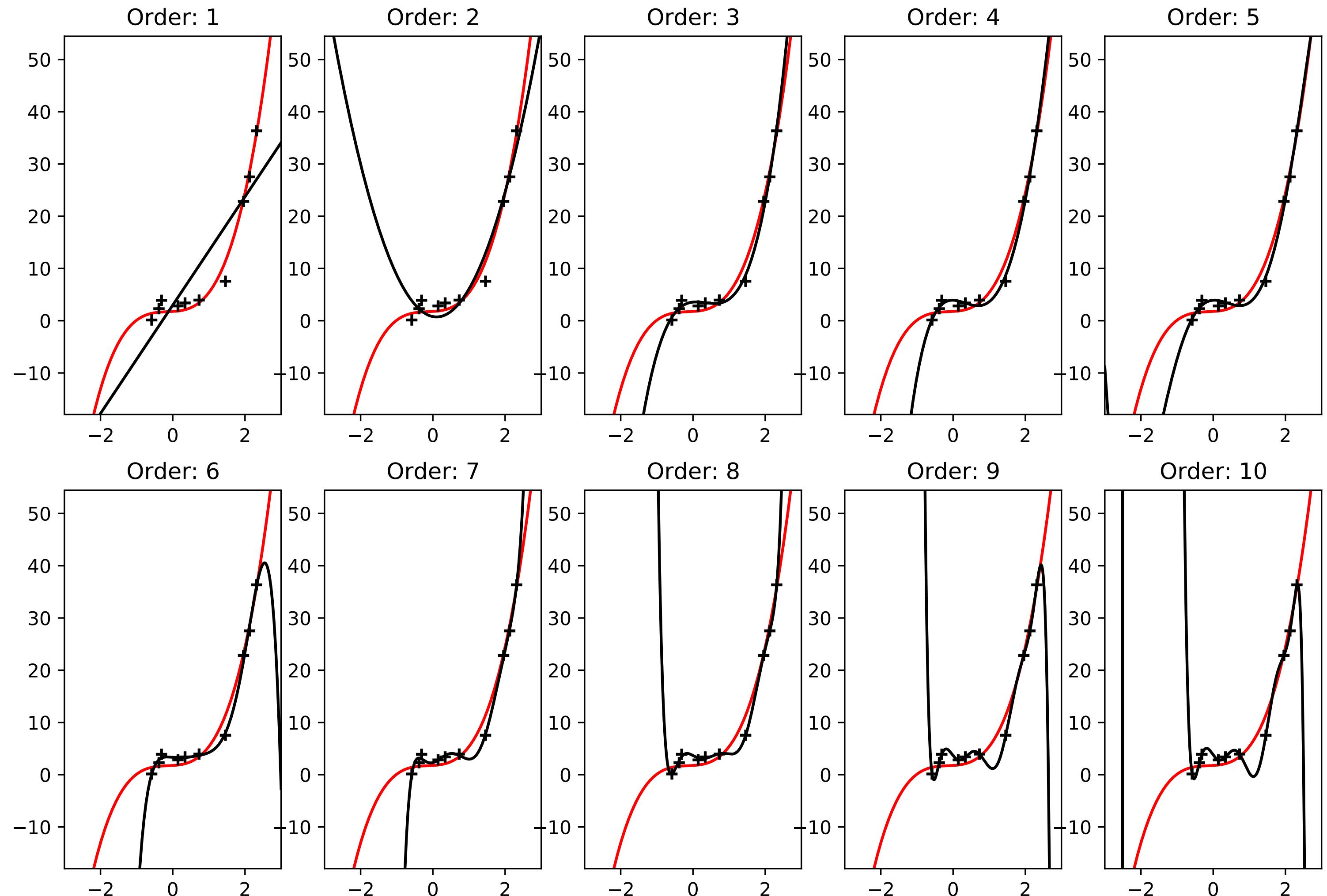
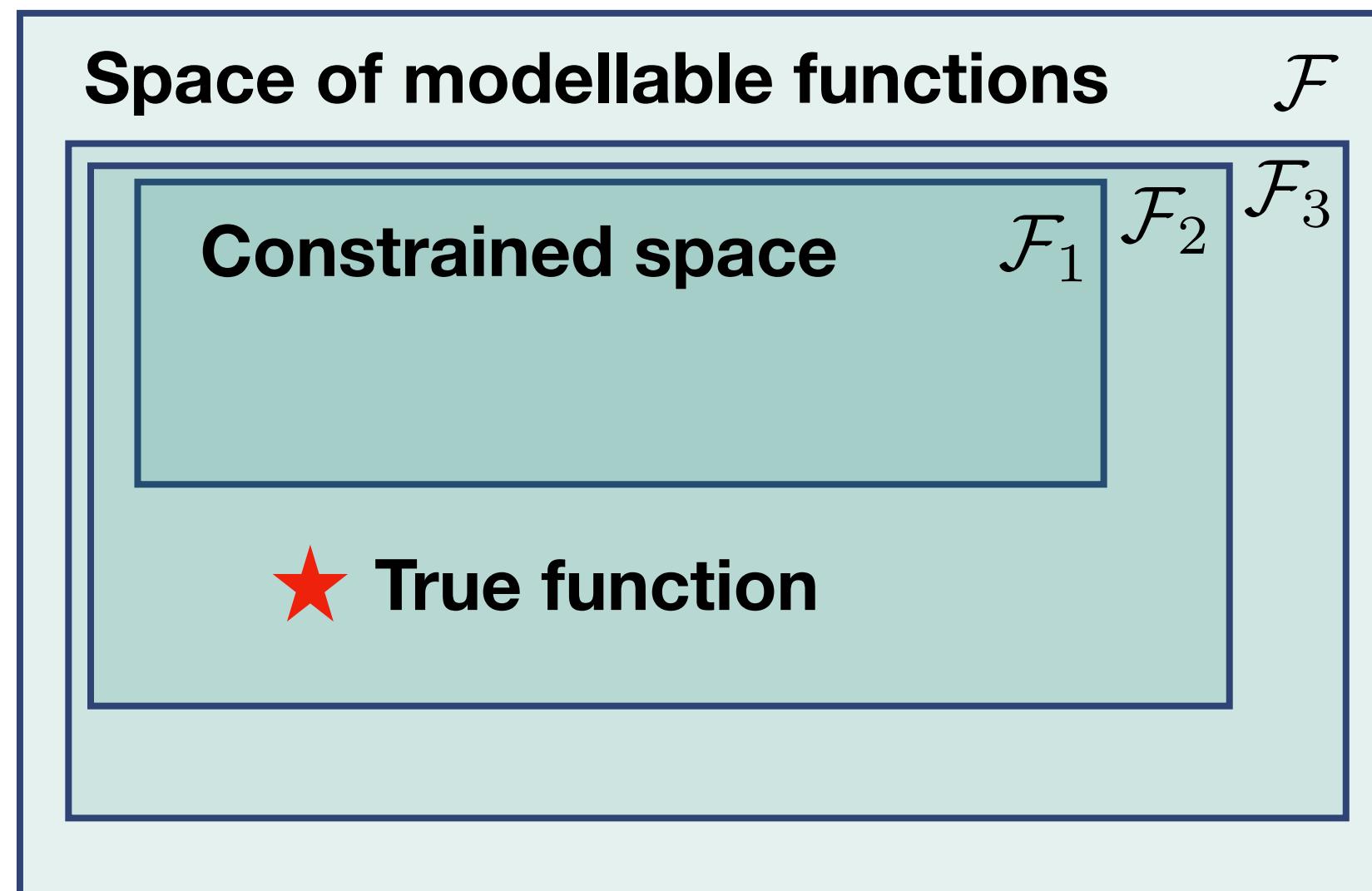
Dilated Residual Networks, Yu et al. (2017)



Inductive biases and overfitting

Remove *degrees of freedom* that do not aid generalization error.

- What assumptions can we make?
- How we encode these assumptions?
- What framework do we use?



Polynomial example

Polynomial fitting to a quintic. What order do we use?

$$y = w_0 + w_1 x + \dots + w_5 x^5 + \epsilon$$

Try multiple orders

Unit Gaussian

$$\mathcal{N}(\mathbf{w} | \mathbf{0}, 10^2 \mathbf{I})$$

$$p(\mathbf{w} | \mathcal{D}, \sigma^2, \tau) = \frac{p(\mathcal{D} | \mathbf{w}, \sigma^2) p(\mathbf{w} | \tau)}{p(\mathcal{D} | \tau)}$$

$$\mathbf{w}_{\text{MAP}} = \arg \max_{\mathbf{w}} p(\mathbf{w} | \mathcal{D}, \tau)$$

Space of modellable functions

\mathcal{F}

Constrained space

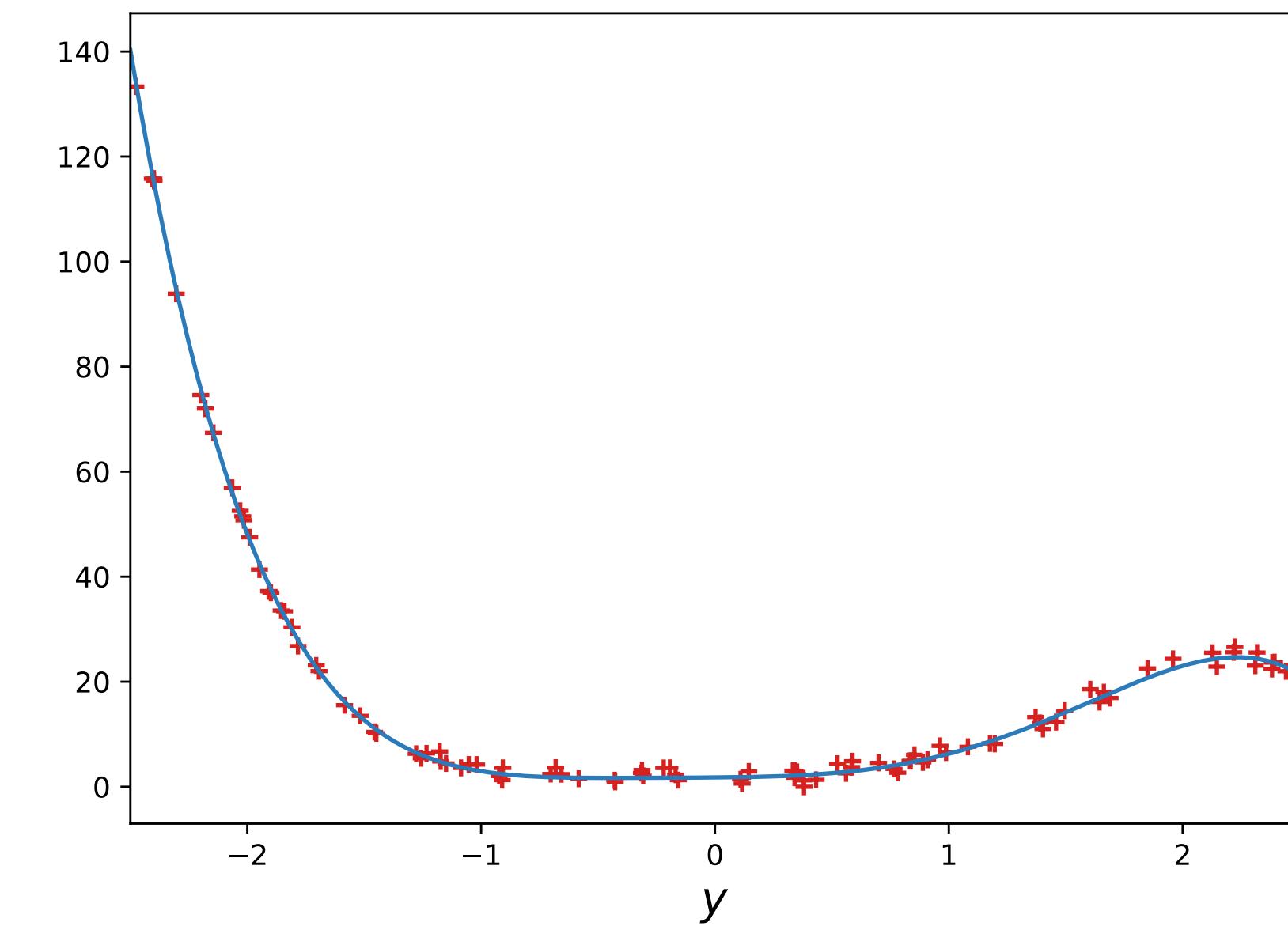
\mathcal{F}_1

\mathcal{F}_2

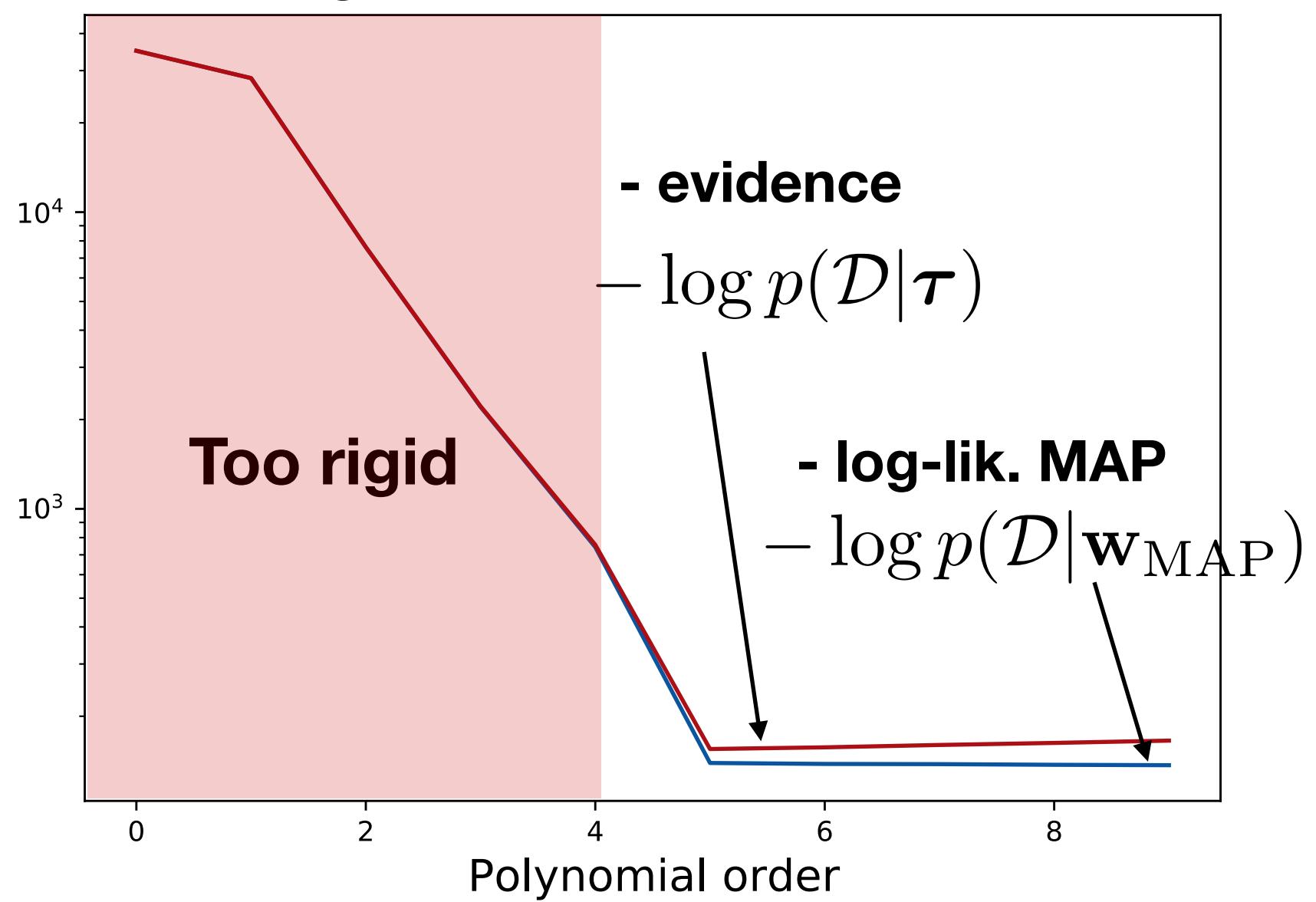
\mathcal{F}_3

True function

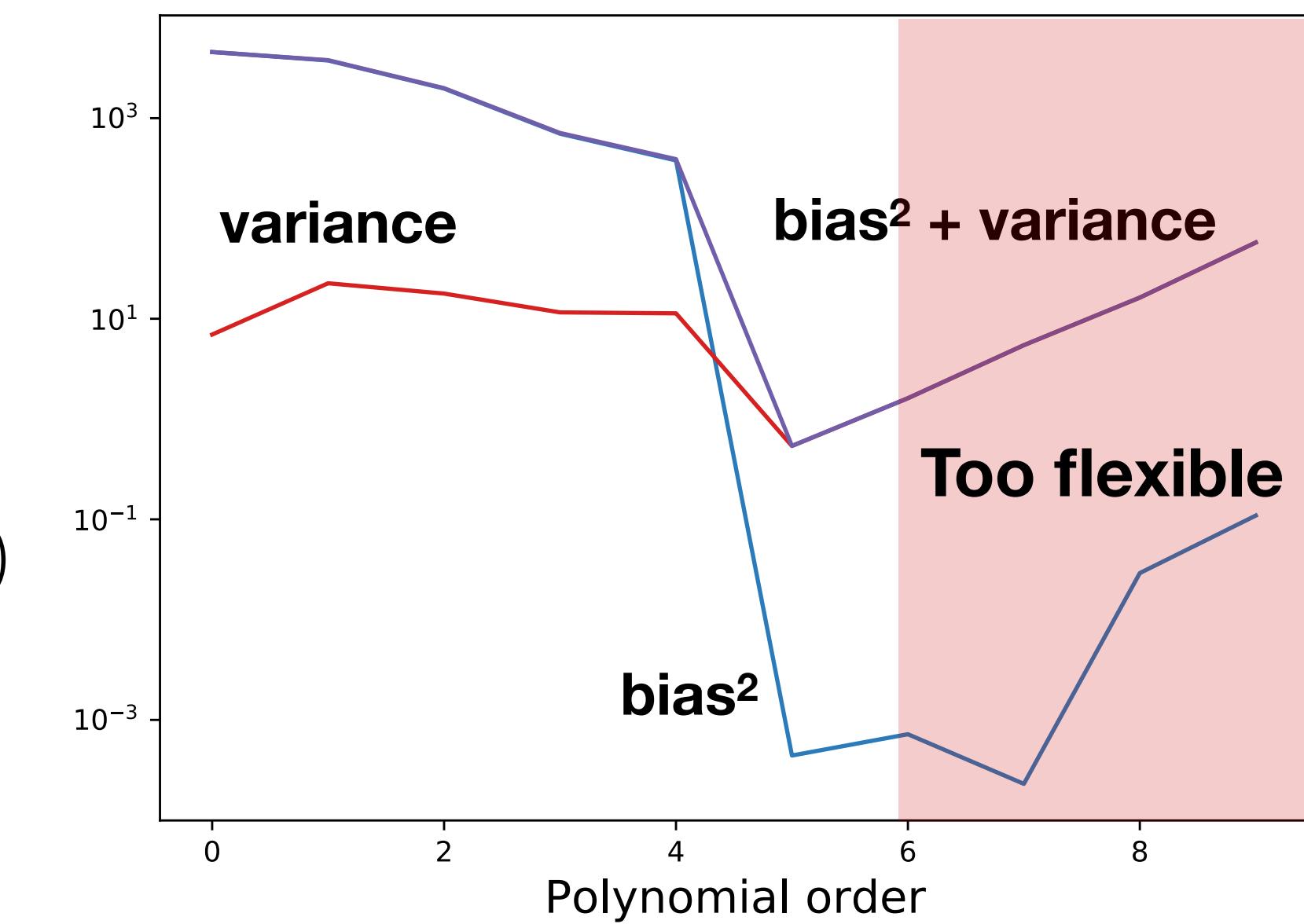
Original quintic polynomial



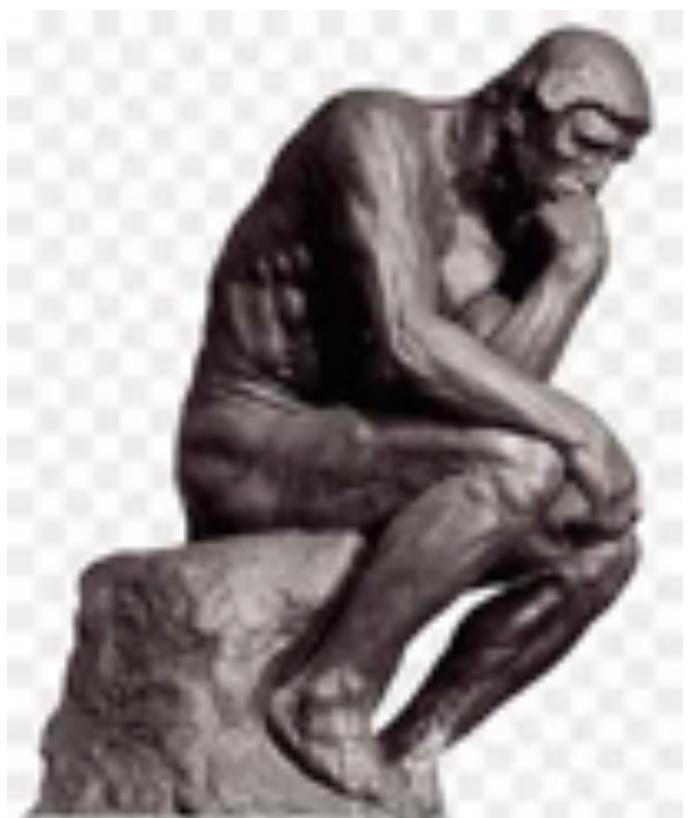
Log-likelihood and evidence



Bias – variance decomposition



White box models



Grey box models

Most ML models sit here.

Regression

- Polynomial order
- Likelihood and prior distribution

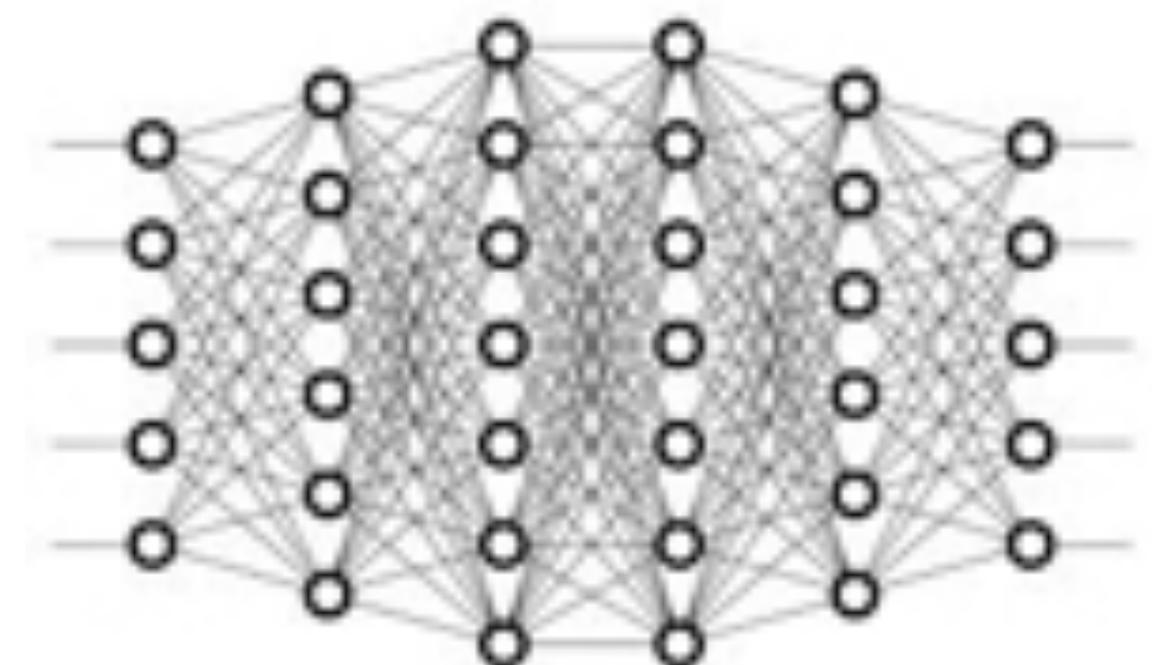
Classification

- Sigmoid function
- Linear features
- ML or MAP?

Deep learning

- Number of layers
- Nonlinearities
- Optimizer
- **Structure: Convolutions**
- ...

Black box models





Equivariance

Batik making

Convolutions

For images we use *convolutions*.

Convolutions use:

1. Translational weight-tying
2. Small reception fields

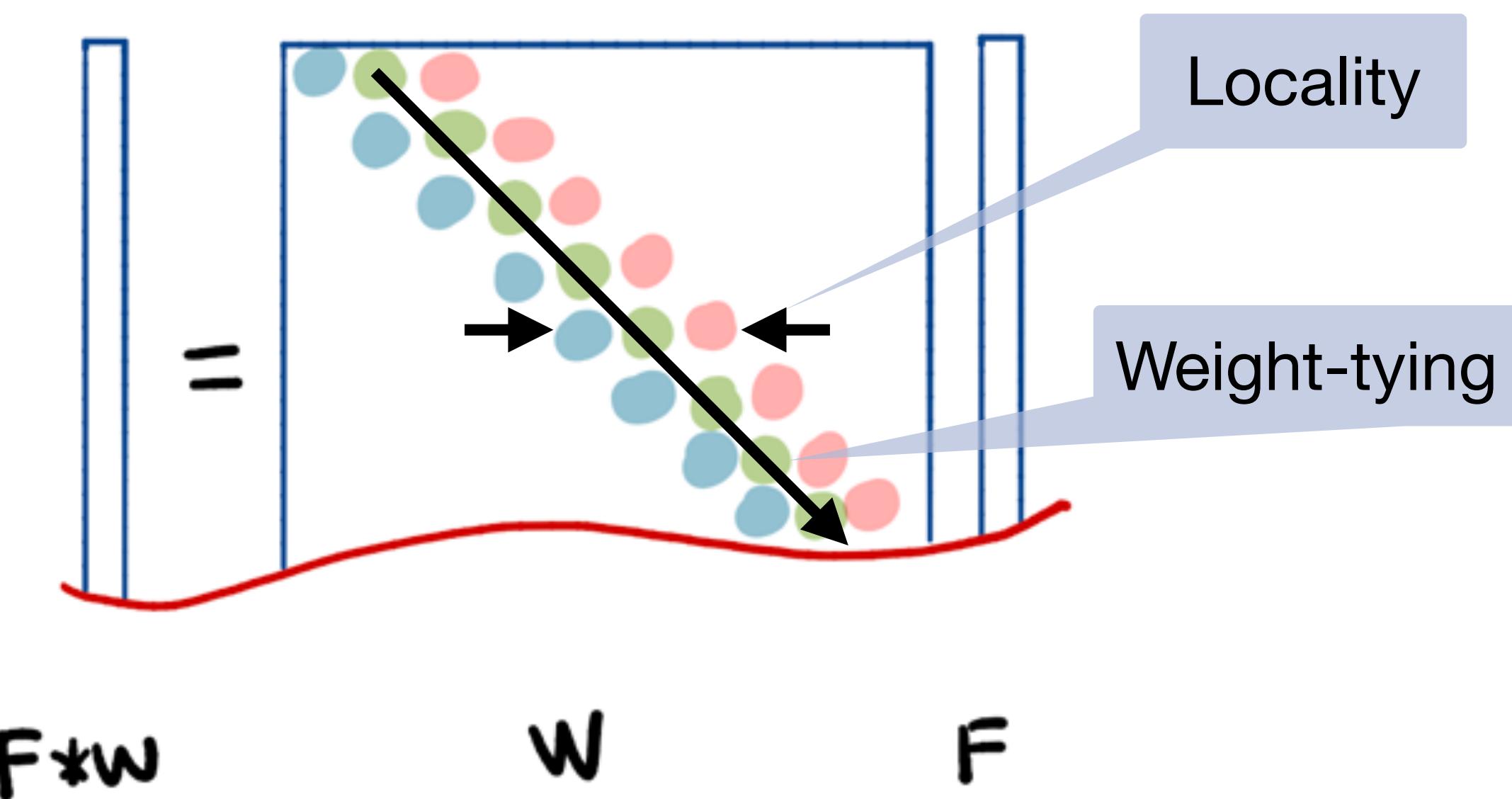
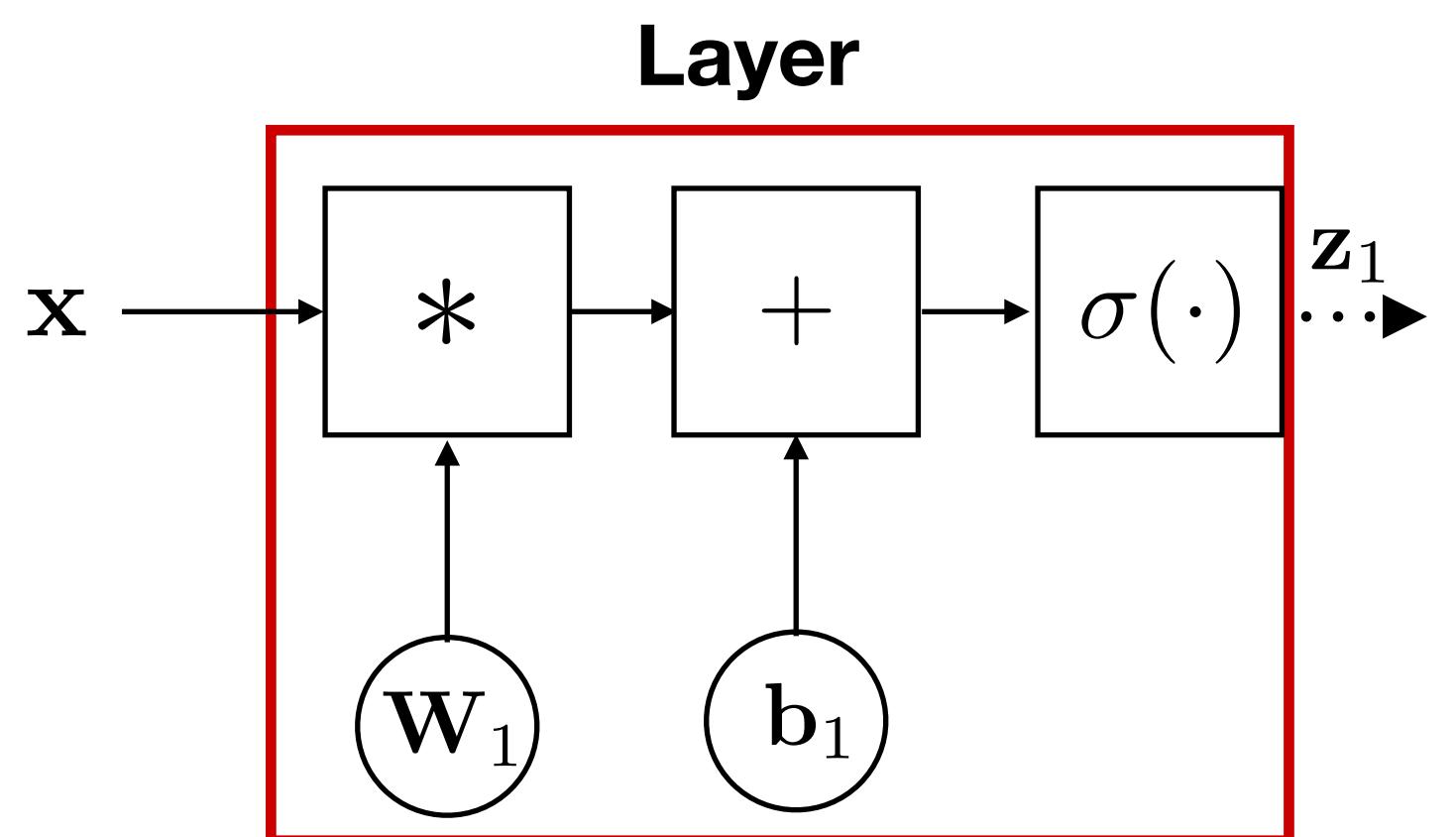
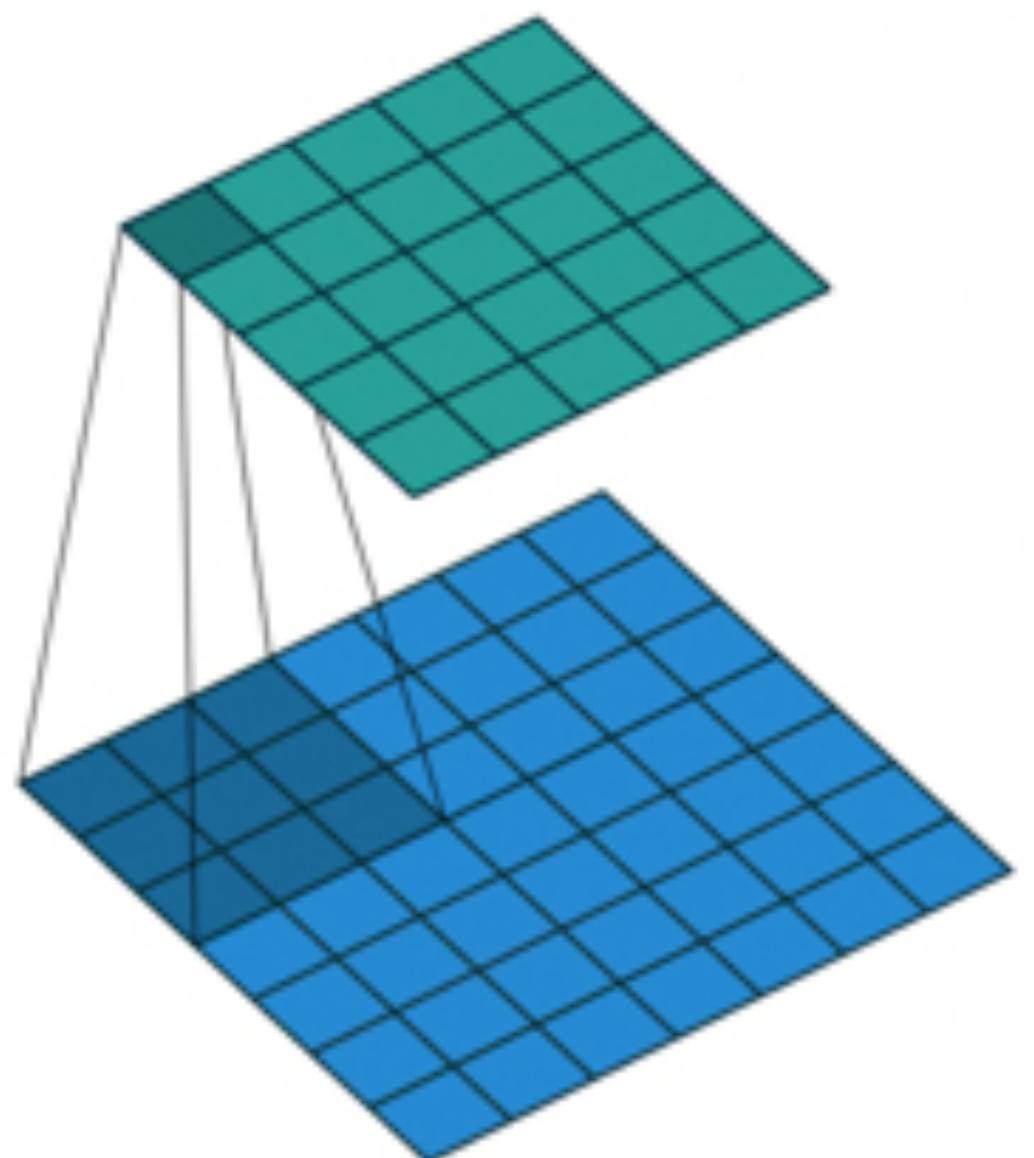
Drop-in replacement
for the linear layer.

Indeed, it is just a
linear layer!

Standard convolution

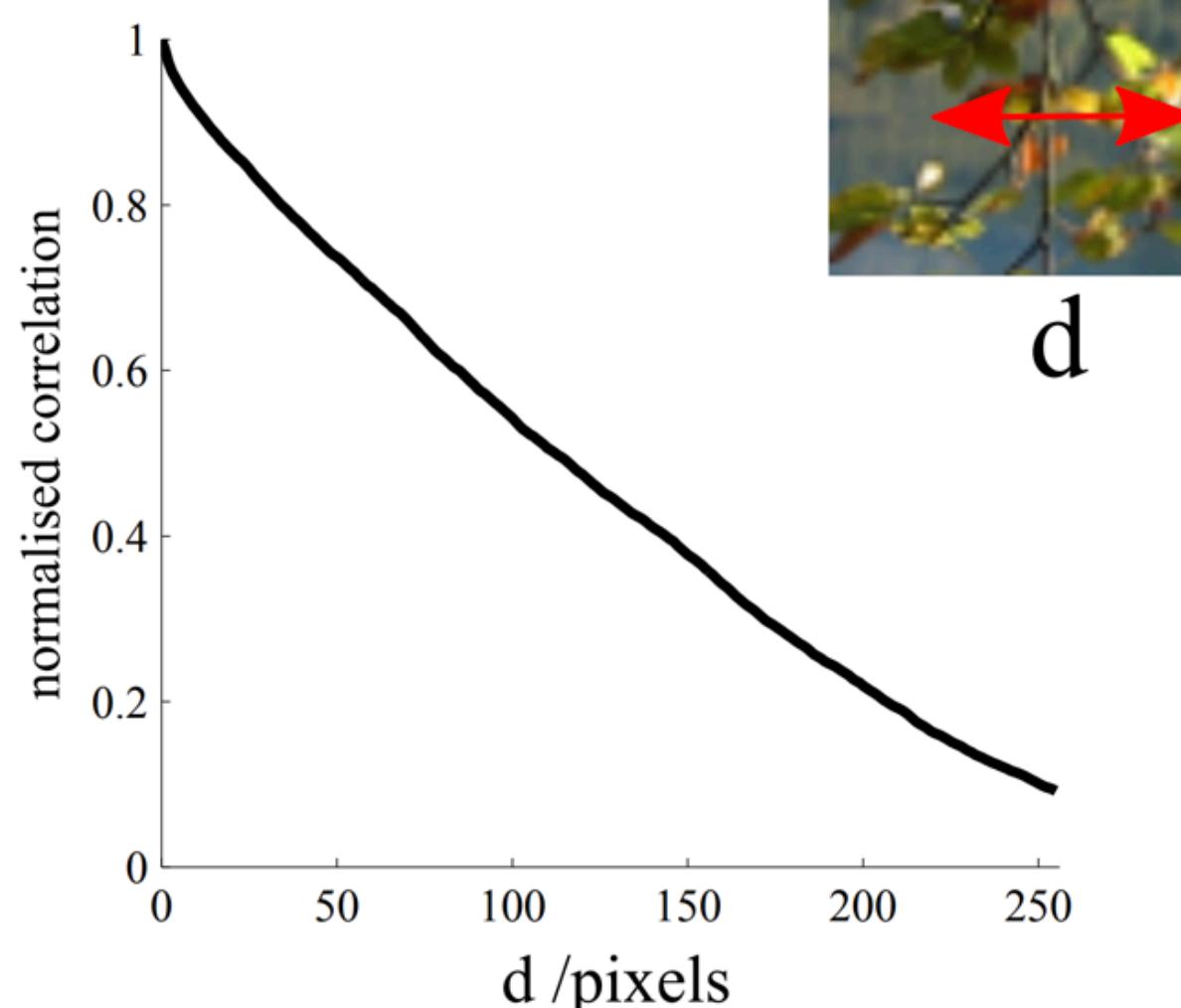
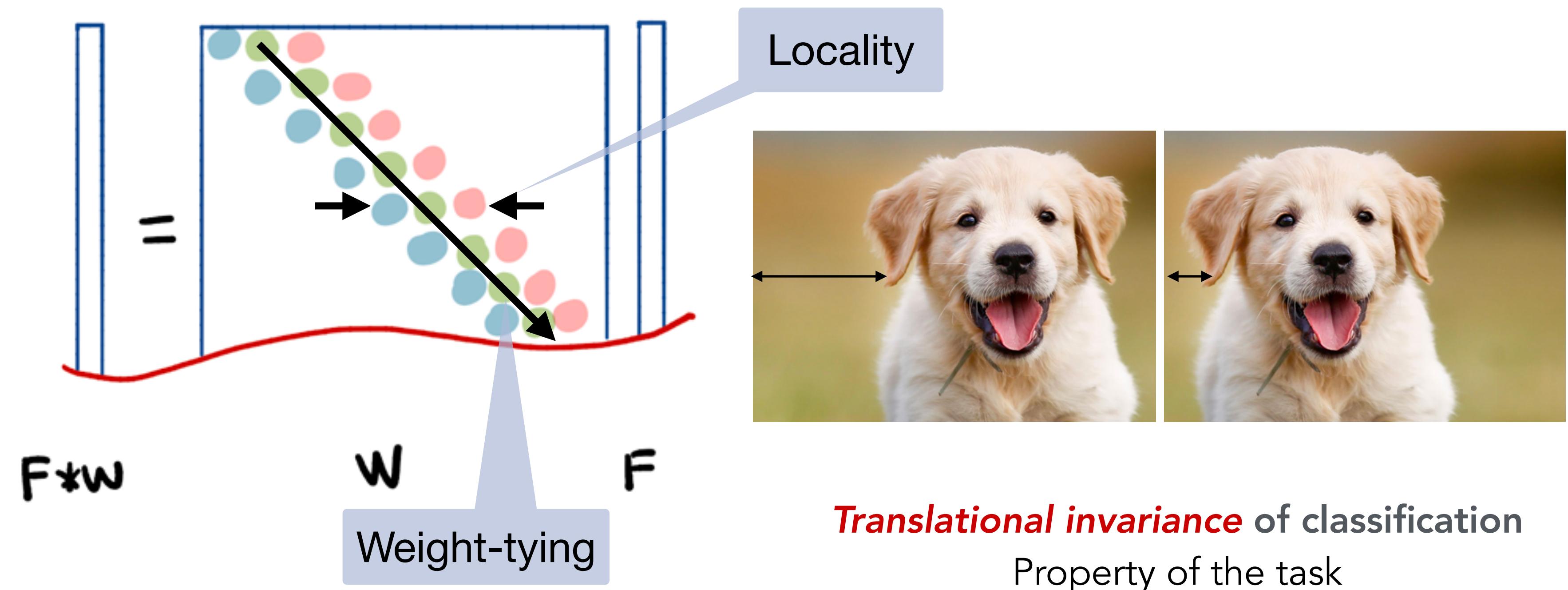
$$[\mathbf{F} * \mathbf{W}](\mathbf{x}) = \sum_{\mathbf{y} \in \mathbb{Z}^2} \mathbf{F}(\mathbf{y}) \mathbf{W}(\mathbf{y} - \mathbf{x})$$

Filter Feature map
e.g. LeCun et al. (1991)



Convolutions can be “reshaped” into matrix-vector products, revealing the weight-tying and locality

Convolutions are special



Locality of pixel statistics
Property of the data

Fewer learnable parameters

Parameter efficient: same function — fewer parameters

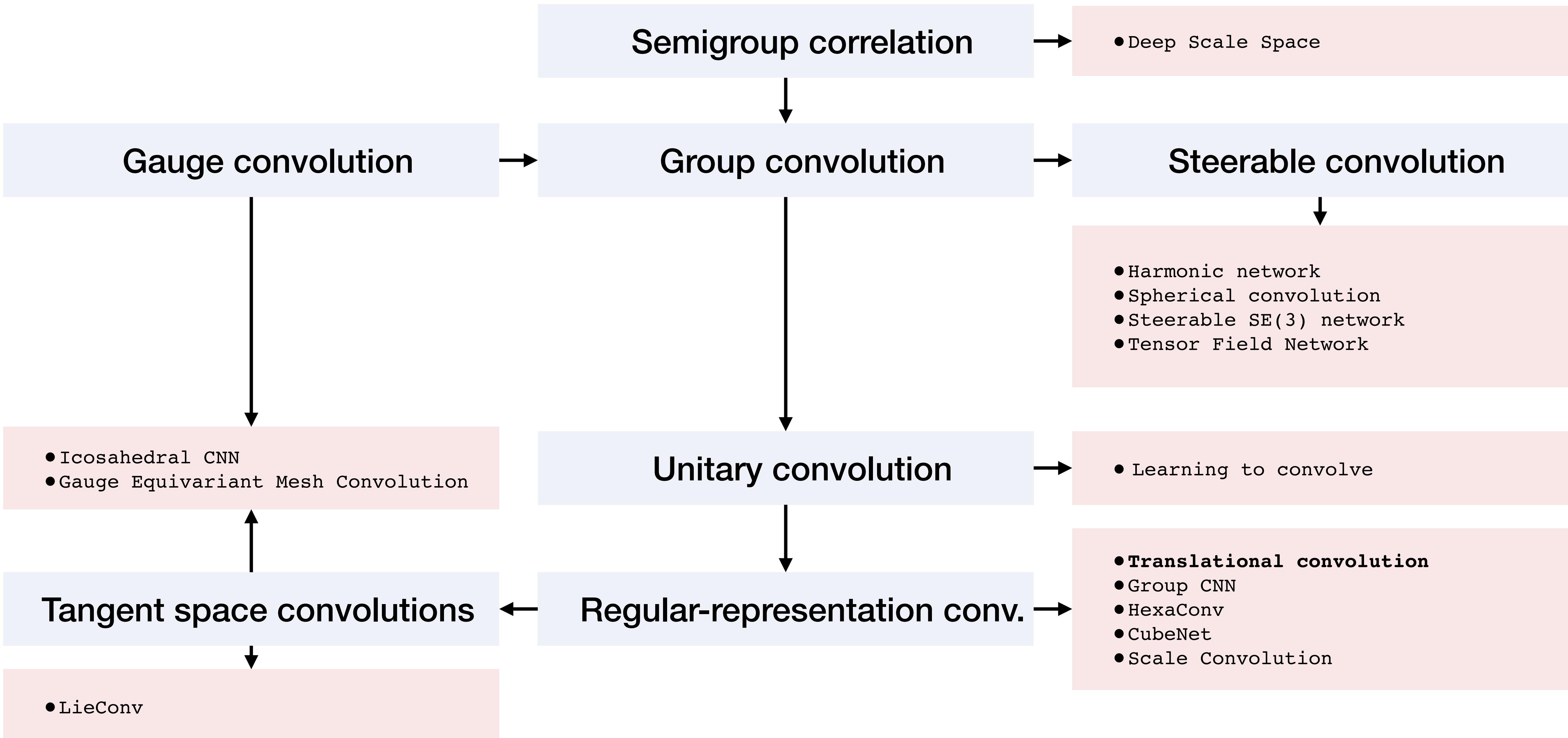
Statistically efficient: need less data

Computationally efficient: need less GPU time

Why learn translational weight-tying when we can build it in?

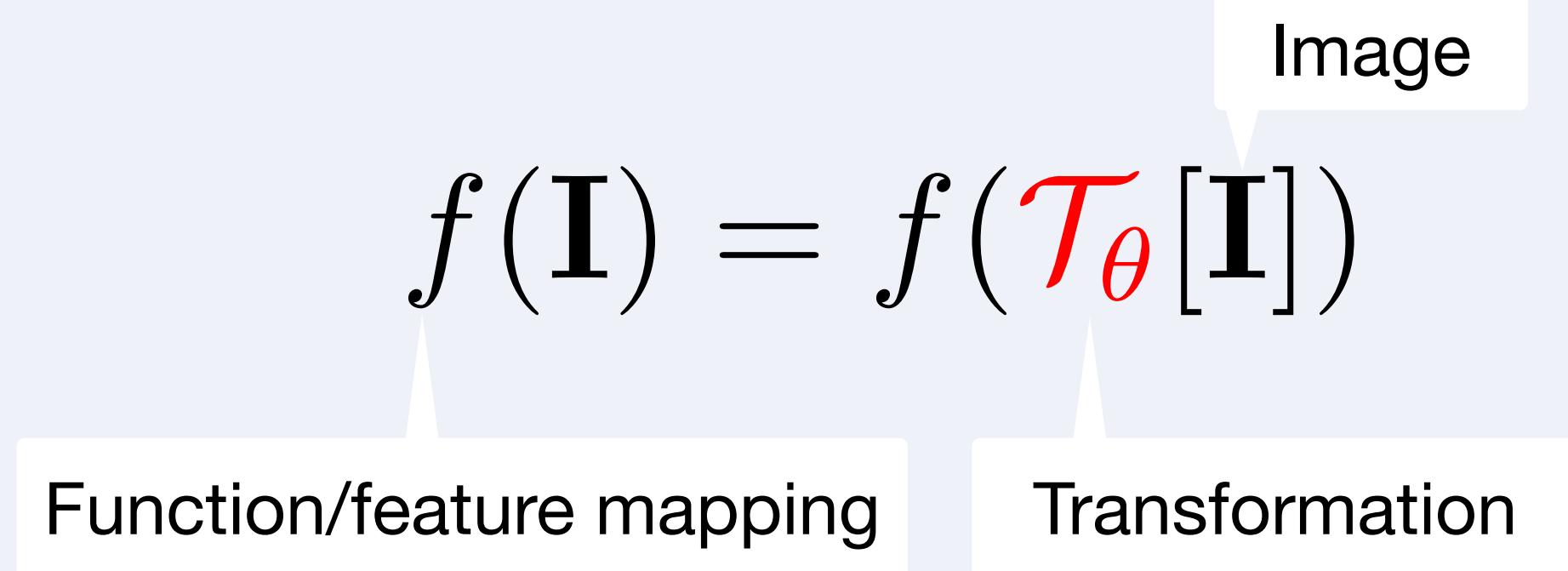
What about rotation, scaling, warps, shears, color jitter, blur, ...?

Convolutional variants



Symmetry: Invariance

Set of input transformations leaving f invariant



Notation

Translation

$$\mathcal{T}_\theta[\mathbf{I}](\mathbf{x}) = \mathbf{I}(\mathbf{x} - \theta)$$

Rotation

$$\mathcal{T}_\theta[\mathbf{I}](\mathbf{x}) = \mathbf{I}(\mathbf{R}_\theta^{-1}\mathbf{x})$$

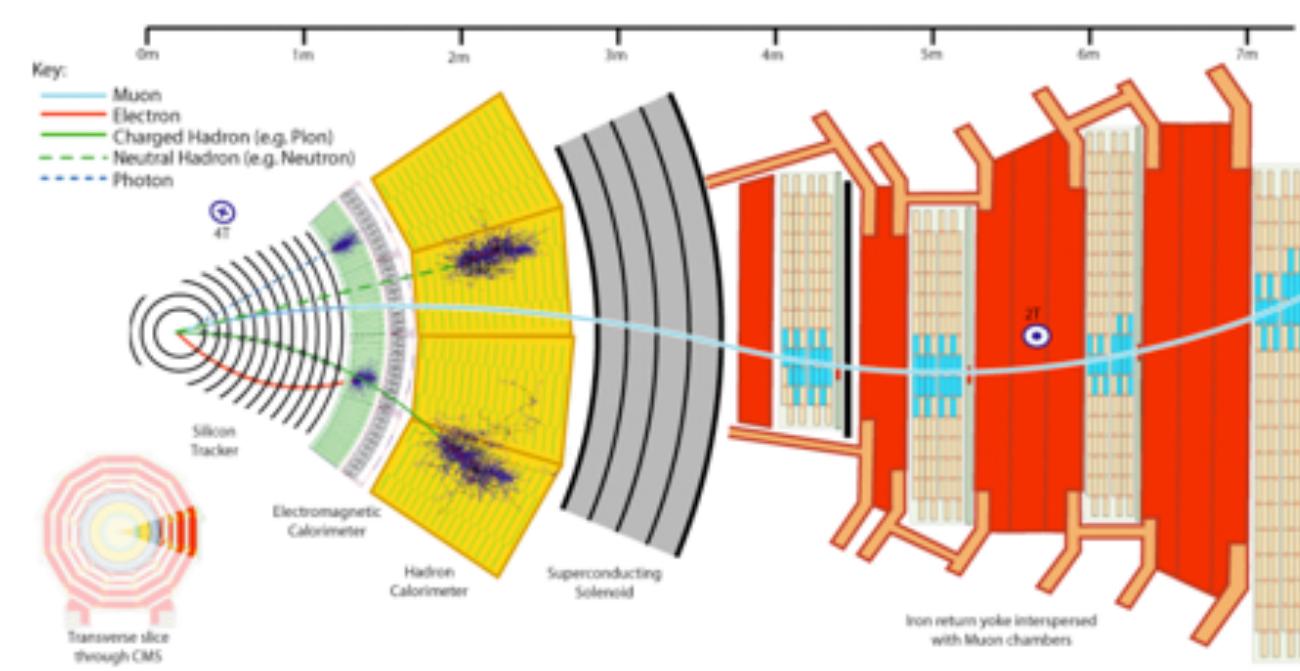
Data whitening

$$\mathcal{T}[\mathbf{I}] = (\mathbf{I} - \mu) / \cdot \sigma^{-1}$$

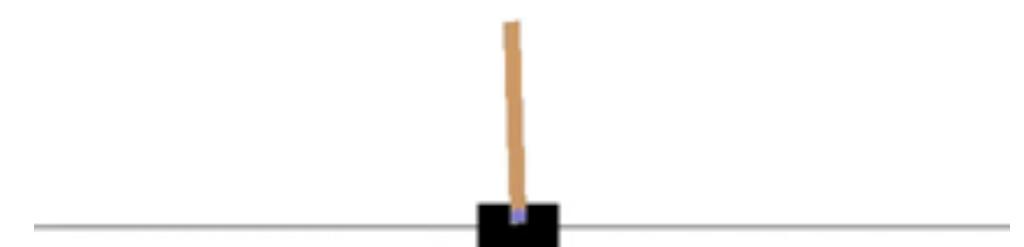
Symmetry is a property of tasks, not of data!



Classification



Signal discovery/detection



Dynamical Systems



Disentangling (cocktail party)

Symmetry: Equivariance

Different representations of same transformation

$$\mathcal{S}_\theta[f](\mathbf{I}) = f(\mathcal{T}_\theta[\mathbf{I}])$$

Transformation in feature space

Invariance

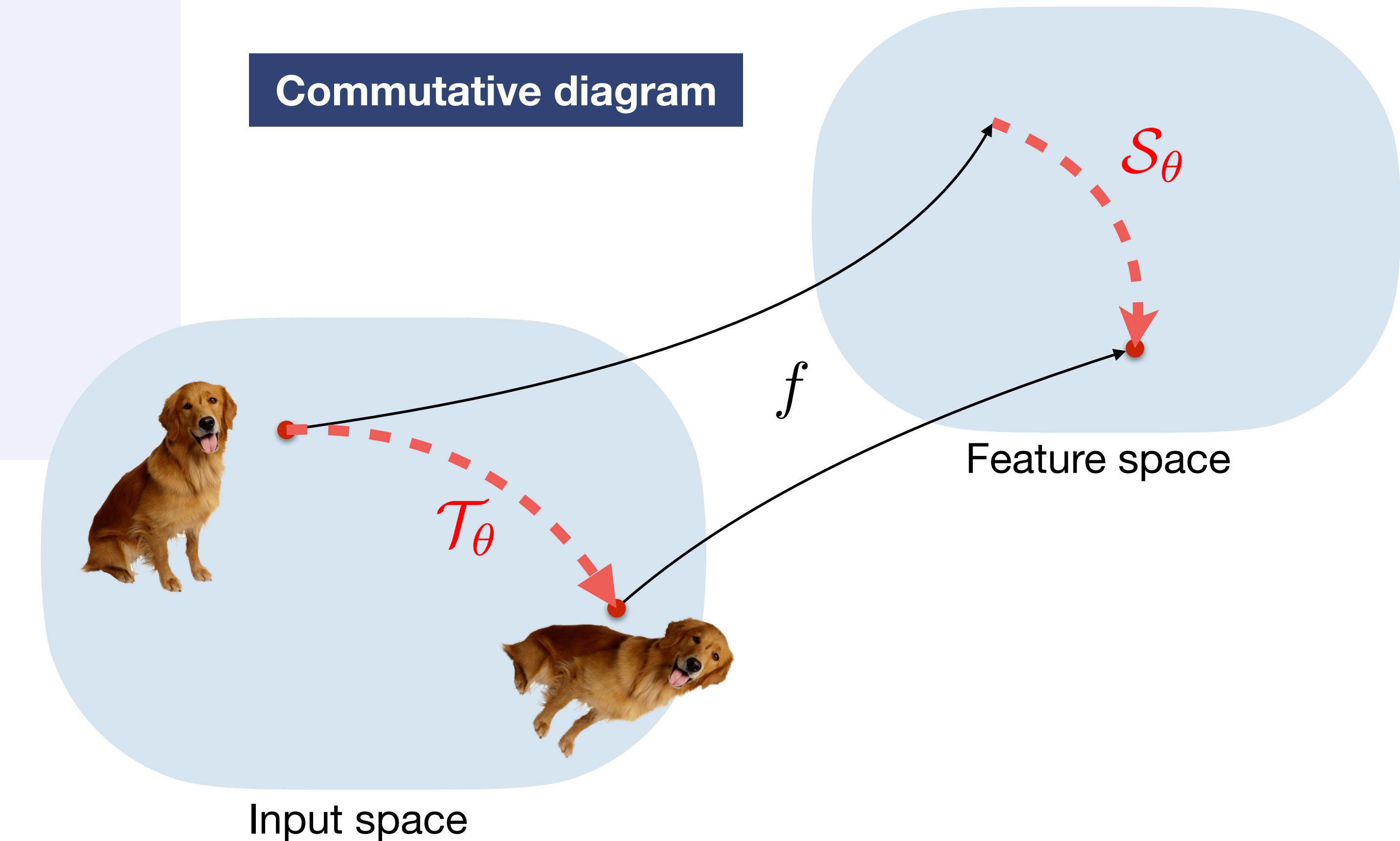
$$\mathcal{S}_\theta = \text{Id}$$

Convolution (and correlation)

$$\underbrace{[\mathbf{I} * \mathbf{W}](\mathbf{x} - \boldsymbol{\theta})}_{\mathcal{S}_\theta[\mathbf{I} * \mathbf{W}](\mathbf{x})} = [\mathcal{T}_\theta[\mathbf{I}] * \mathbf{W}](\mathbf{x})$$

$$\mathcal{S}_\theta[\mathbf{I} * \mathbf{W}](\mathbf{x})$$

Commutative diagram



Theorem [Kondor & Trivedi (2018), Cohen et al. (2020a), Bekkers (2020)]:

Group convolution is the only linear map* equivariant to group-structured transformations**

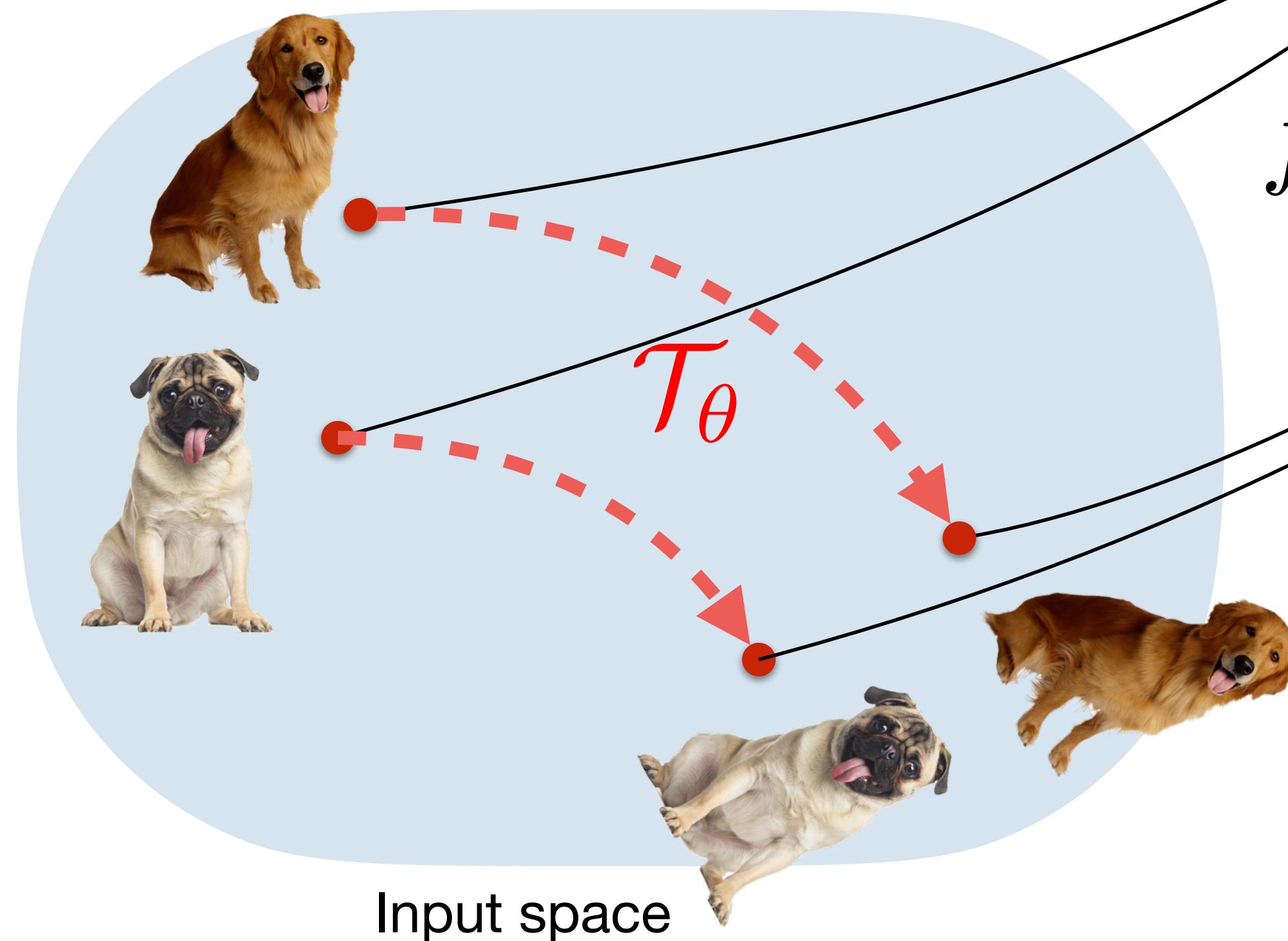
*Linear, bounded map between measurable homogeneous spaces **Countable groups and Lie groups

Symmetry: Equivariance

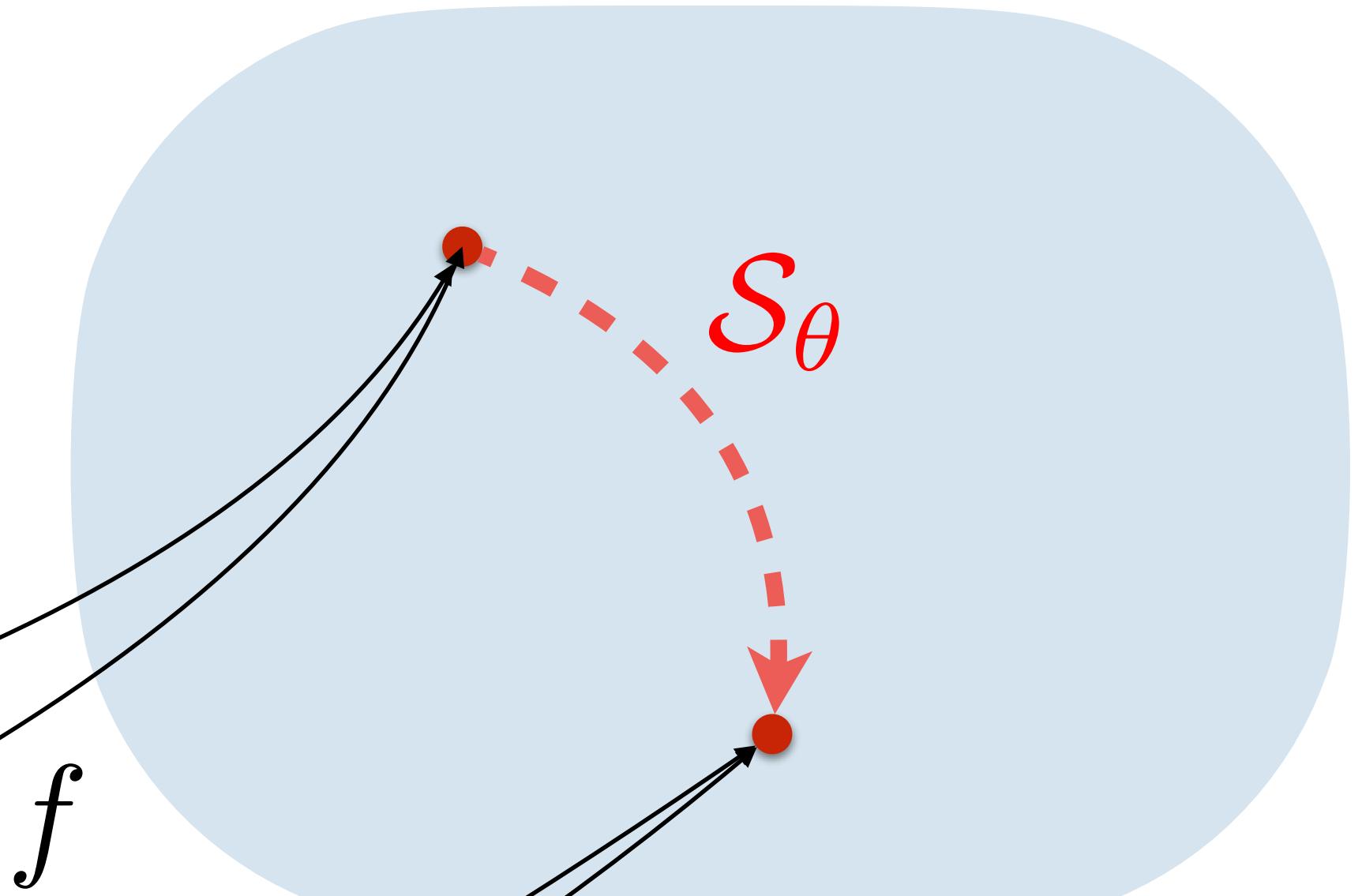
Different representations of same transformation

$$\mathcal{S}_\theta[f](\mathbf{I}) = f(\mathcal{T}_\theta[\mathbf{I}])$$

Transformation in feature space



Commutative diagram



**Sophisticated invariance:
Equivalence classes preserved**

Translational Equivariance Proof

$$[\mathcal{T}_{\mathbf{t}}[\mathbf{I}] * \mathbf{W}](\mathbf{x}) = \sum_{\mathbf{y} \in \mathbb{Z}^2} \mathcal{T}_{\mathbf{t}}[\mathbf{I}](\mathbf{y}) \mathbf{W}(\mathbf{y} - \mathbf{x})$$

Write out convolution in full

$$= \sum_{\mathbf{y} \in \mathbb{Z}^2} \mathbf{I}(\mathbf{y} - \mathbf{t}) \mathbf{W}(\mathbf{y} - \mathbf{x})$$

Expand translation operator

$$= \sum_{\mathbf{y}' \in \mathbb{Z}^2} \mathbf{I}(\mathbf{y}') \mathbf{W}(\mathbf{y}' - (\mathbf{x} - \mathbf{t}))$$

Change of variables
 $\mathbf{y}' = \mathbf{y} - \mathbf{t}$

$$= [\mathbf{I} * \mathbf{W}](\mathbf{x} - \mathbf{t}) = \mathcal{T}_{\mathbf{t}}[\mathbf{I} * \mathbf{W}](\mathbf{x})$$

Oh look, it's a convolution!

Hints

$$[\mathbf{I} * \mathbf{W}](\mathbf{x}) = \sum_{\mathbf{y} \in \mathbb{Z}^2} \mathbf{I}(\mathbf{y}) \mathbf{W}(\mathbf{y} - \mathbf{x})$$

$$\mathcal{T}_{\mathbf{t}}[\mathbf{I}](\mathbf{x}) = \mathbf{I}(\mathbf{x} - \mathbf{t})$$

Group theory

Mathematical abstraction
modeling compositional
structure.

Can be used to model
transformations

Abstraction

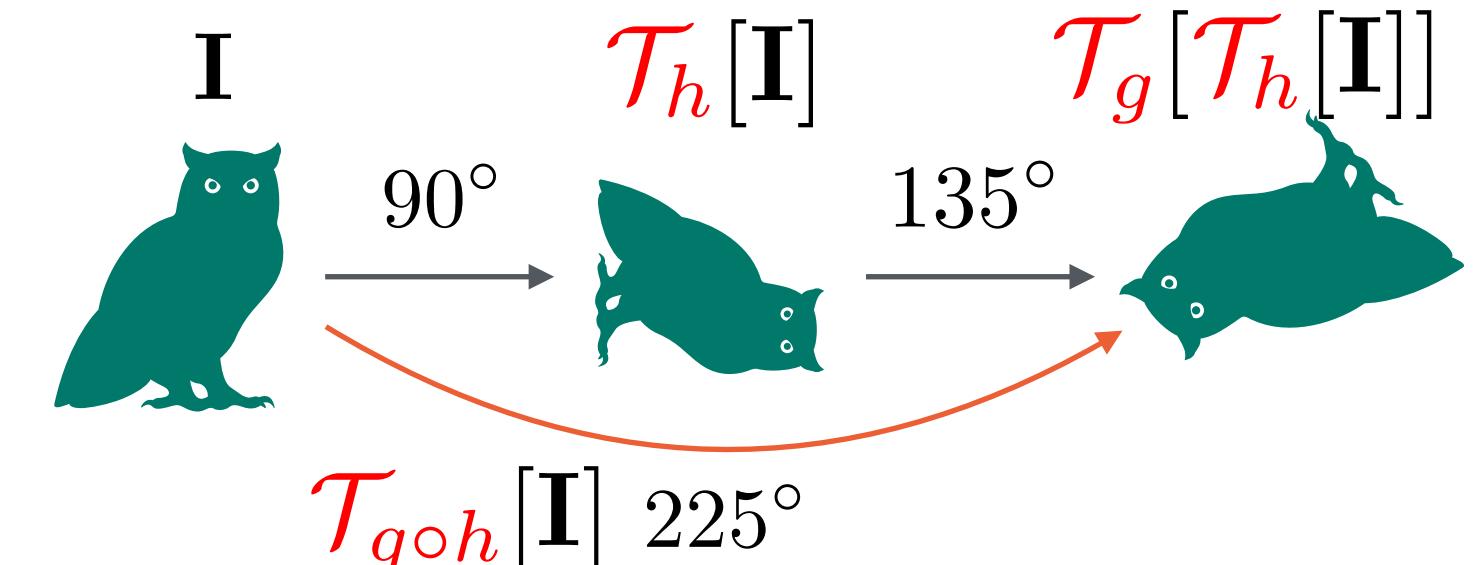
1. **Closure:** compositions well-behaved

$$g \circ h \in G$$

Composition

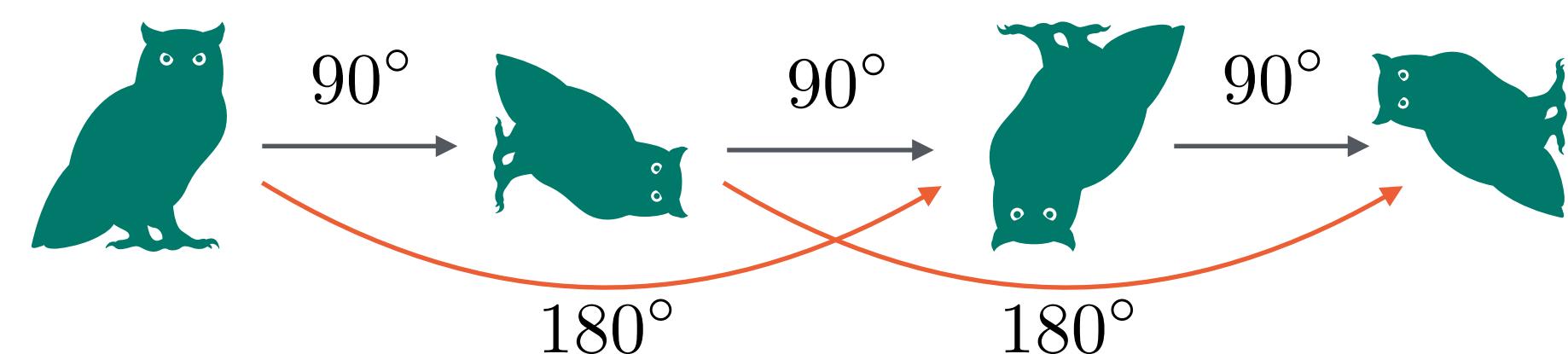
Set of transformations

Action/Transformation



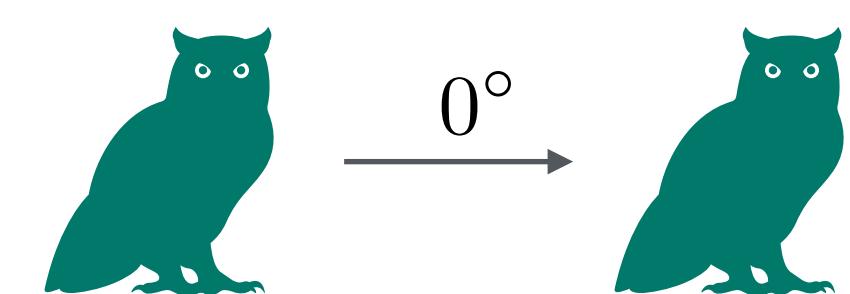
2. **Associativity:** brackets unnecessary

$$(g \circ h) \circ k = g \circ (h \circ k) = g \circ h \circ k$$



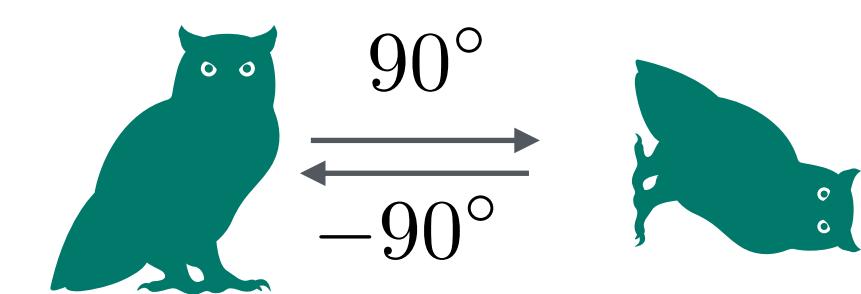
3. **Identity:** “do nothing” transformation

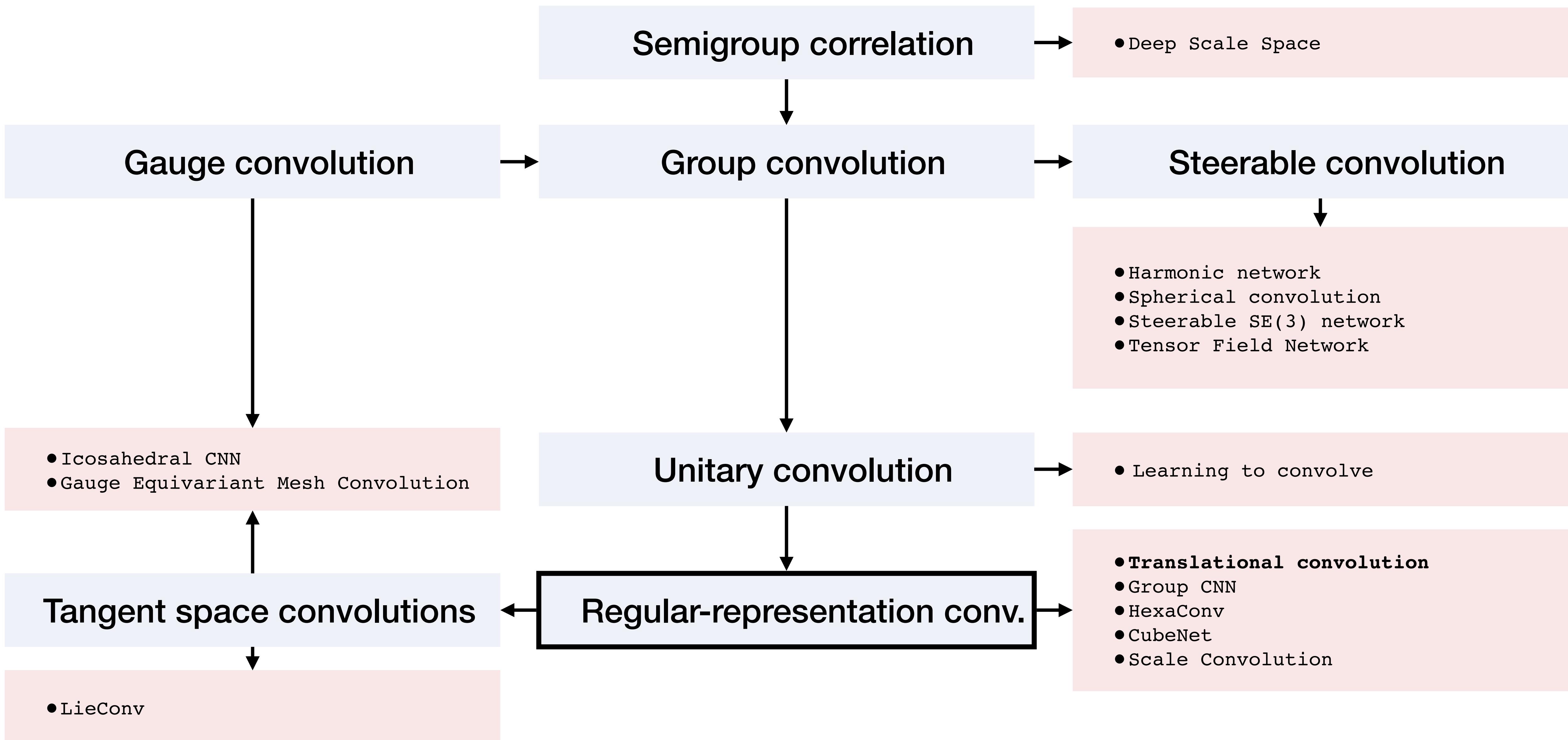
$$e \circ g = g \circ e = g$$



4. **Invertibility:** transformation reversible

$$g \circ g^{-1} = g^{-1} \circ g = e$$





The Regular Group Convolution

Standard convolution

Inner product

$$[F * W](x) = \sum_{y \in \mathbb{Z}^2} F(y)W(y - x)$$

Translations

Group convolution

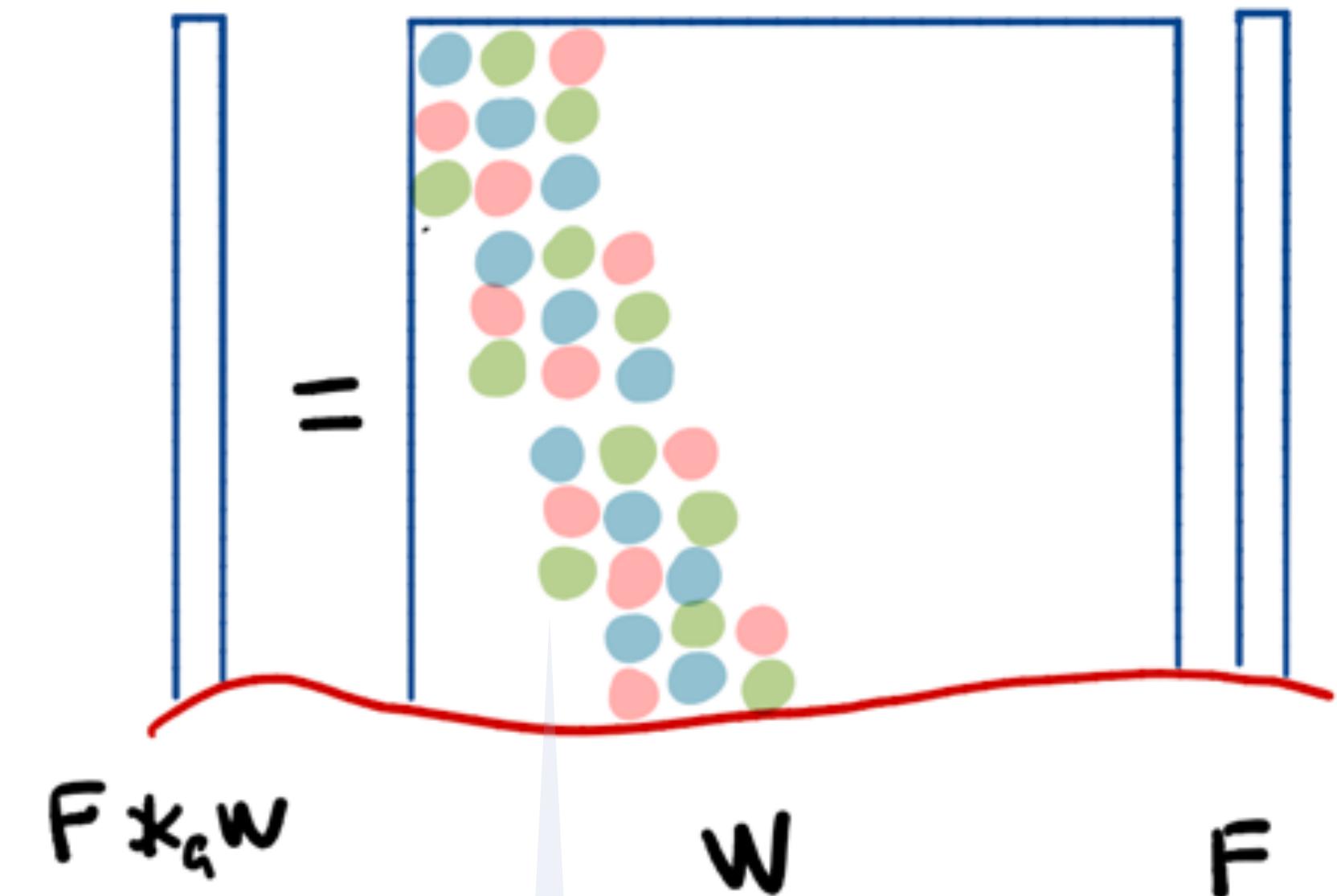
Inner product

$$[F * W](x) = \sum_{y \in \mathcal{Y}} F(y)W(\mathcal{T}_x^{-1}[y])$$

x is transformation parameter

Transformations

Adjusted domain



At each location multiple transformed filter copies

Hints

Translation

$$\mathcal{T}_x[y] = y + x$$

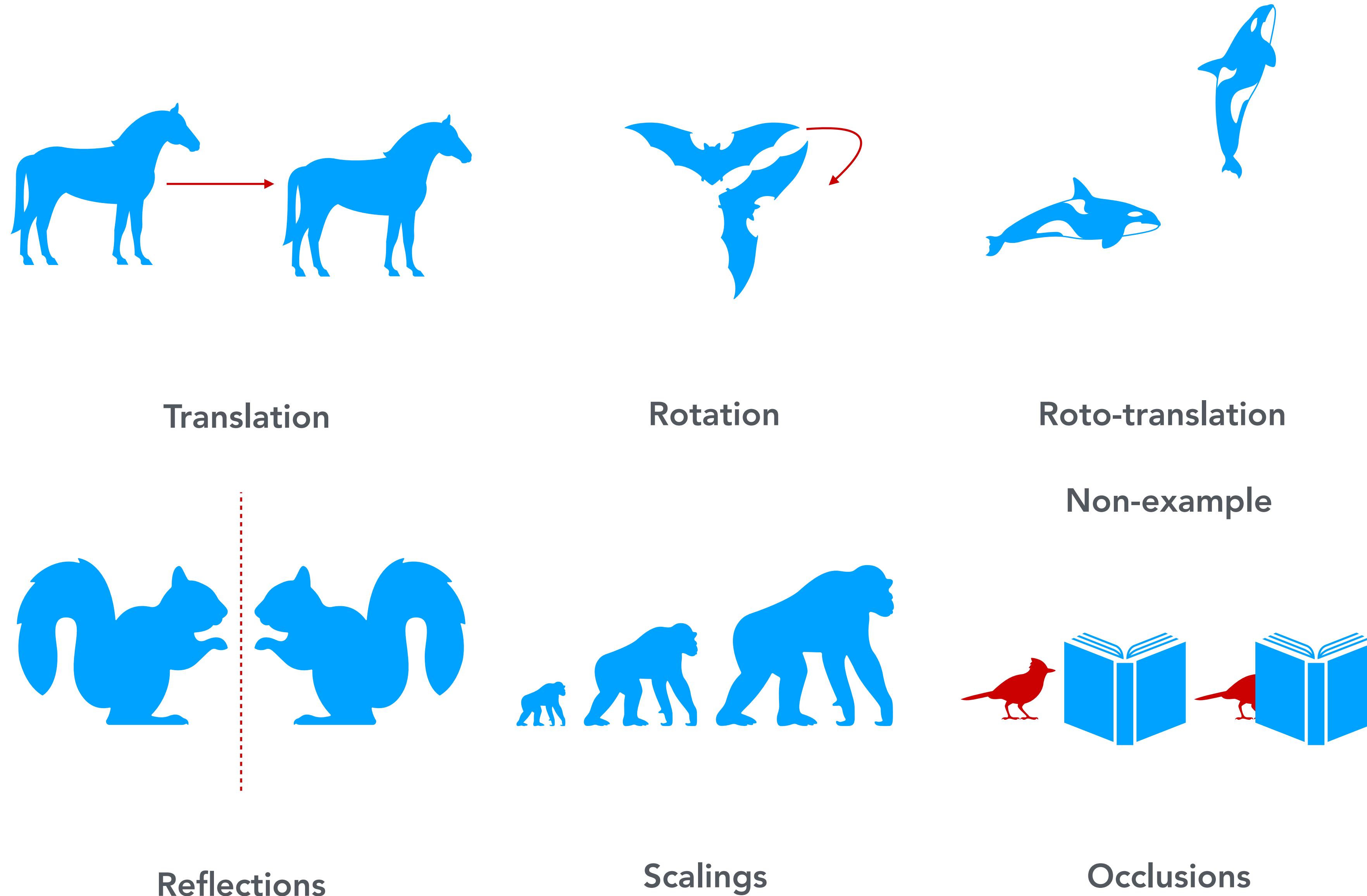
Rotation

$$\mathcal{T}_x[y] = R_x y$$

Roto-translation

$$\mathcal{T}_x[y] = R_x y + t_x$$

Group Transformation Examples



SO(2) Rotation

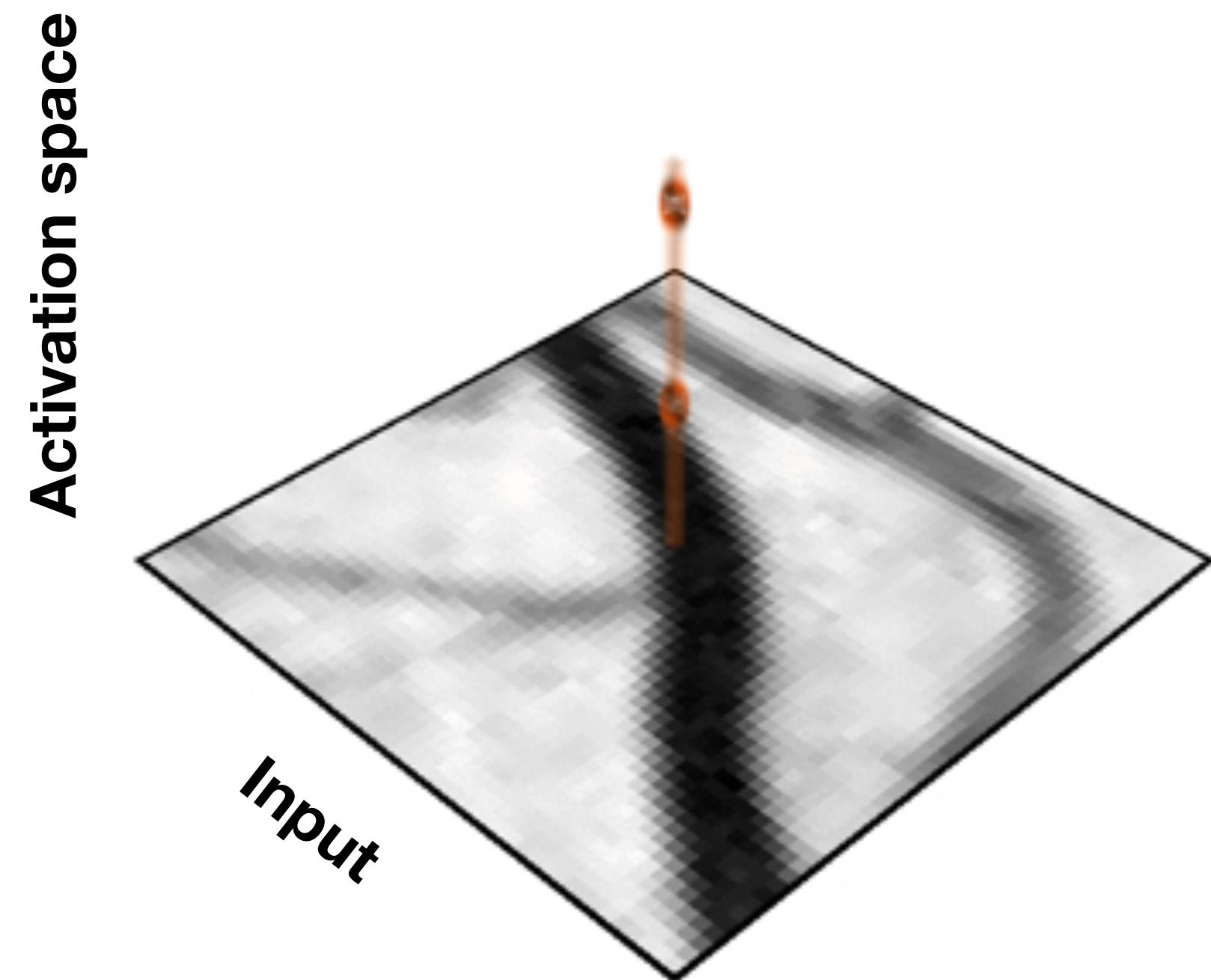
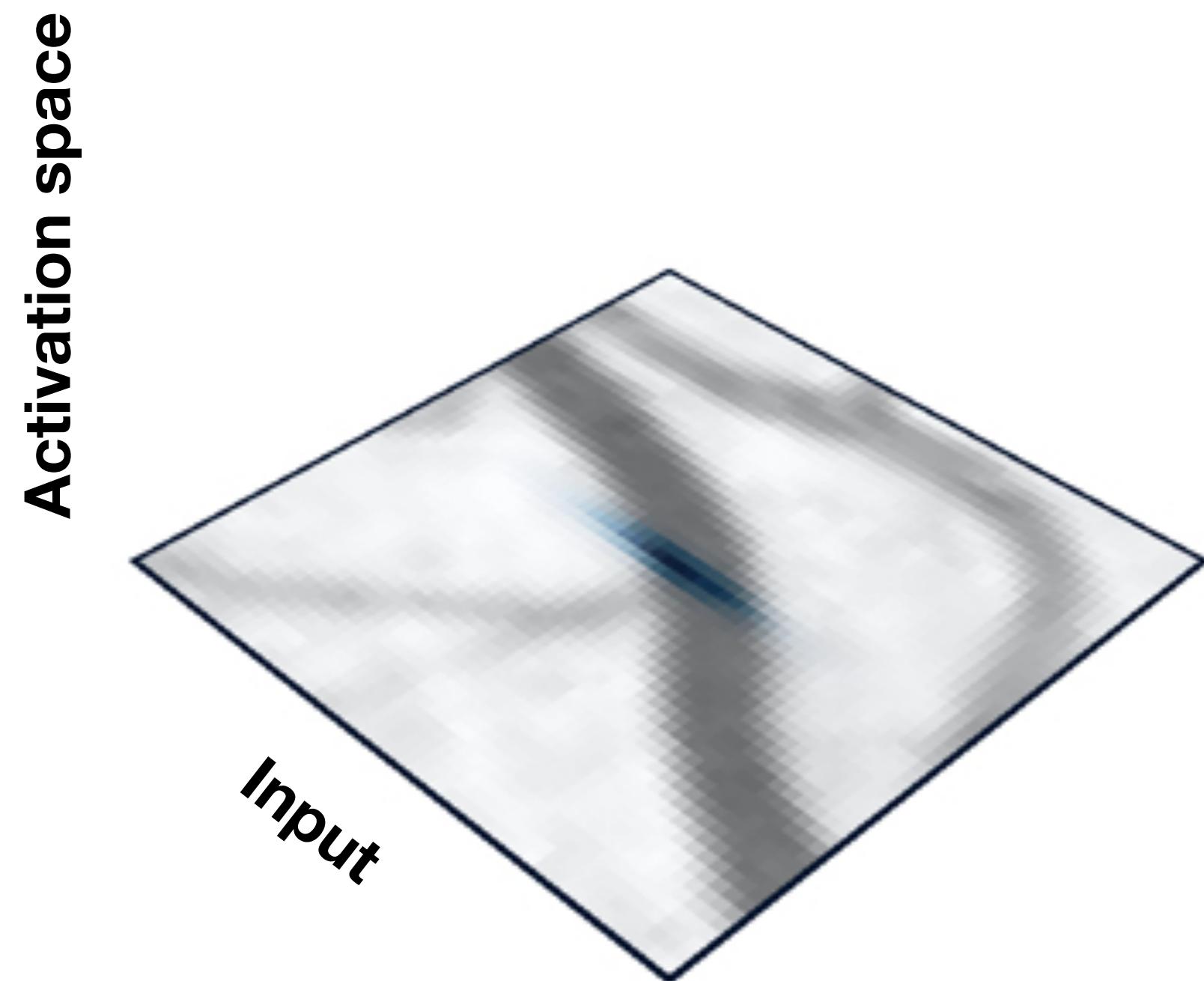
Group convolution

$$[\mathbf{F} * \mathbf{W}](\mathbf{x}) = \sum_{\mathbf{y} \in \mathcal{Y}} \mathbf{F}(\mathbf{y}) \mathbf{W}(\mathcal{T}_{\mathbf{x}}^{-1}[\mathbf{y}])$$

Notice index of convolution

$$[\mathbf{F} * \mathbf{W}](\mathbf{R}_{\theta}) = \sum_{\mathbf{y} \in \mathcal{Y}} \mathbf{F}(\mathbf{y}) \mathbf{W}(\mathcal{T}_{\mathbf{R}_{\theta}^{-1}}[\mathbf{x}])$$

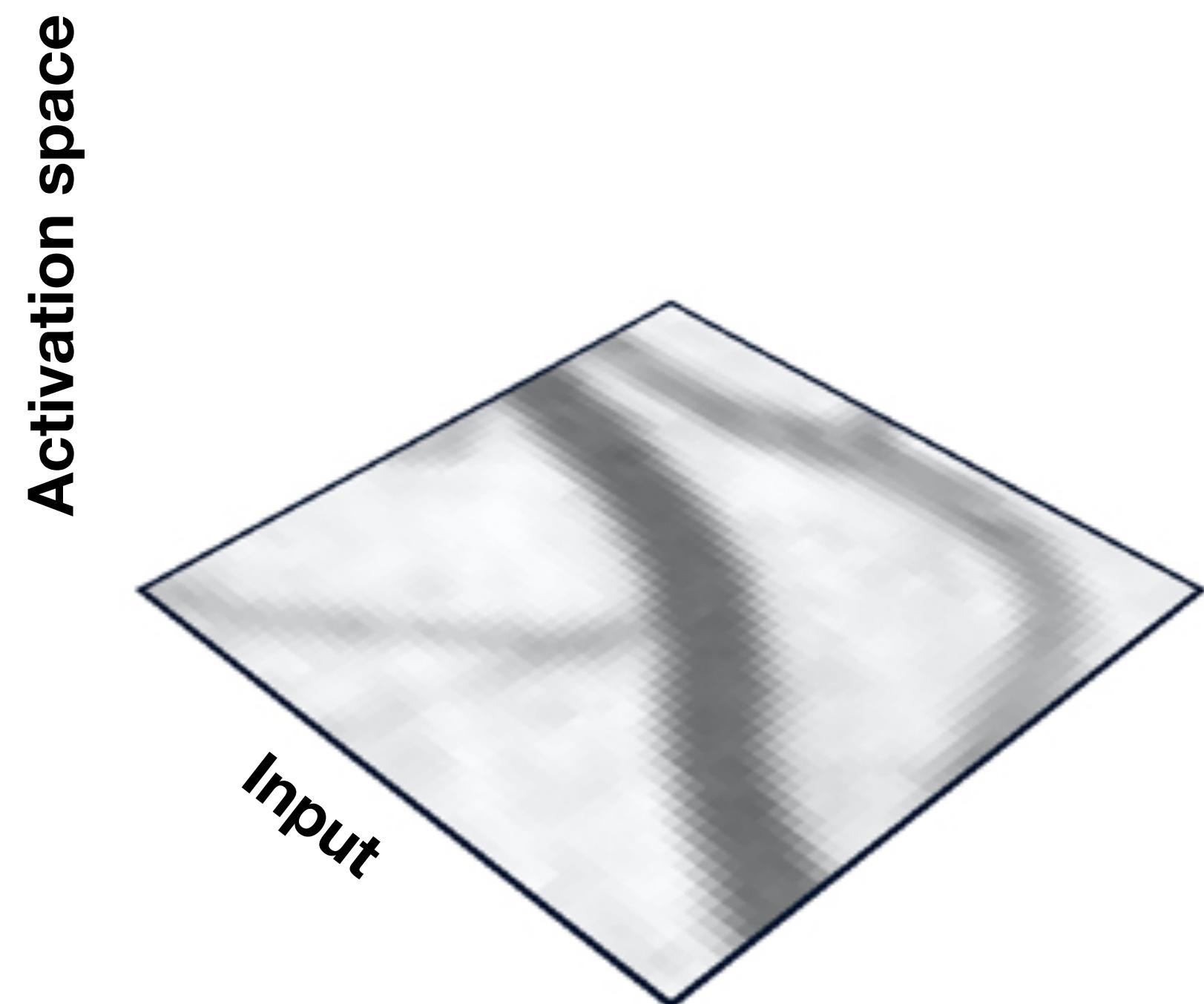
Rotating kernel



$$[\mathcal{T}_{\mathbf{R}_{\psi}}[\mathbf{F}] * \mathbf{W}](\mathbf{R}_{\theta}) = [\mathbf{F} * \mathbf{W}](\mathbf{R}_{\psi}^{-1}\mathbf{R}_{\theta})$$

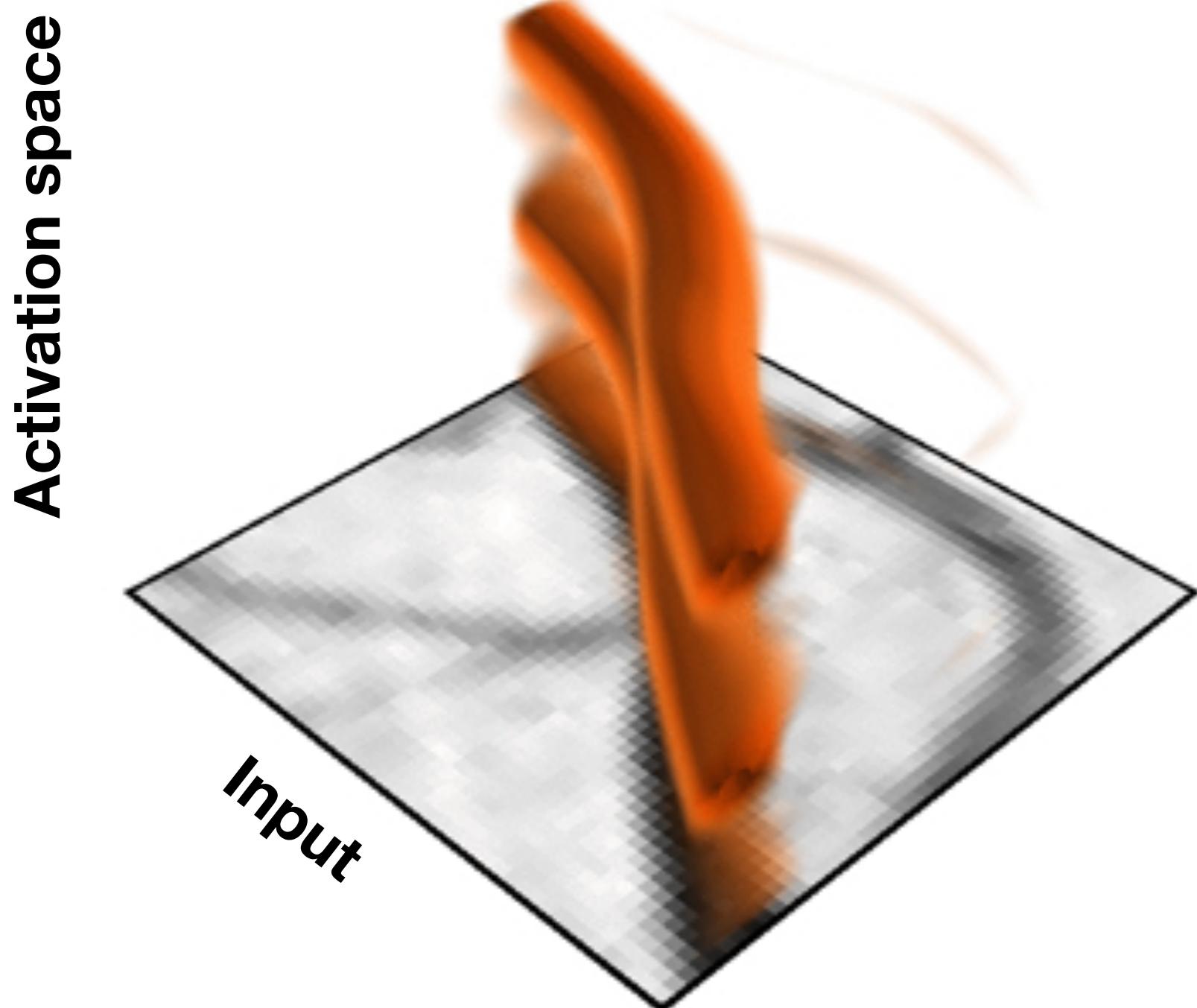
Group convolution

$$[\mathbf{F} * \mathbf{W}](\mathbf{x}) = \sum_{\mathbf{y} \in \mathcal{Y}} \mathbf{F}(\mathbf{y}) \mathbf{W}(\mathcal{T}_{\mathbf{x}}^{-1}[\mathbf{y}])$$



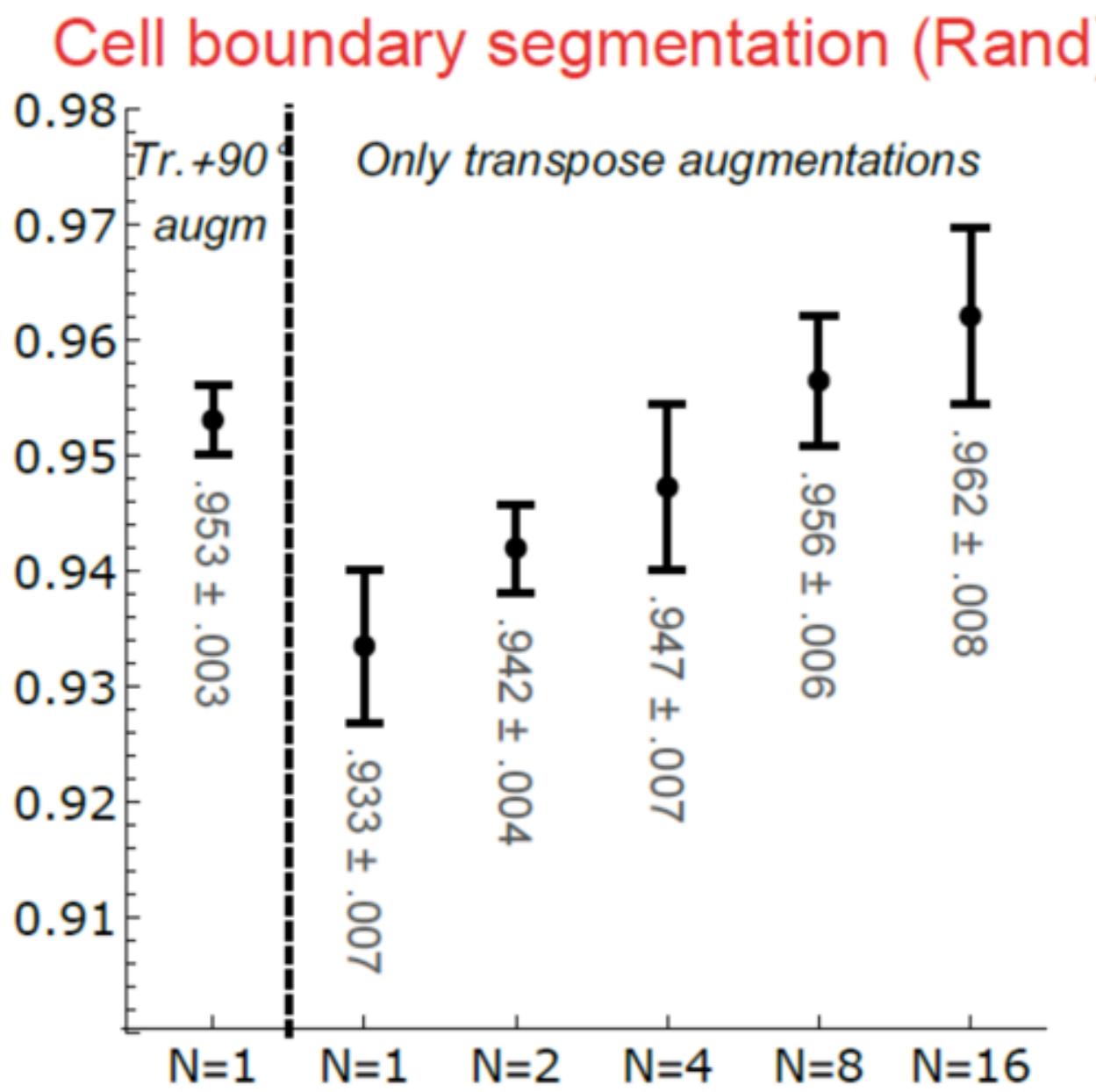
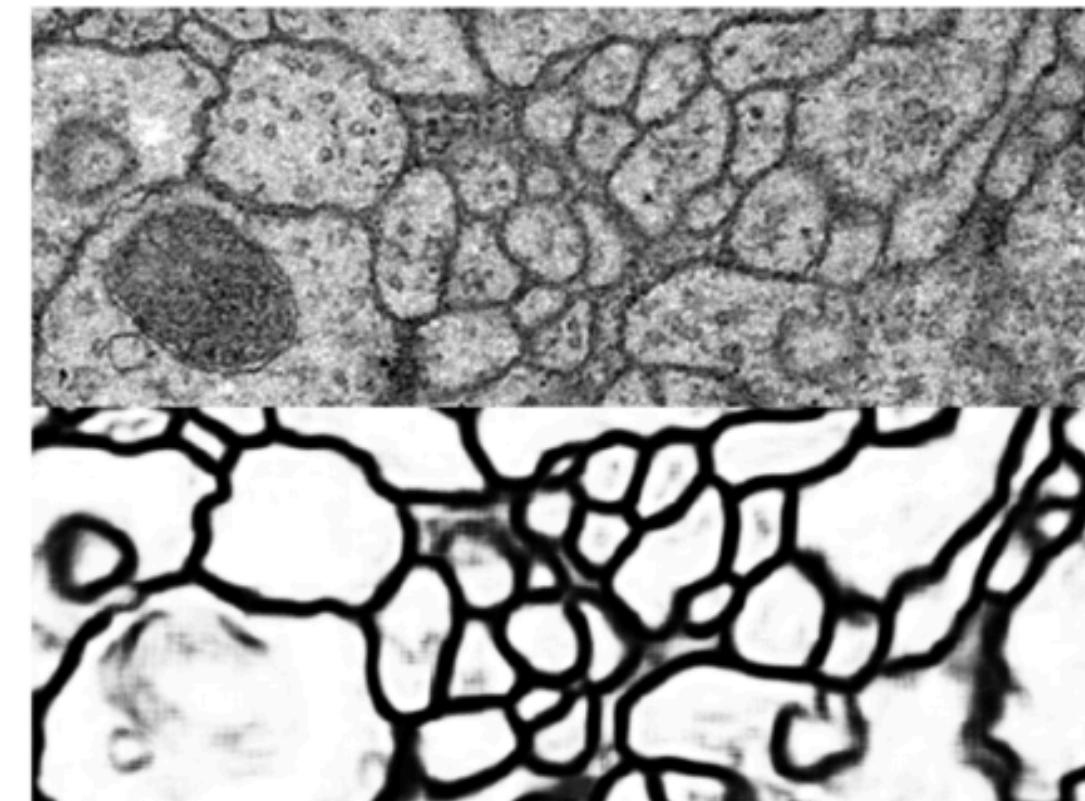
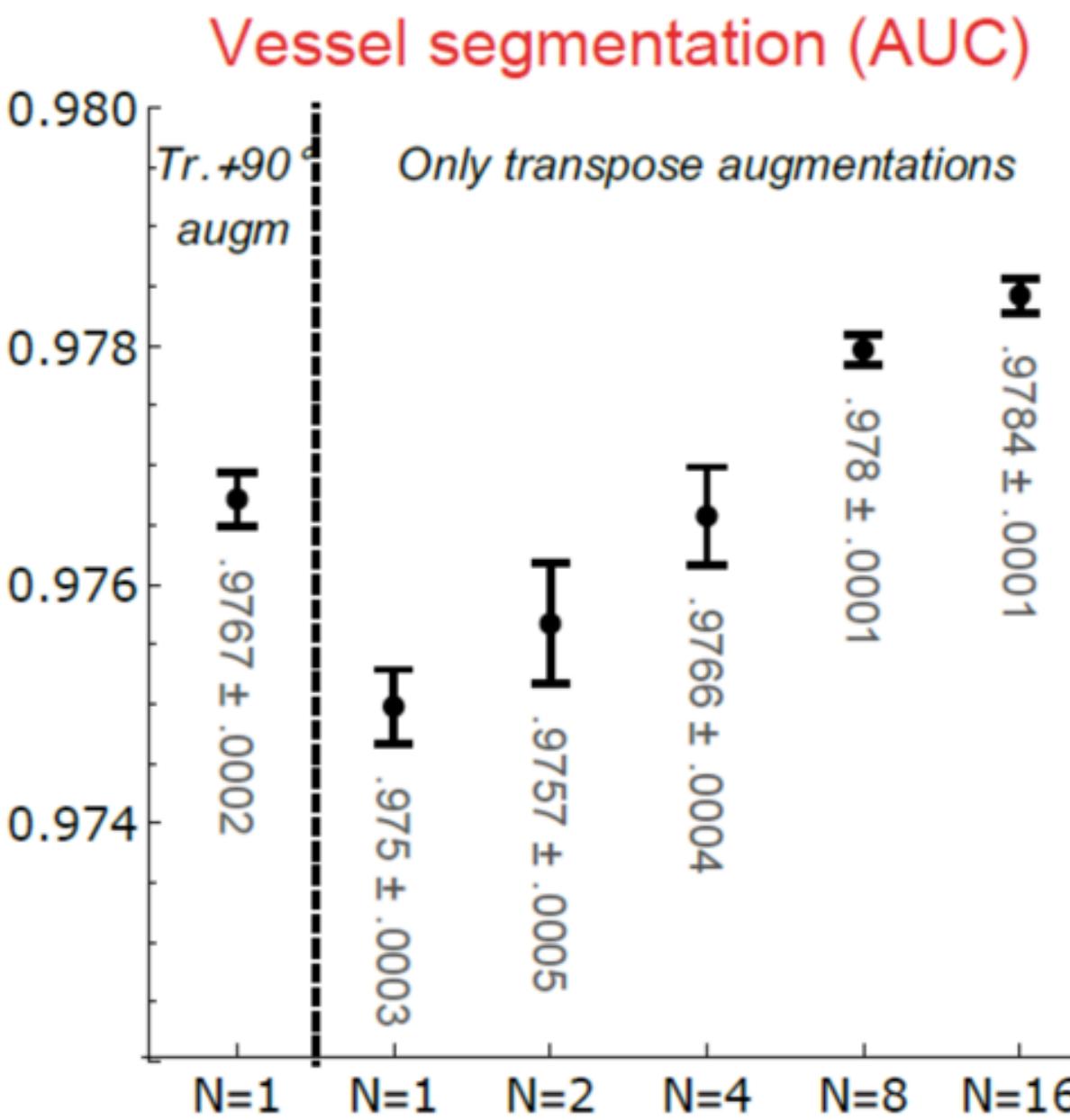
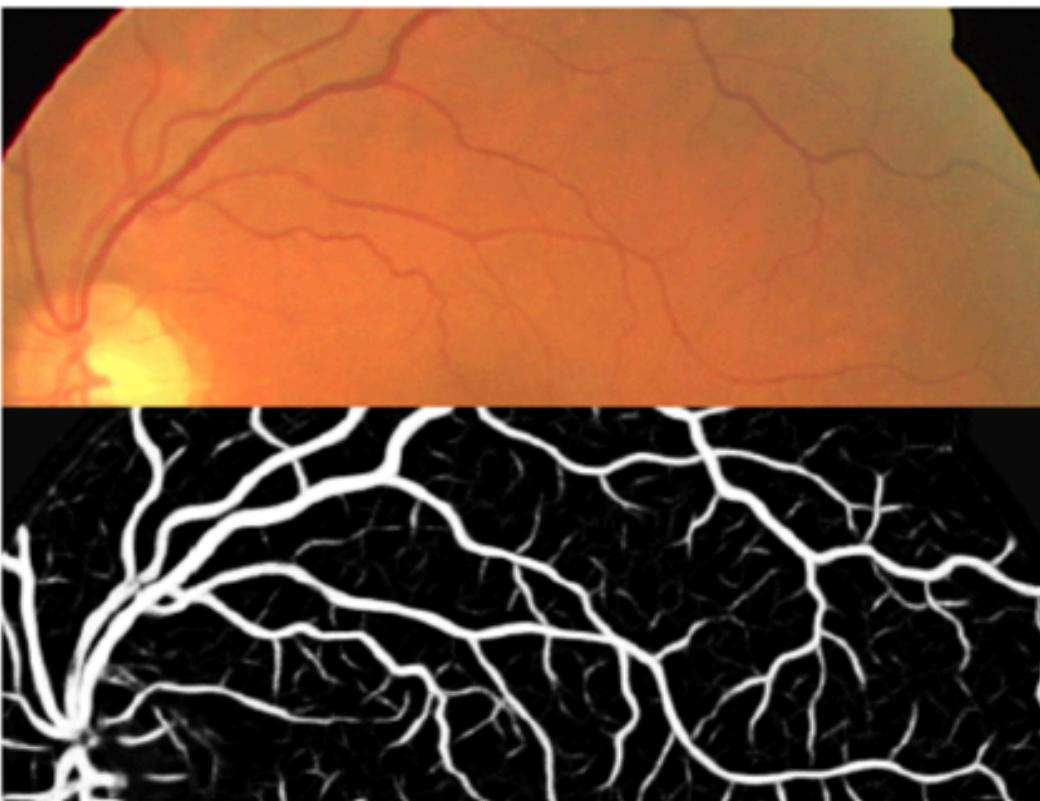
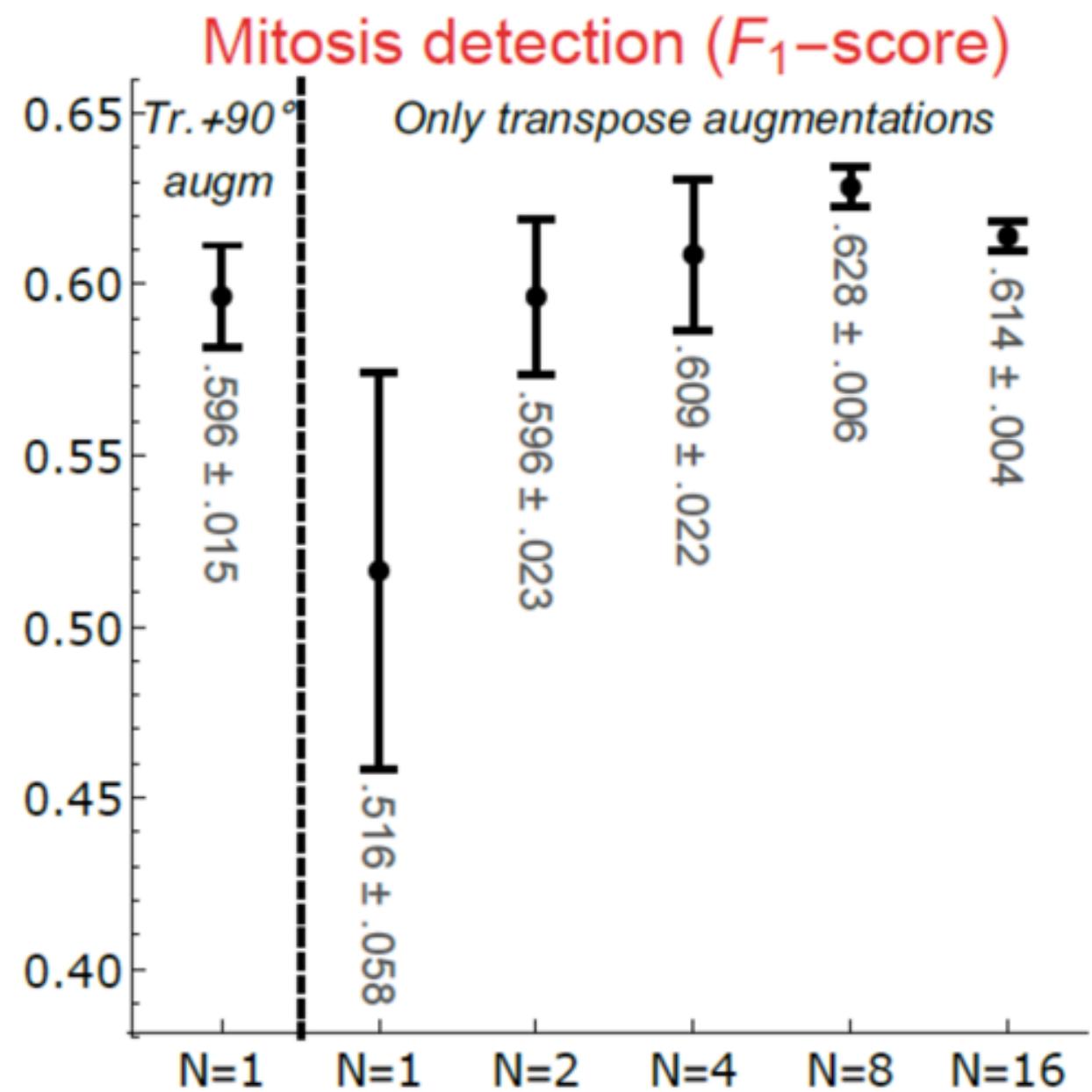
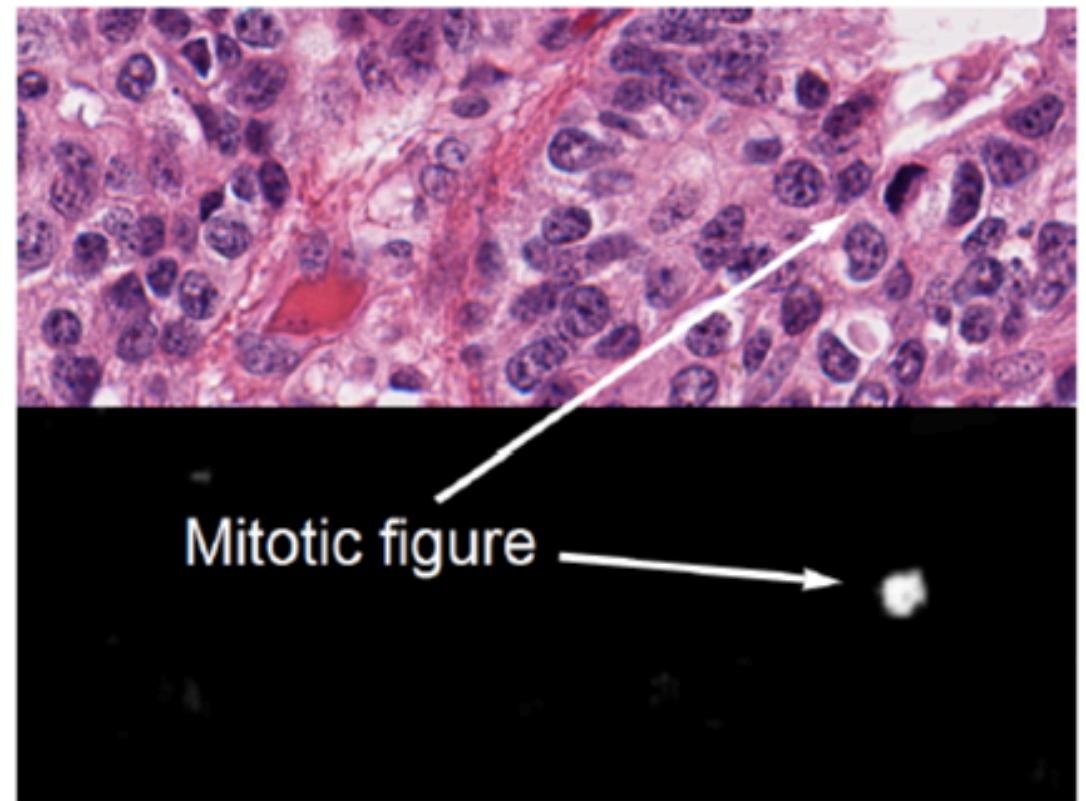
$$[\mathbf{F} * \mathbf{W}](\mathbf{R}_{\theta}, \mathbf{x}) = \sum_{\mathbf{y} \in \mathbb{Z}^2} \mathbf{F}(\mathbf{y}) \mathbf{W}(\mathbf{R}_{\theta}^{-1}(\mathbf{y} - \mathbf{x}))$$

Rotating + translating kernel



$$[\mathcal{T}_{\mathbf{R}_{\psi}, \mathbf{z}}[\mathbf{F}] * \mathbf{W}](\mathbf{R}_{\theta}, \mathbf{x}) = [\mathbf{F} * \mathbf{W}](\mathbf{R}_{\theta - \psi}, \mathbf{R}_{\psi}^{-1}(\mathbf{x} - \mathbf{z}))$$

Sample efficiency



Roto-Translation Covariant Convolutional Networks for Medical Image Analysis

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

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

1 Introduction

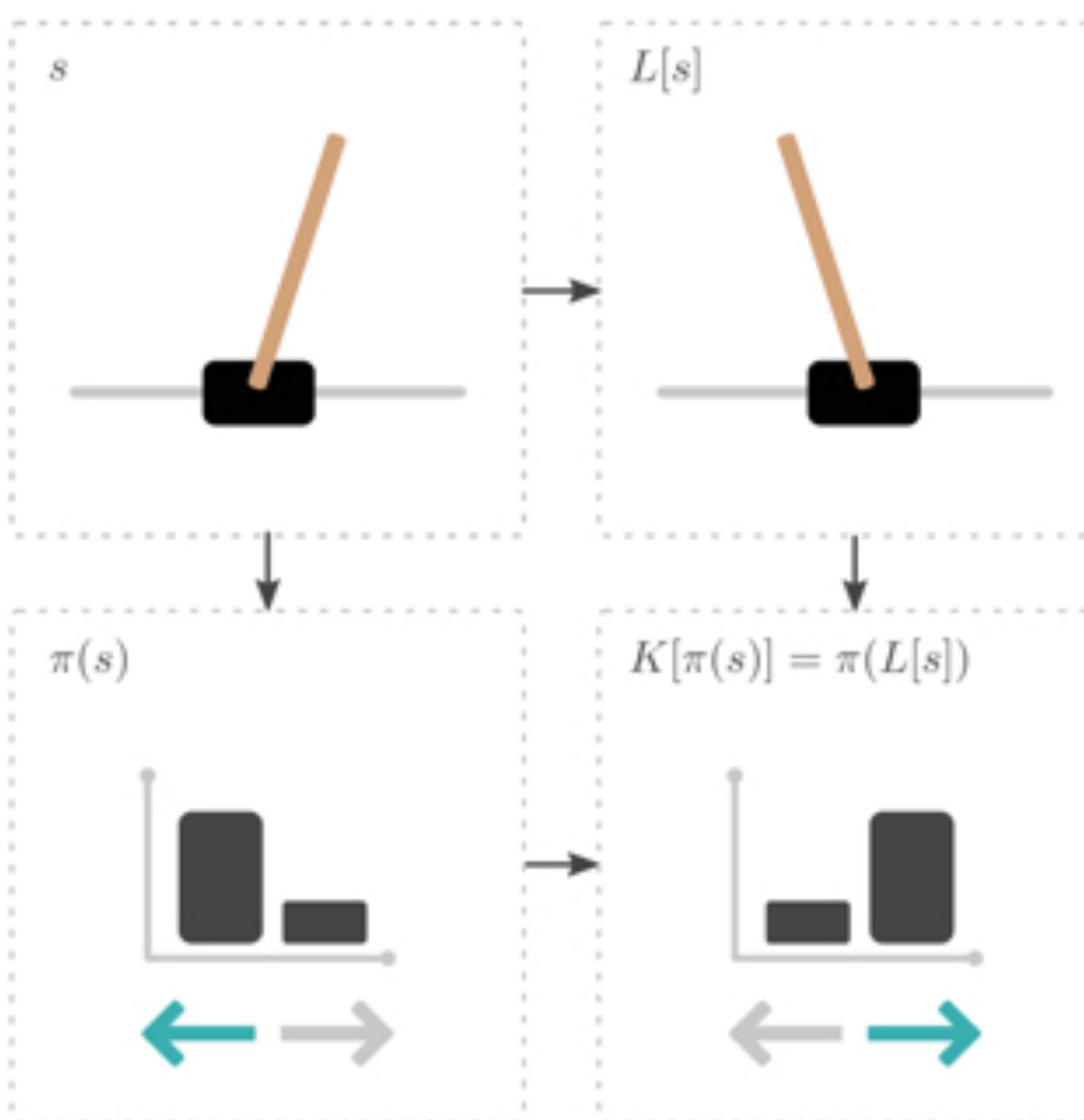
In this work we generalize \mathbb{R}^2 convolutional neural networks (CNNs) to $SE(2)$ group CNNs (G-CNNs) in which the data lives on position orientation space, and in which the convolution layers are defined in terms of representations of the

Bekkers et al., 2018

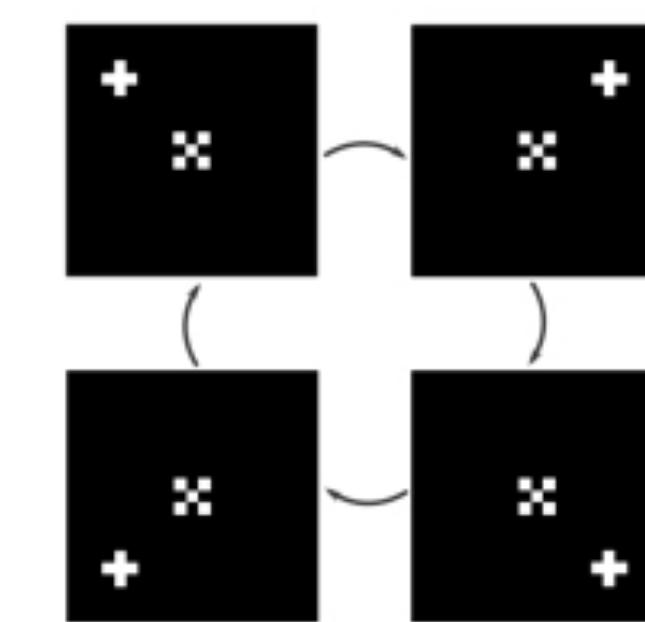
Sample efficiency

RL sample hungry: exploit symmetries

Transformation equivariant policies via
MDP homomorphism theory



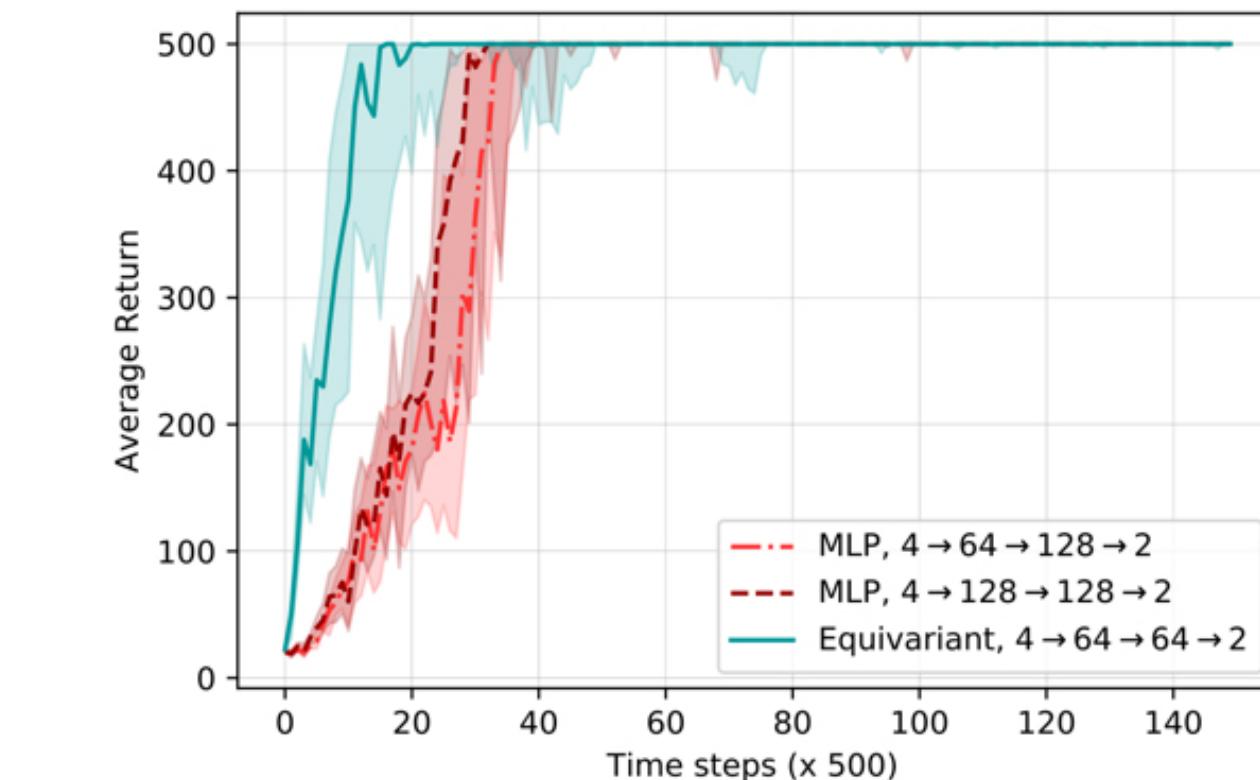
Cartpole



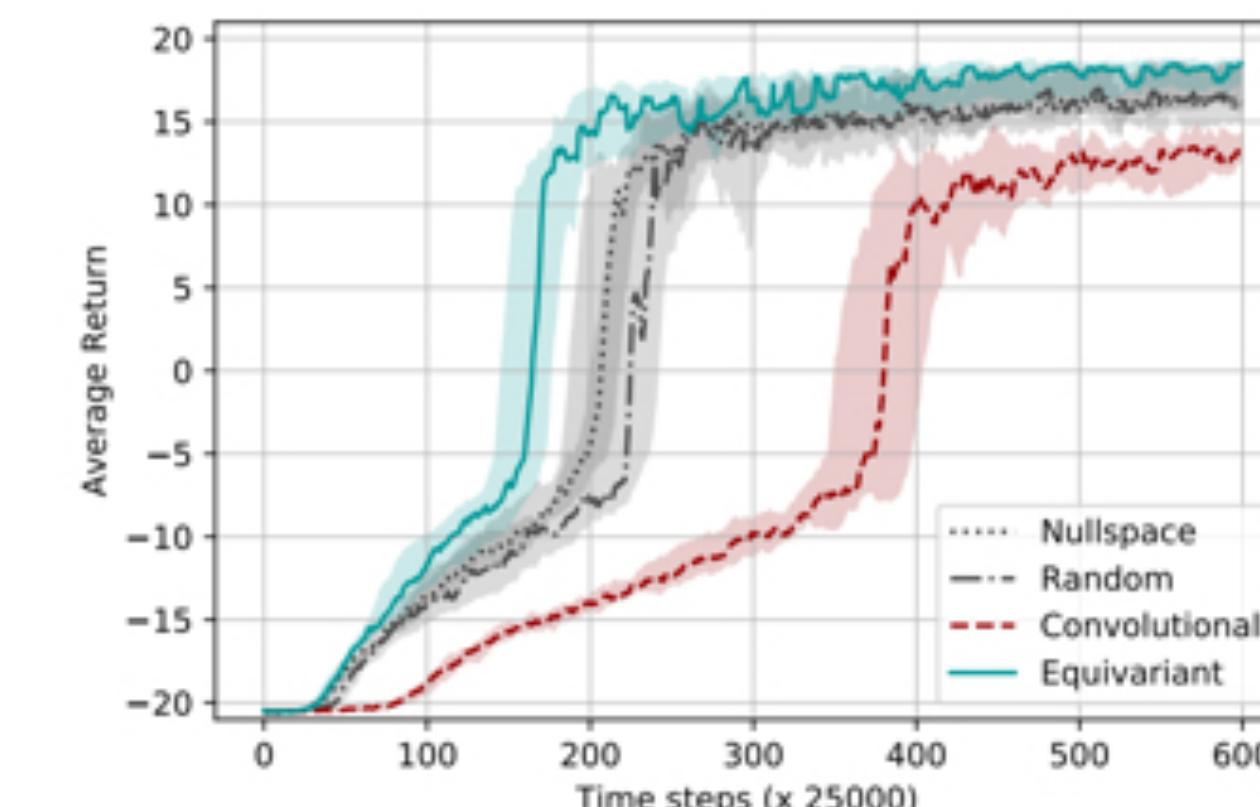
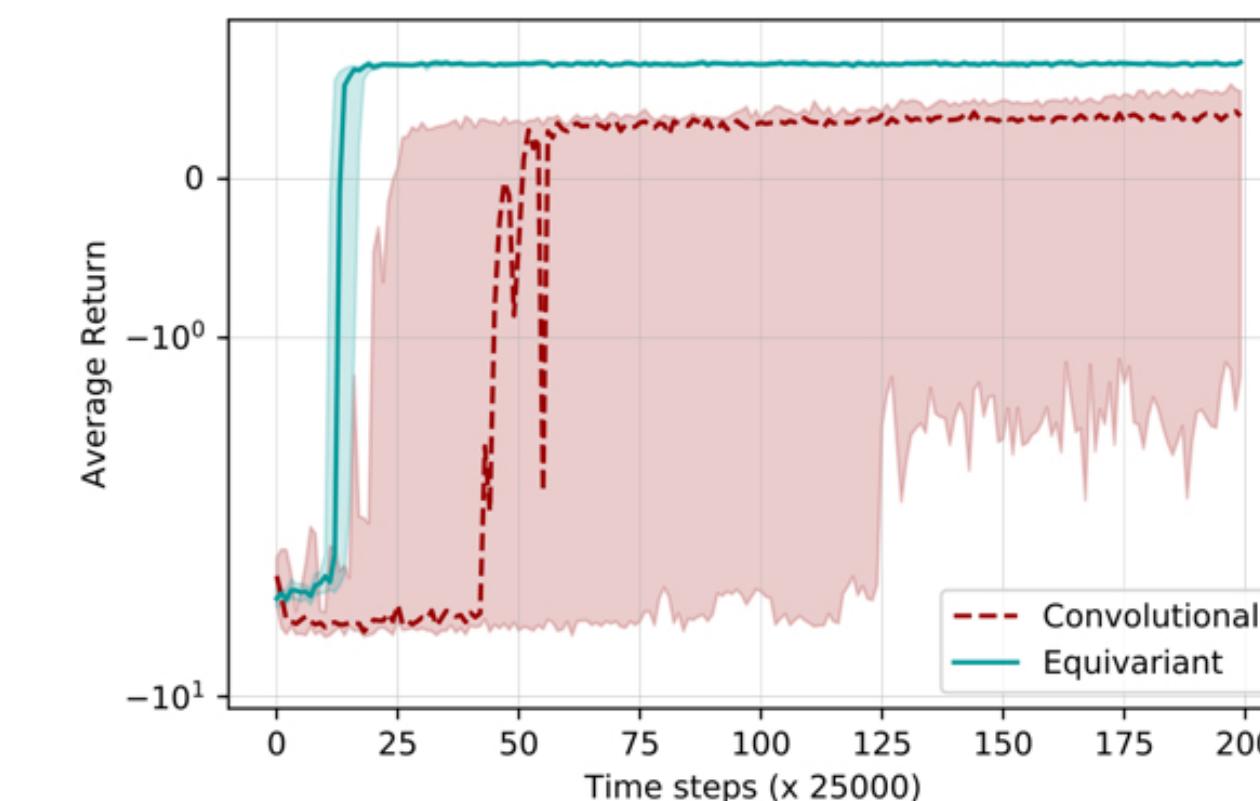
GridWorld



Pong



[S,LG] 30 Jun 2020



MDP Homomorphic Networks: Group Symmetries in Reinforcement Learning

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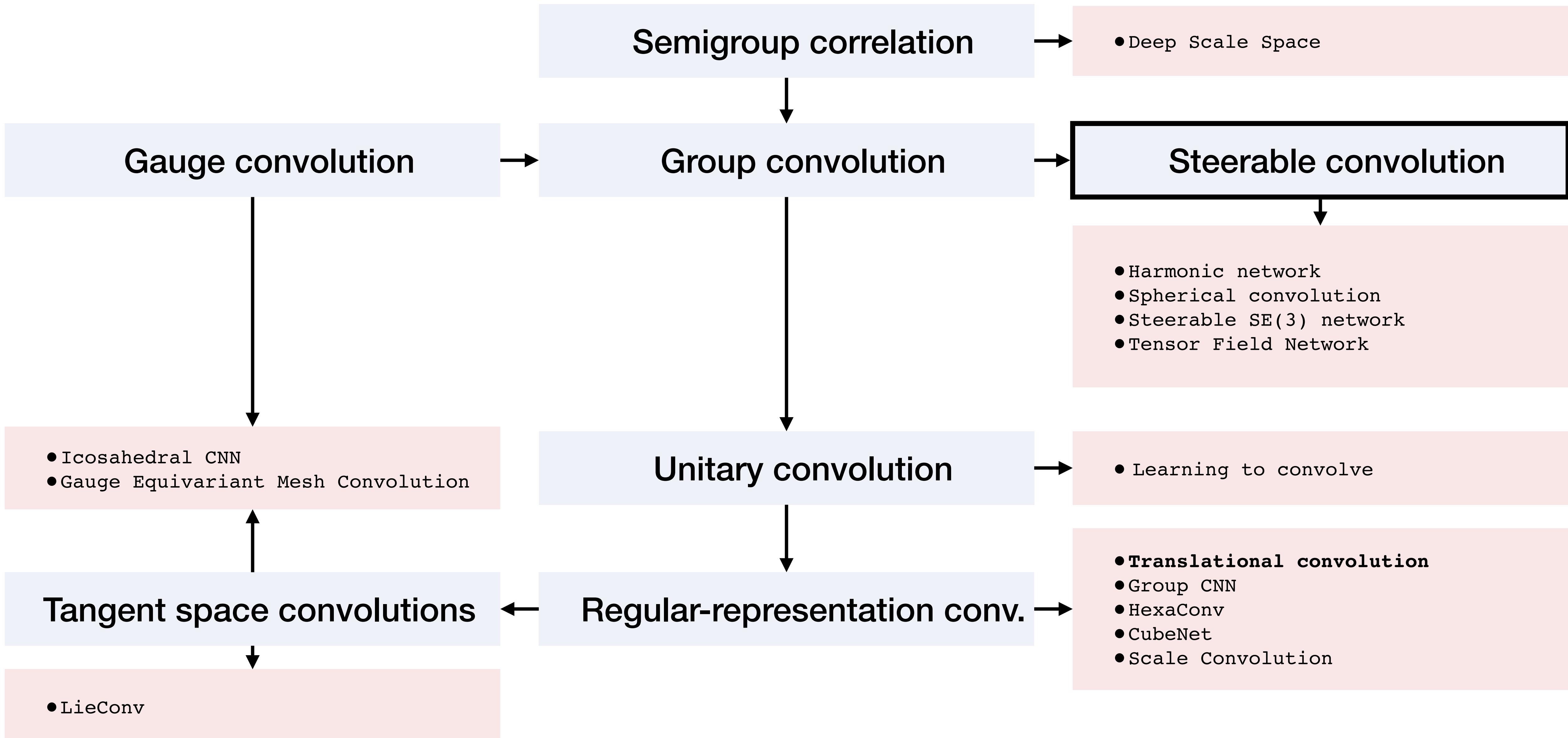
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Abstract

This paper introduces MDP homomorphic networks for deep reinforcement learning. MDP homomorphic networks are neural networks that are equivariant under symmetries in the joint state-action space of an MDP. Current approaches to deep

van der Pol et al. (2020)

Convolutions are special

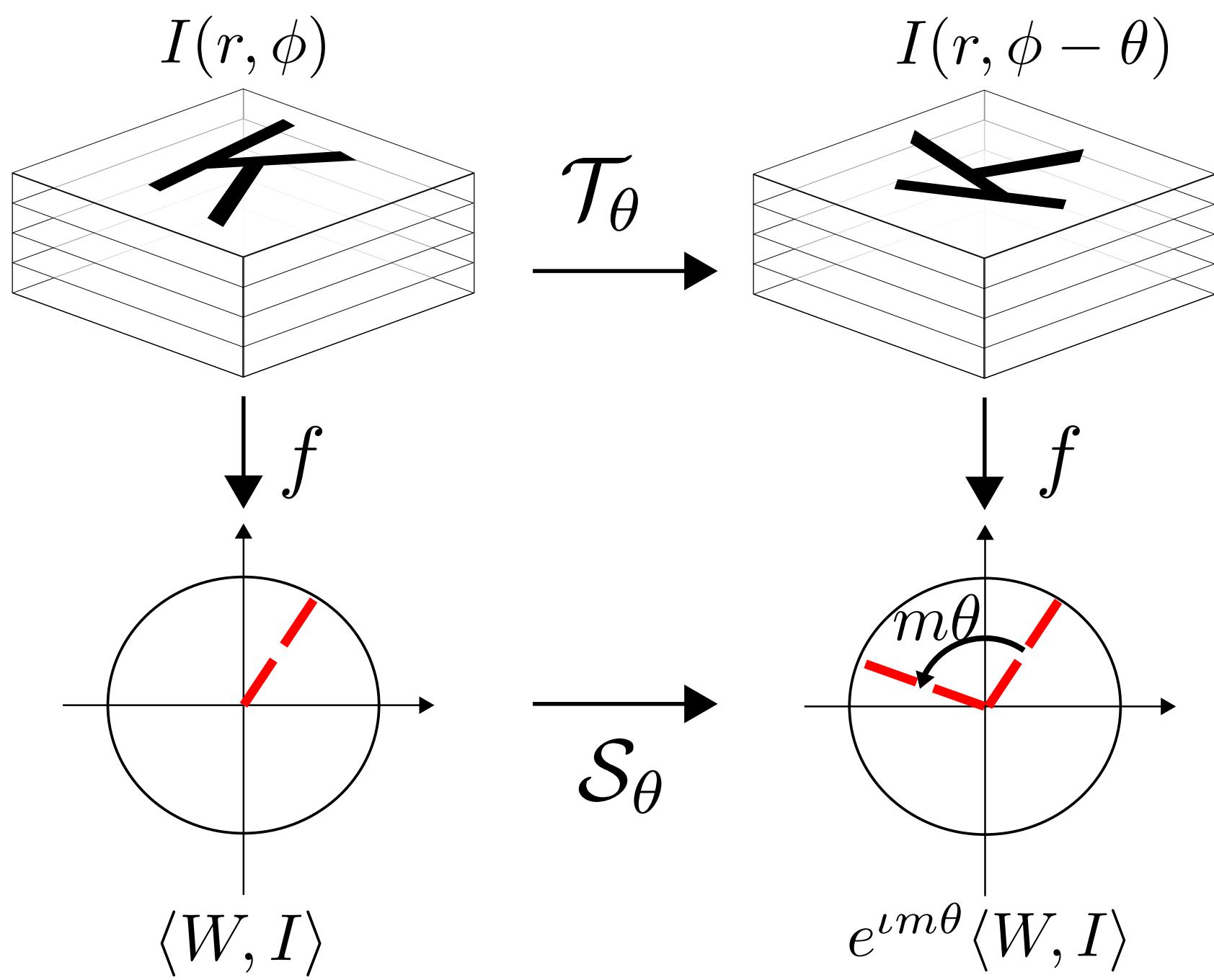


Steerable Convolutions

Another equivariant mapping is the *Fourier transform*

$$\mathcal{F}\{F\}(m) = \int_{-\pi}^{\pi} F(\phi) e^{-\imath m\phi} d\phi$$

Inner product!



Can be generalized to other transformation groups

Fourier Shift Theorem

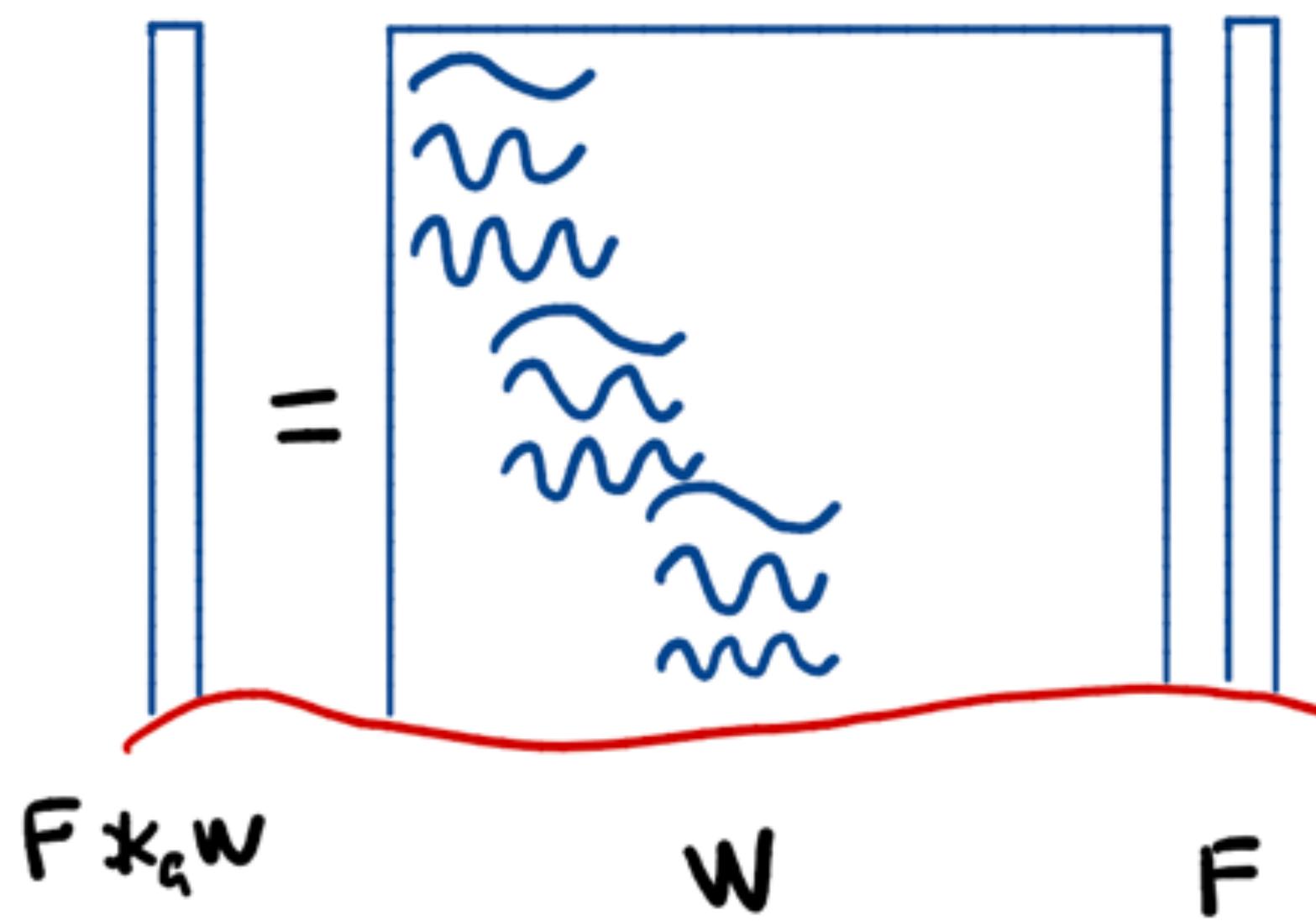
$$\begin{aligned} \int_{-\pi}^{\pi} F(\phi - \theta) e^{-\imath m\phi} d\phi &= \int_{-\pi - \theta}^{\pi - \theta} F(\phi') e^{-\imath m(\phi' + \theta)} d\phi' \\ &= e^{-\imath m\theta} \int_{-\pi}^{\pi} F(\phi') e^{-\imath m\phi'} d\phi' \end{aligned}$$

Equivariant

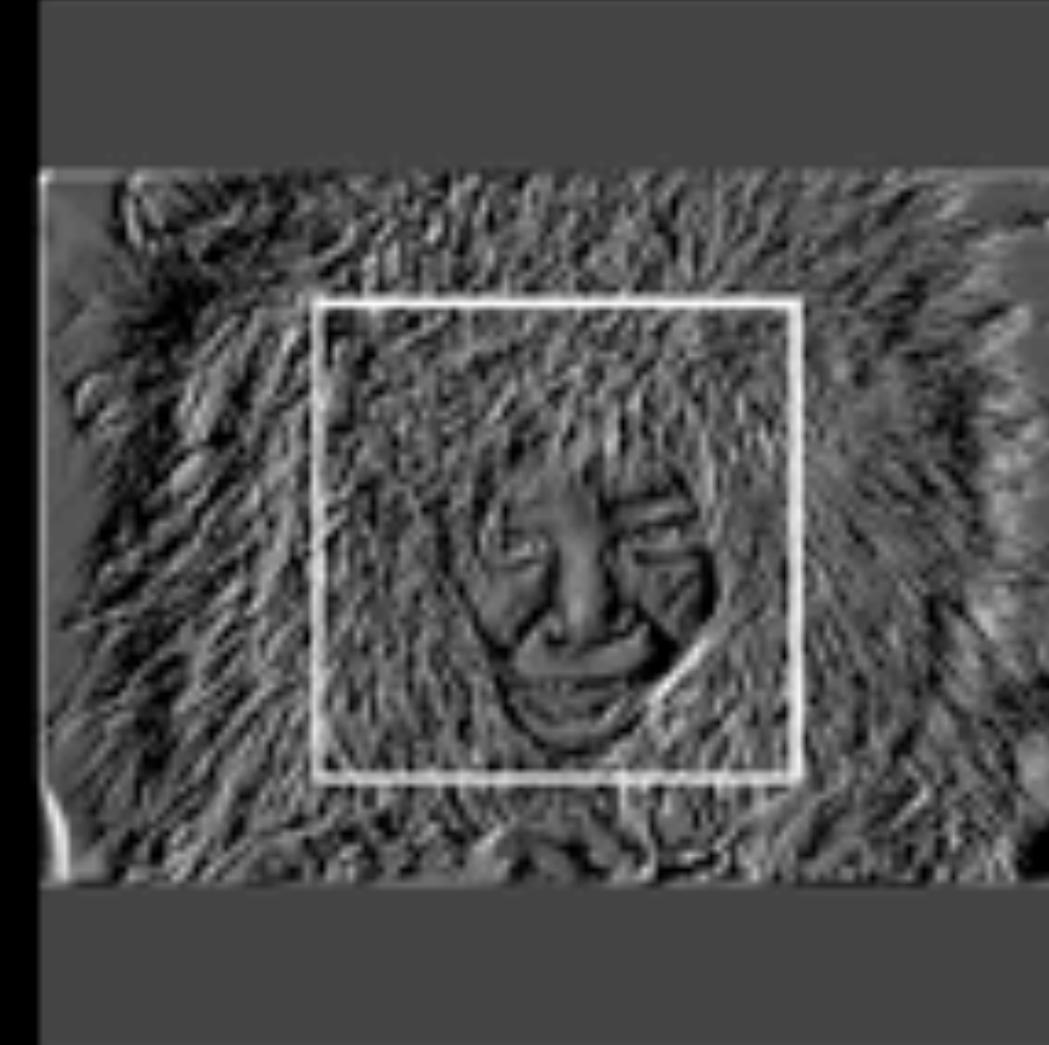
Invariant

$$\mathcal{F}\{\mathcal{T}_\theta[F]\}(m) = e^{-\imath m\theta} \mathcal{F}\{F\}(m) = \mathcal{S}_\theta[\mathcal{F}]\{F\}(m)$$

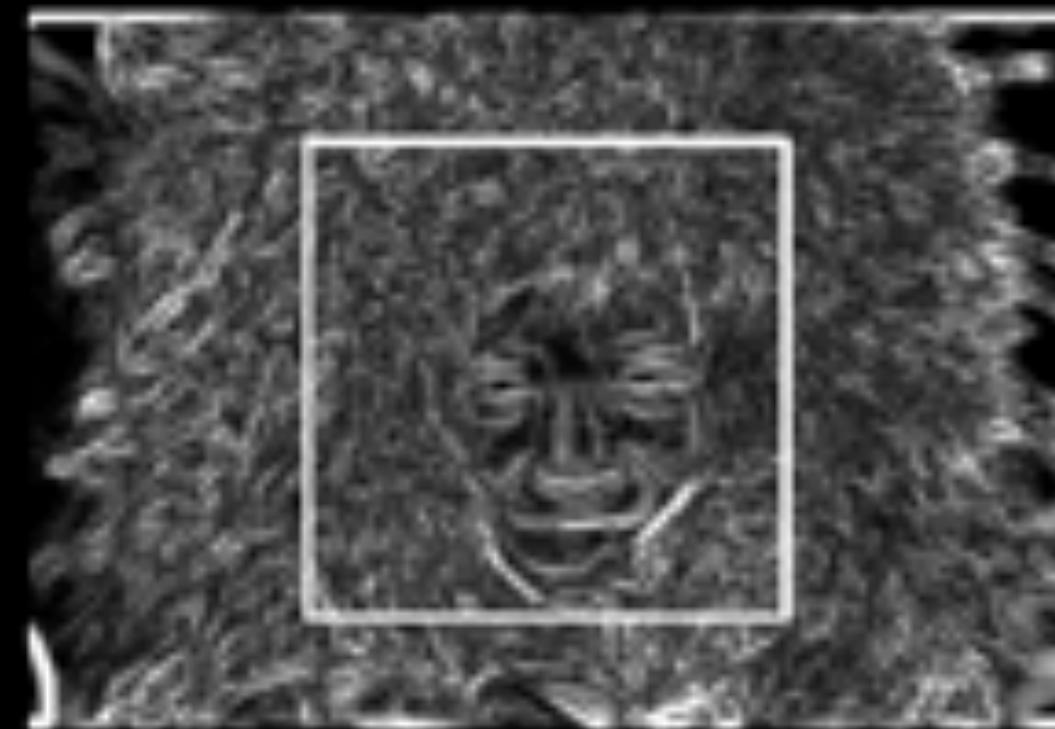
Learnable Learnable
 $W_m(r; \phi) = R(r) e^{\imath(m\phi + \beta)}$
 Fixed



Lack of Rotation Equivariance



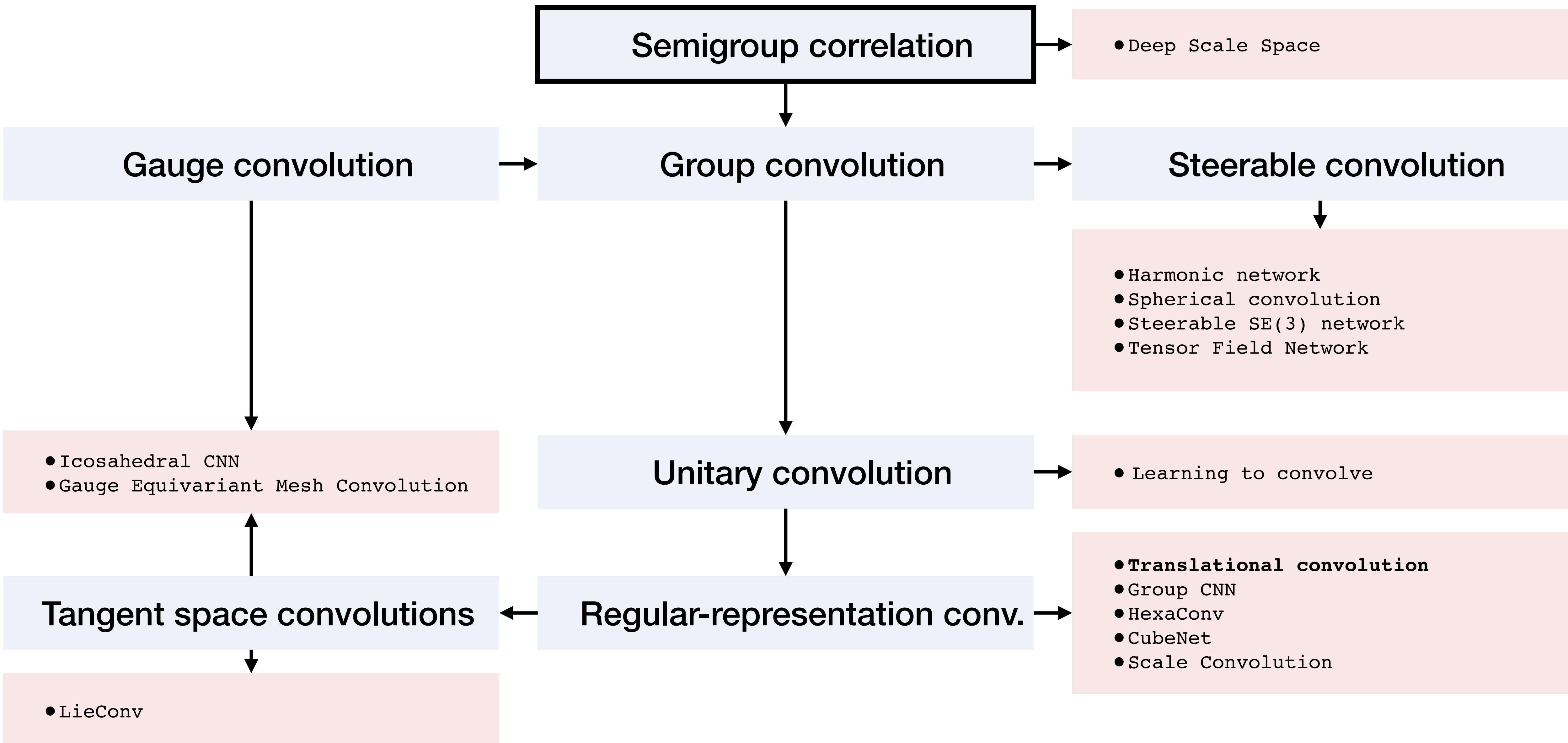
Steerable Equivariance



Comparison



Convolutional variants: Semigroup Correlations



Semigroups: How not to rescale

x2

Original



Subsample



Bandlimit + subsample



Semigroups: How not to rescale

x4

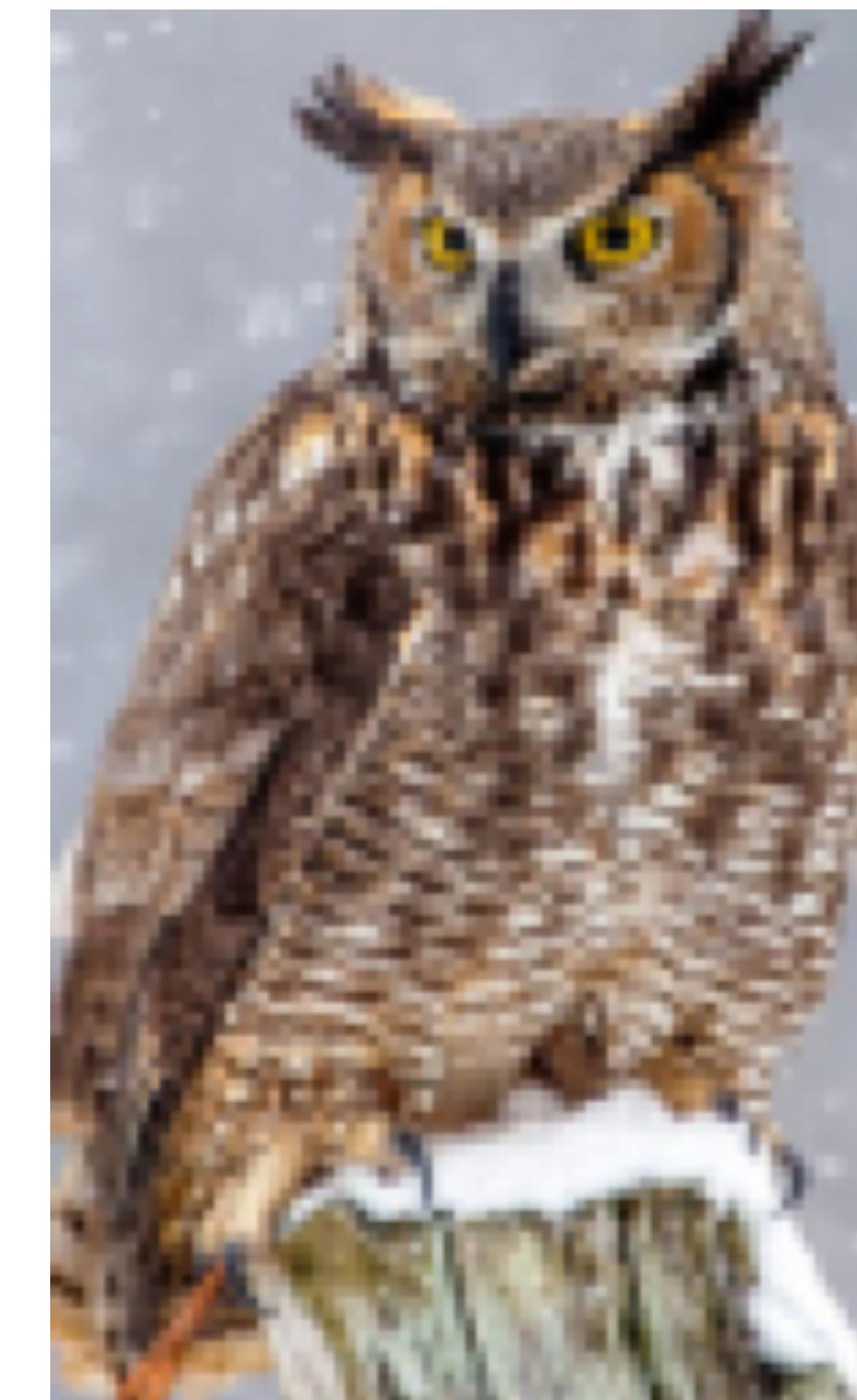
Original



Subsample



Bandlimit + subsample



Semigroups: How not to rescale

x4

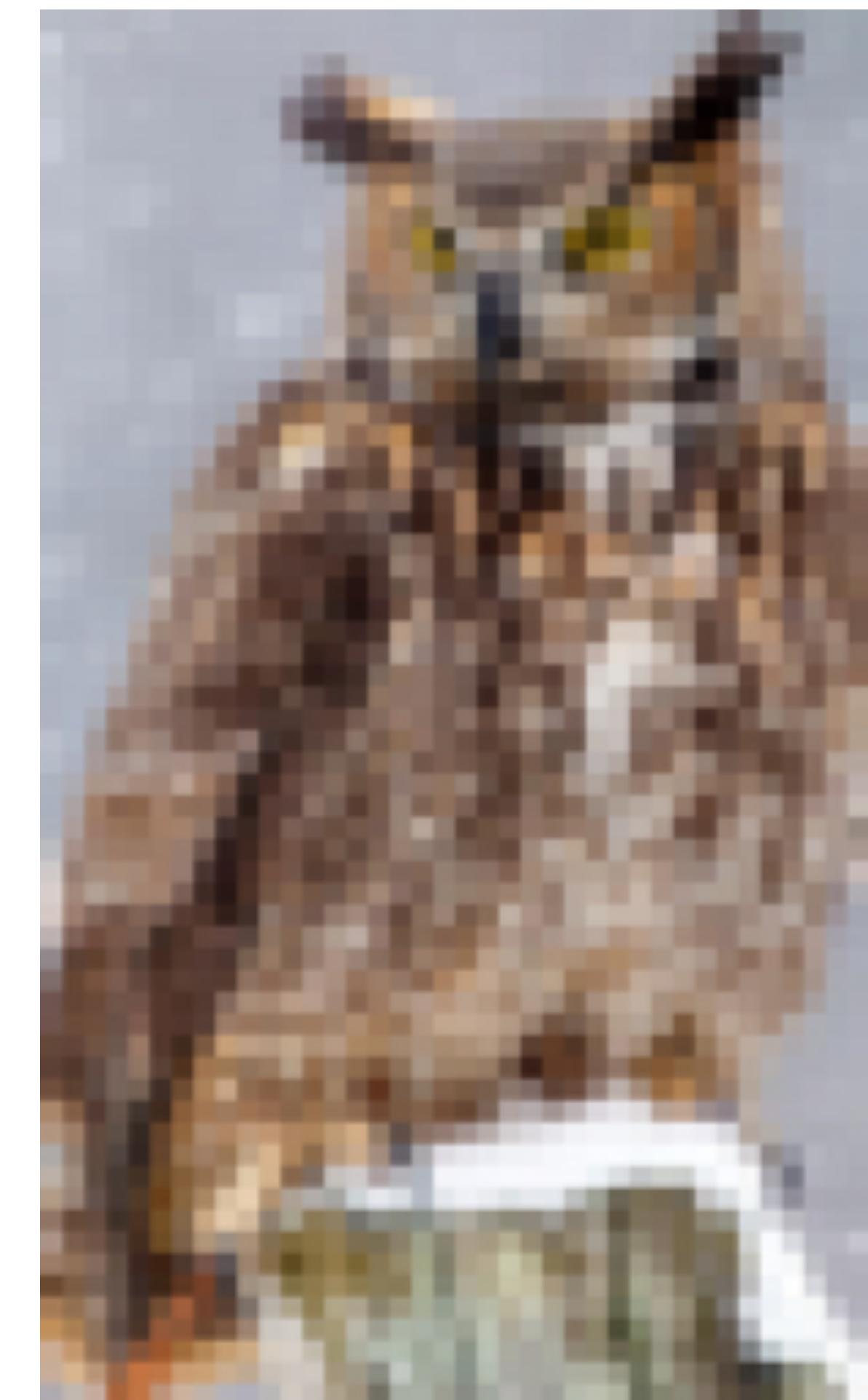
Original



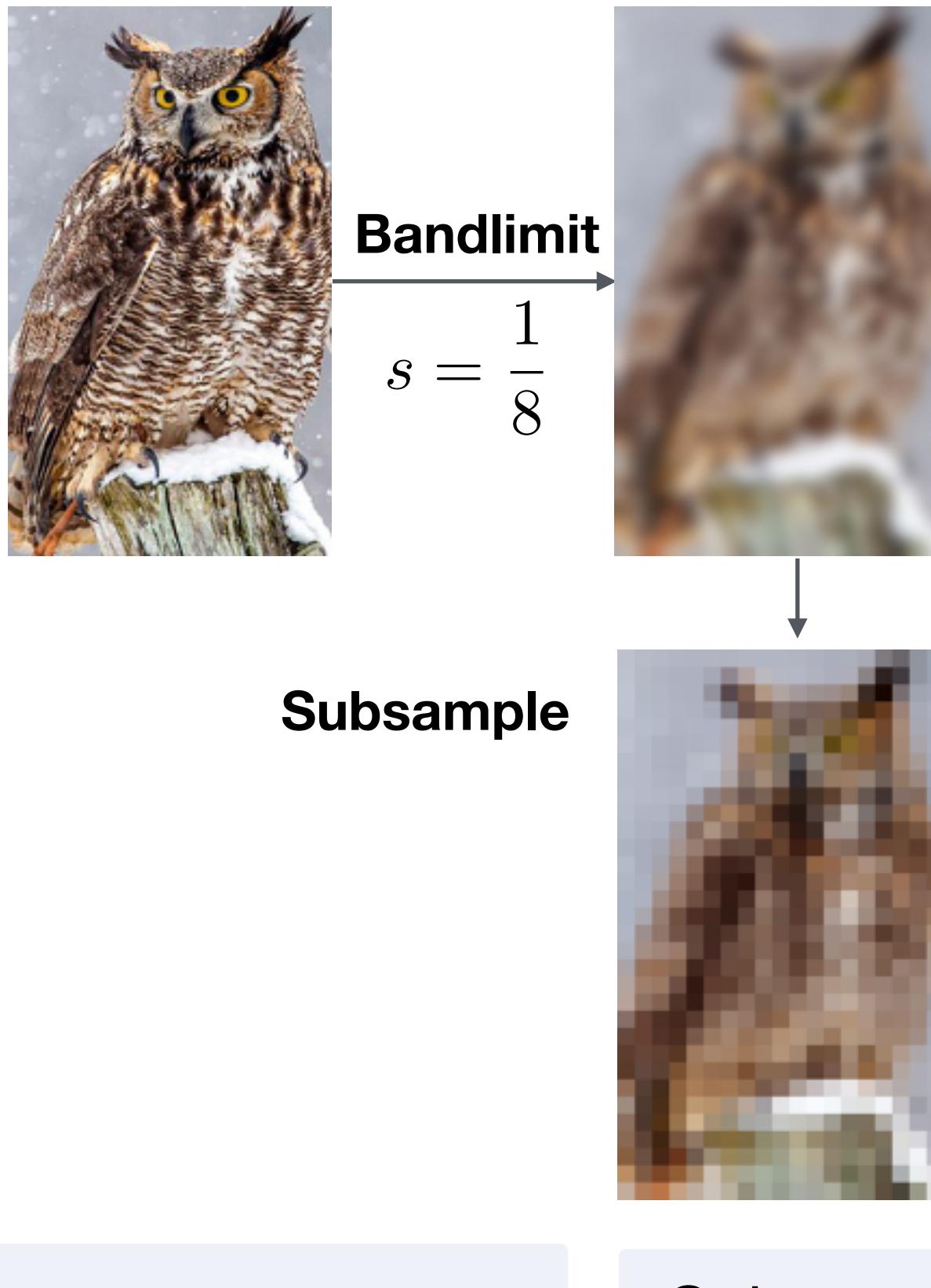
Subsample



Bandlimit + subsample



Semigroups: How to rescale



Blur appropriately

$$\mathcal{T}_s[\mathbf{F}](\mathbf{x}) = \text{Blur}_s[\mathbf{F}](s^{-1}\mathbf{x})$$

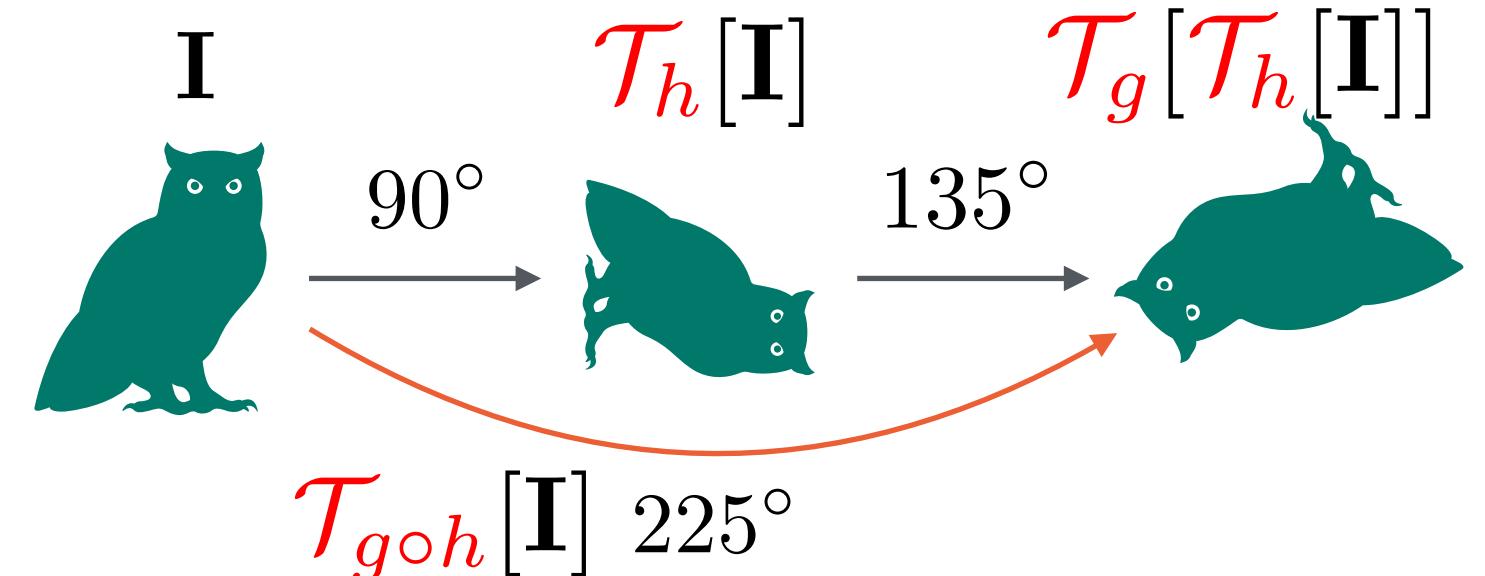
$\mathcal{T}_s^{-1}[\mathbf{F}](\mathbf{x})$ does not exist!!!

Abstraction

1. **Closure:** compositions well-behaved

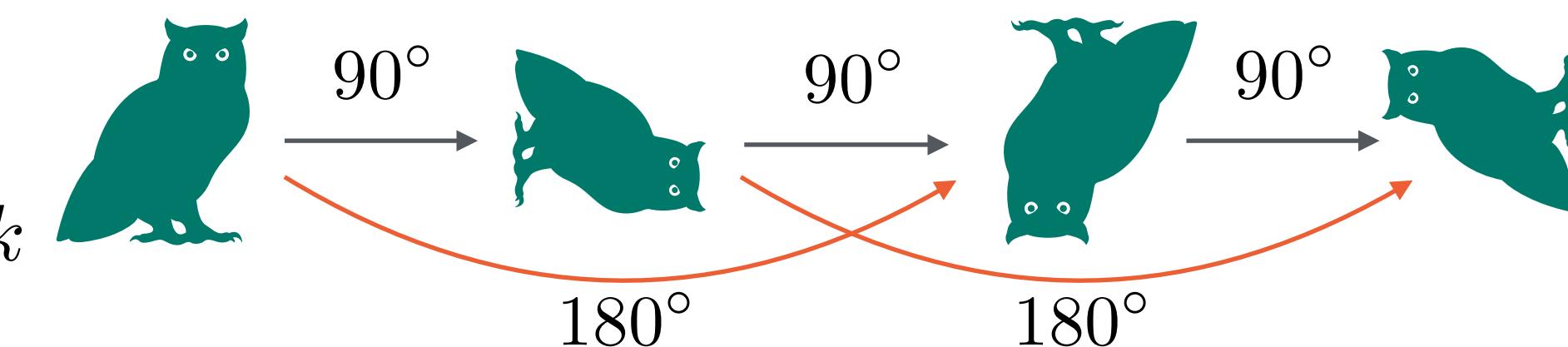
$$g \circ h \in G$$

Action/Transformation



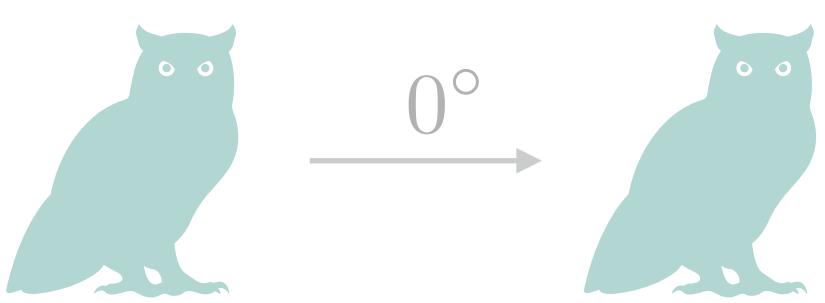
2. **Associativity:** brackets unnecessary

$$(g \circ h) \circ k = g \circ (h \circ k) = g \circ h \circ k$$



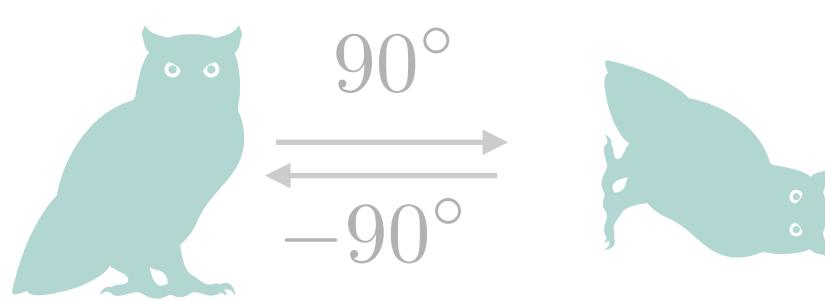
3. **Identity:** “do nothing” transformation

$$e \circ g = g \circ e = g$$



4. **Invertibility:** transformation reversible

$$g \circ g^{-1} = g^{-1} \circ g = e$$



Group convolution

e.g. Cohen & Welling (2016)

$$[I * W](x) = \sum_{y \in \mathcal{Y}} I(y) W(\mathcal{T}_x^{-1}[y])$$

1) Rescaling \neq shuffling pixel locations

Unitary Group Convolution

e.g. Diaconu & Worrall (2019)

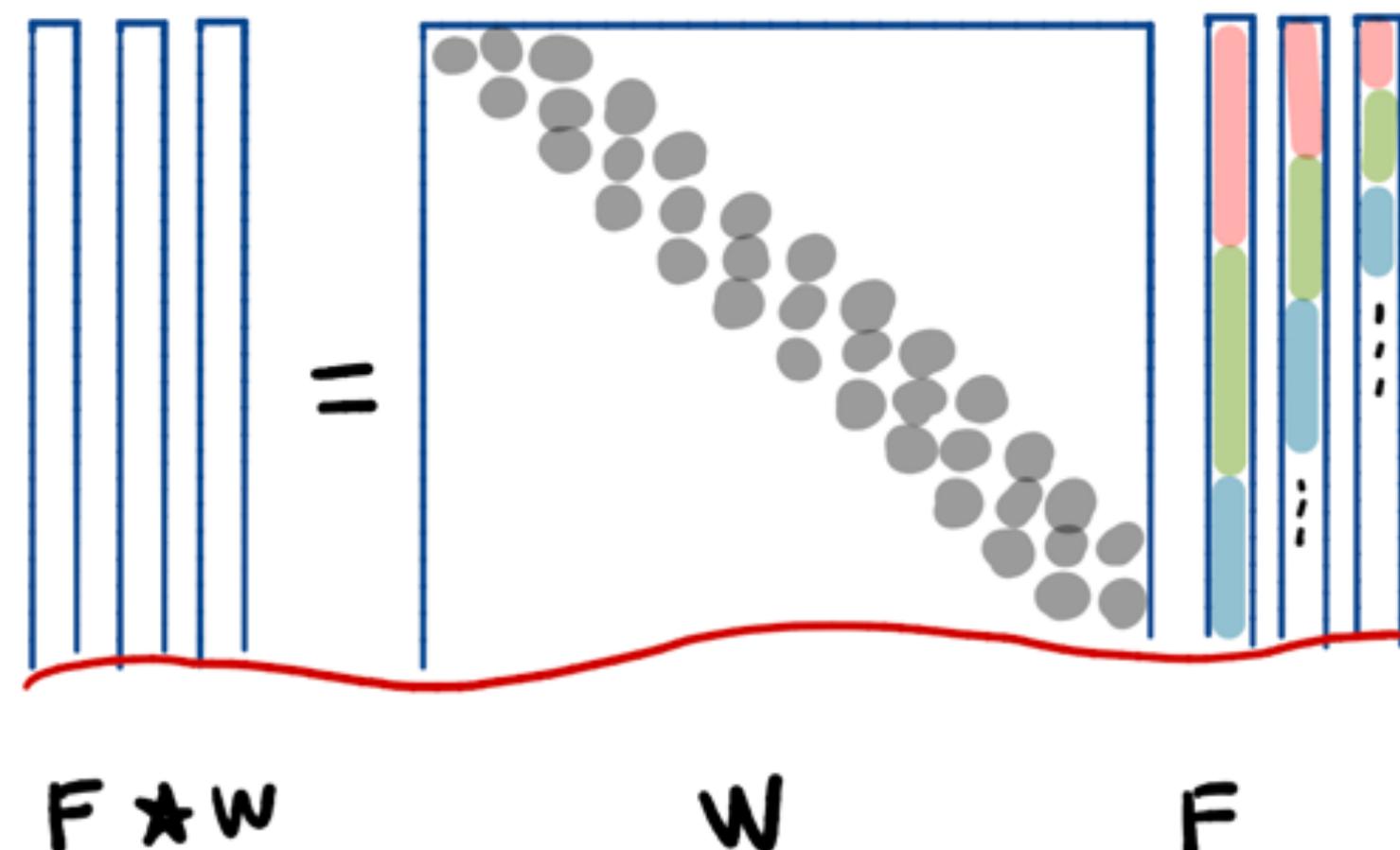
$$[I * W](x) = \sum_{y \in \mathcal{Y}} I(y) \mathcal{T}_x^{-1}[W](y)$$

2) Use non-invertible transformations

Semigroup correlation

e.g. Worrall & Welling (2019)

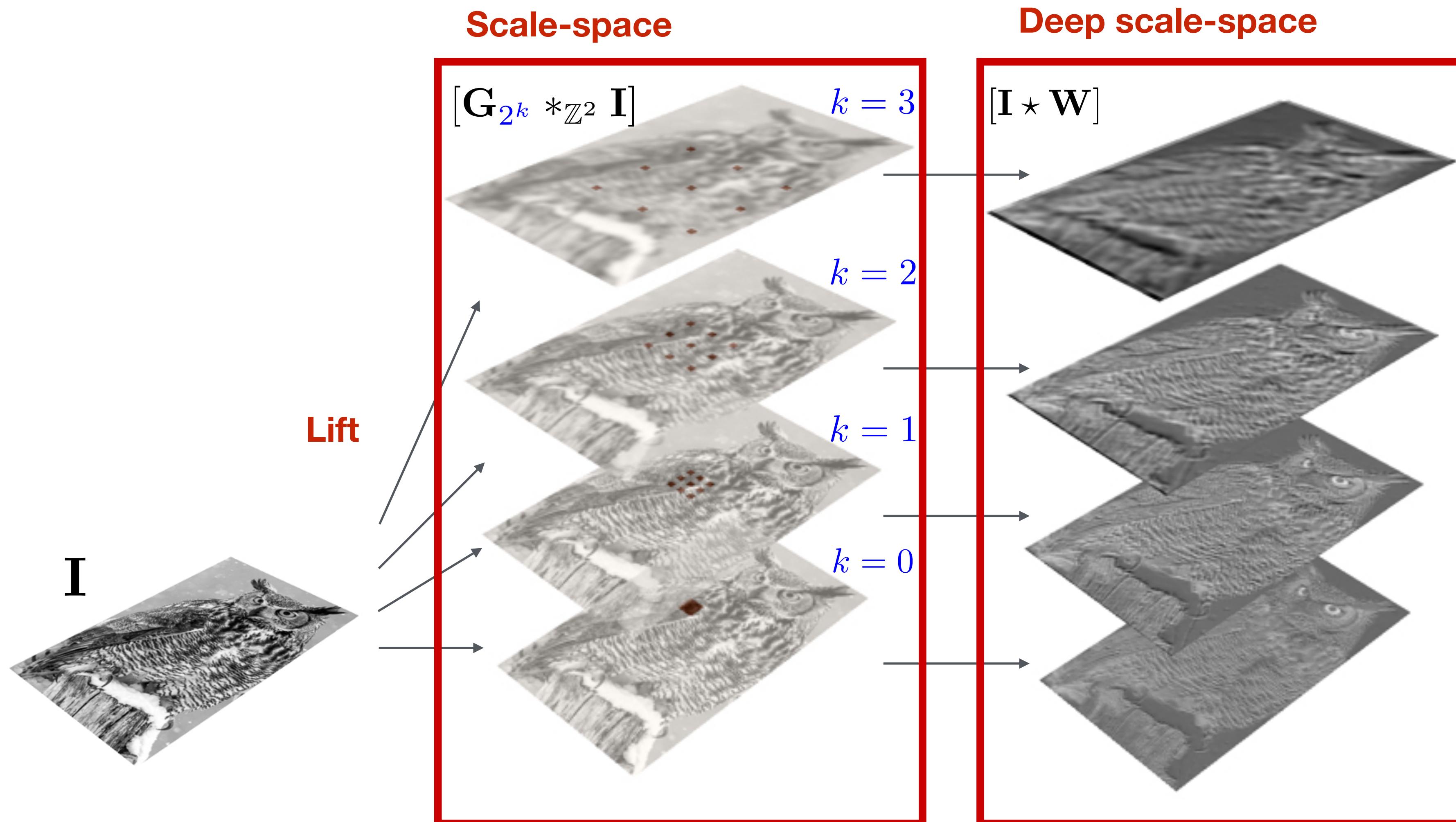
$$[I \star W](x) = \sum_{y \in \mathcal{Y}} \mathcal{T}_x[I](y) W(y)$$



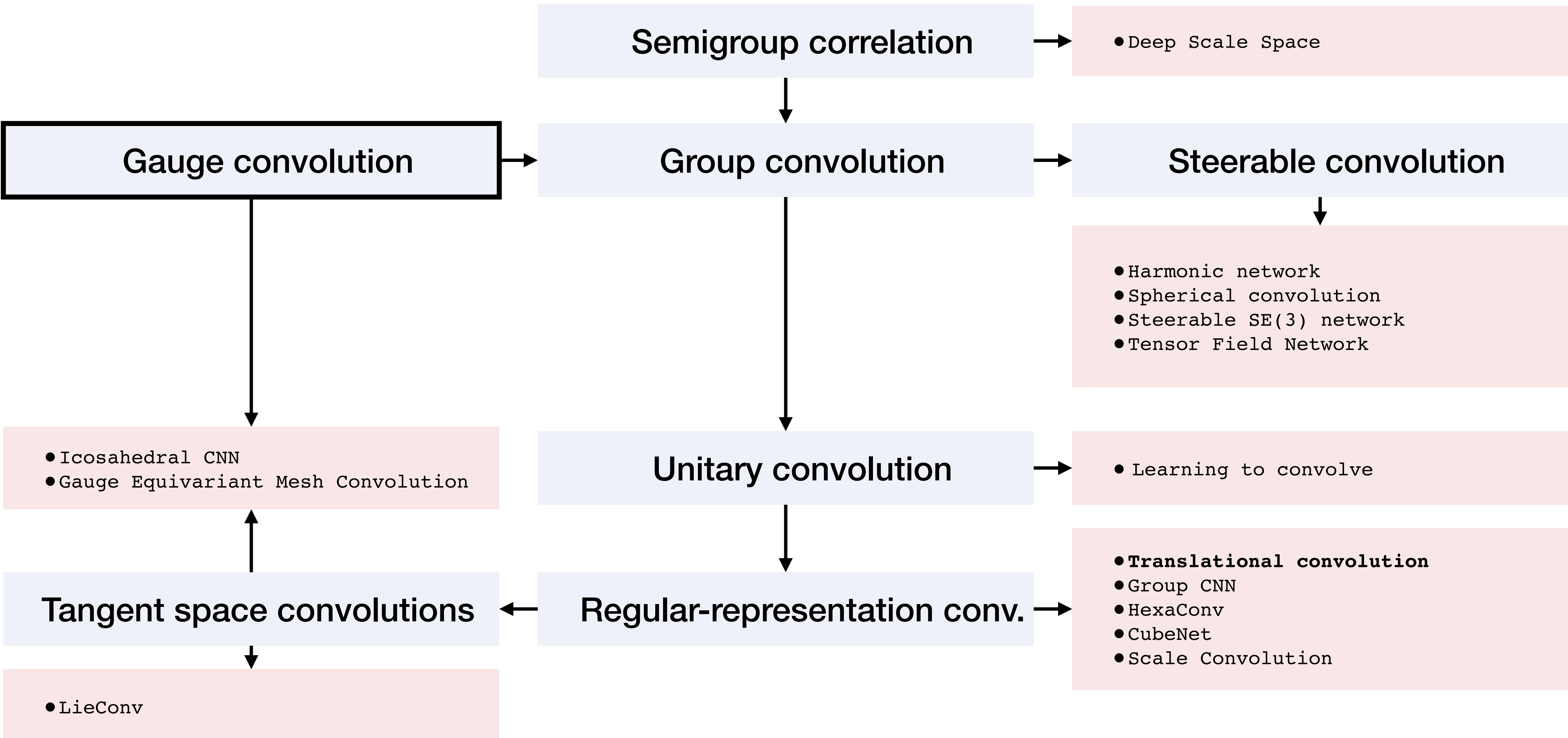
The Semigroup Correlation

$$[\mathbf{I} \star \mathbf{W}](k, t) = \sum_{y \in \mathbb{Z}^2} [\mathbf{G}_{2^k} *_{\mathbb{Z}^2} \mathbf{I}](2^k y + t) \mathbf{W}(y)$$

y $\in \mathbb{Z}^2$ blur dilated convolution

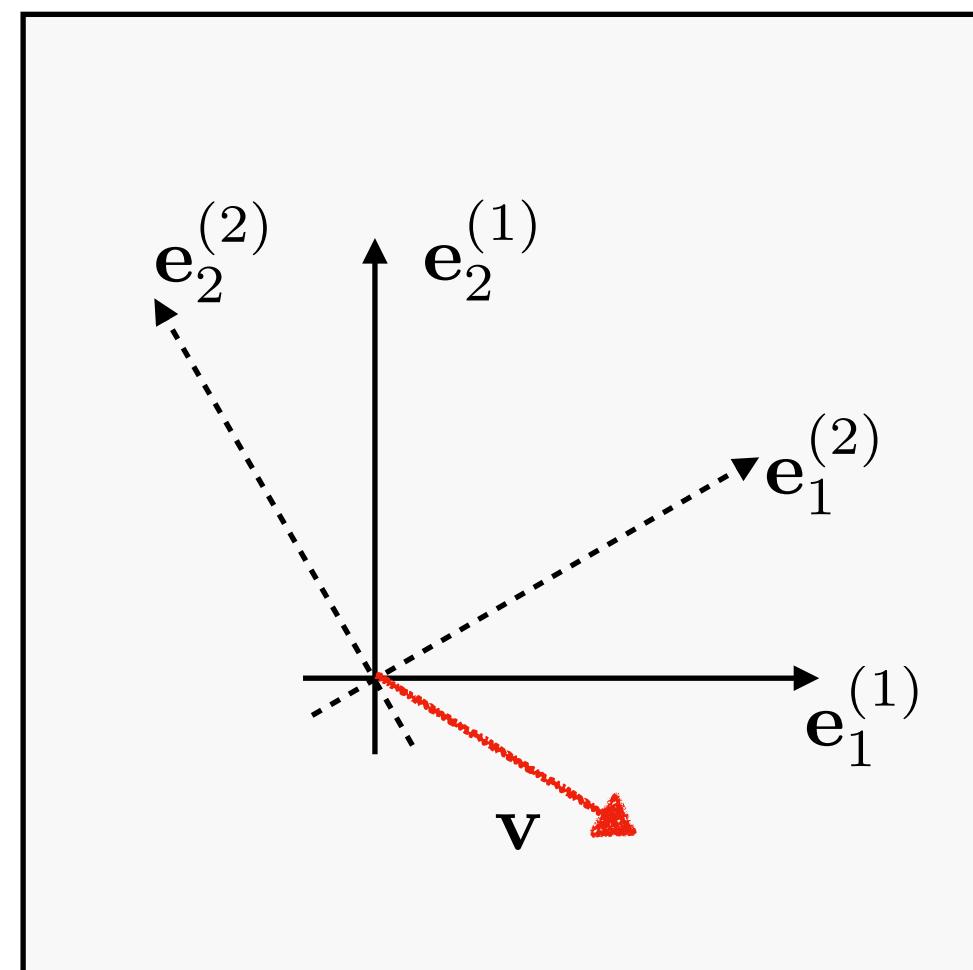


Convolutional variants: Gauge Equivariance



Gauge Convolutions

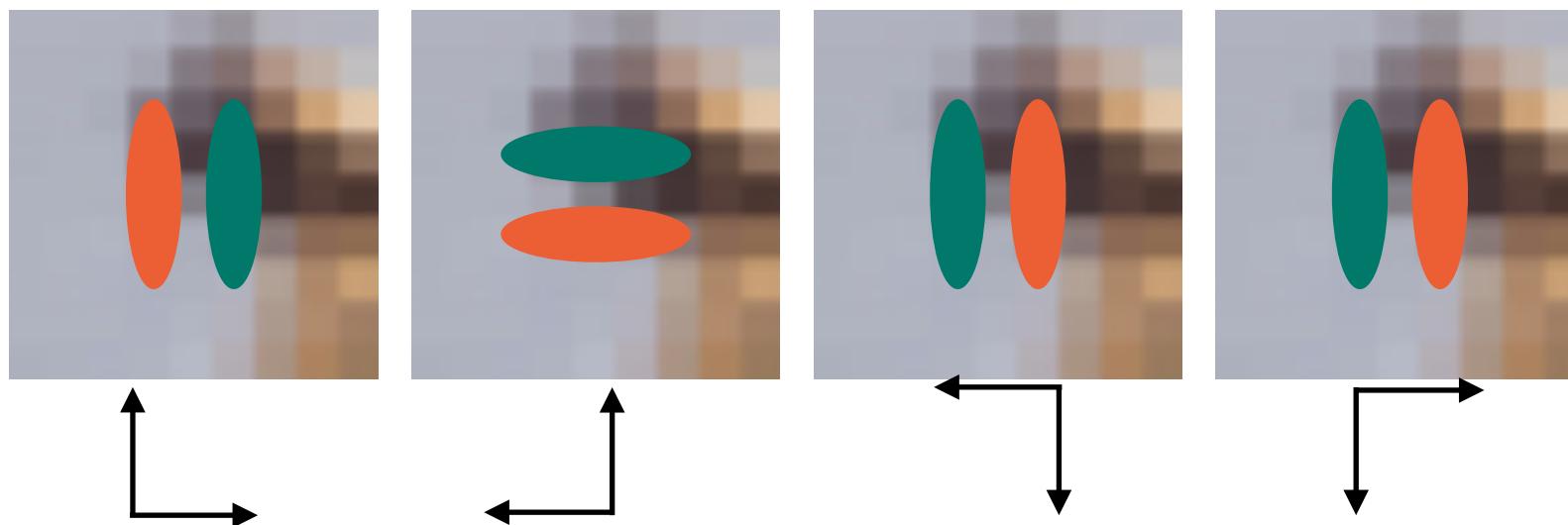
An alternative route to equivariance is to consider *local gauge transformations*



$$v_1^{(1)} \mathbf{e}_1^{(1)} + v_2^{(1)} \mathbf{e}_2^{(1)} = v_1^{(2)} \mathbf{e}_1^{(2)} + v_2^{(2)} \mathbf{e}_2^{(2)}$$

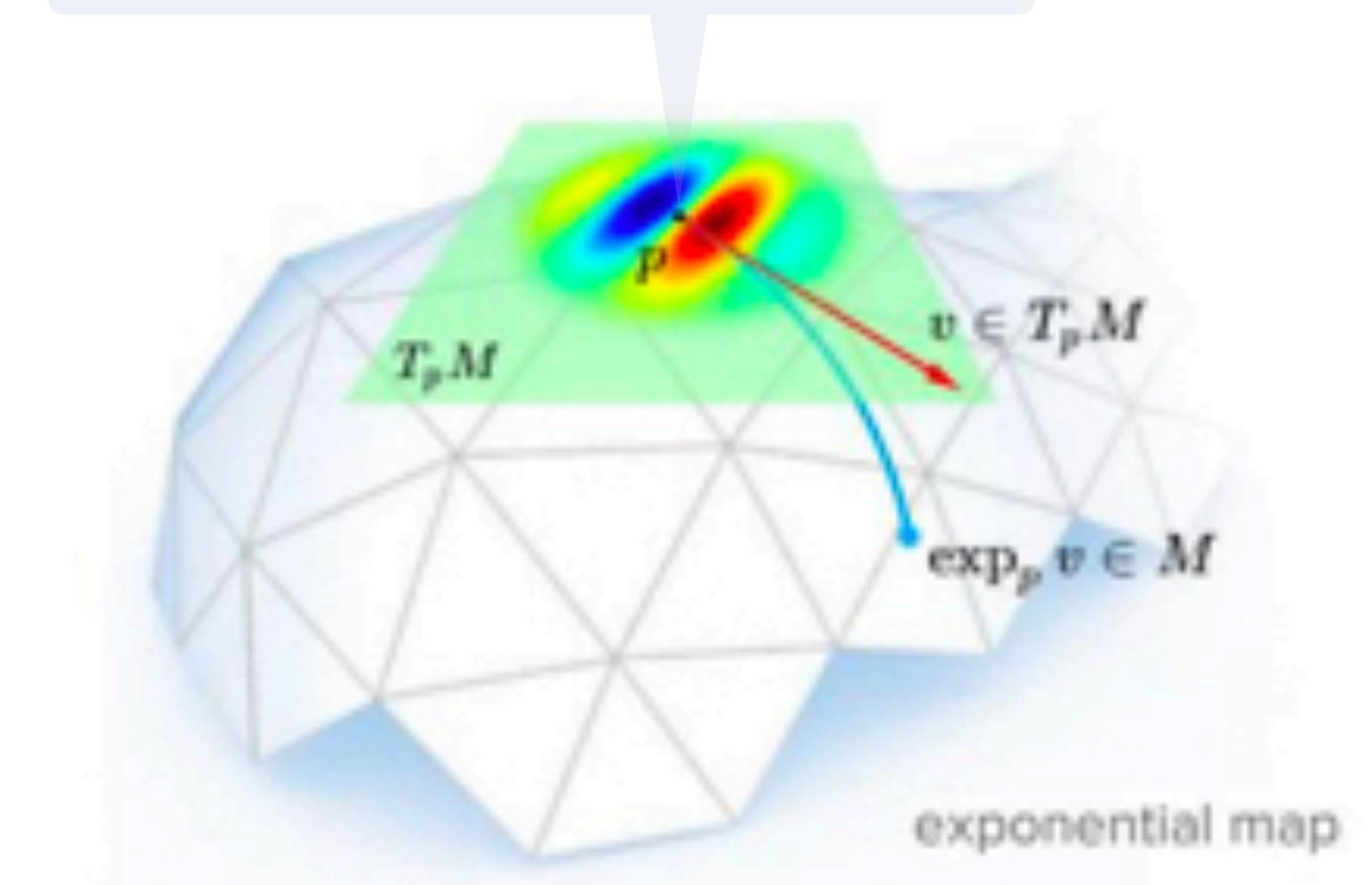
A *frame* is another name for coordinates.
How to make frame independent?

Take inner product between signal and filter represented in all frame orientations

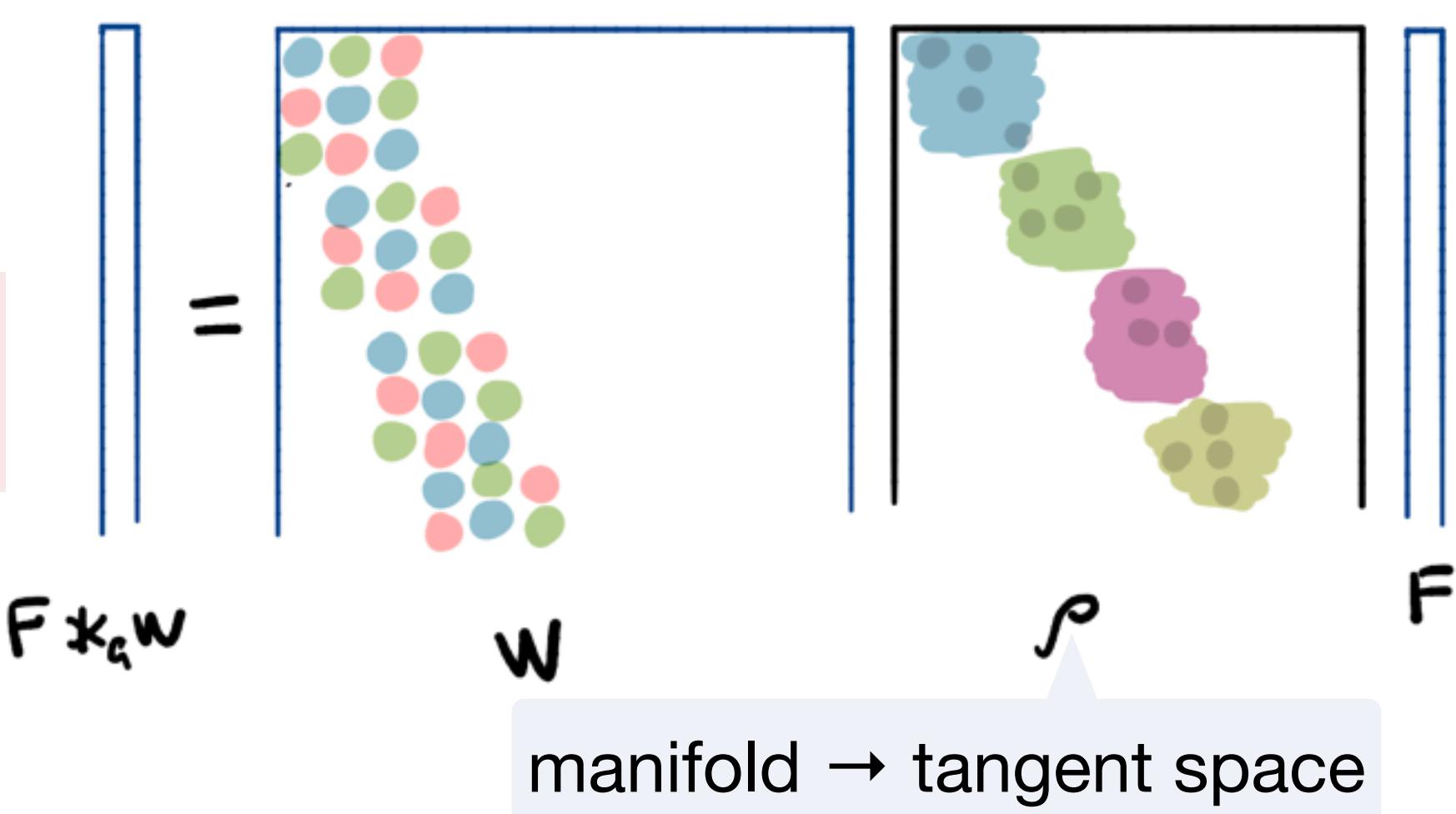


Like a group convolution, but...:
• Defined locally
• Can work on manifolds

Need to map signal manifold → tangent space

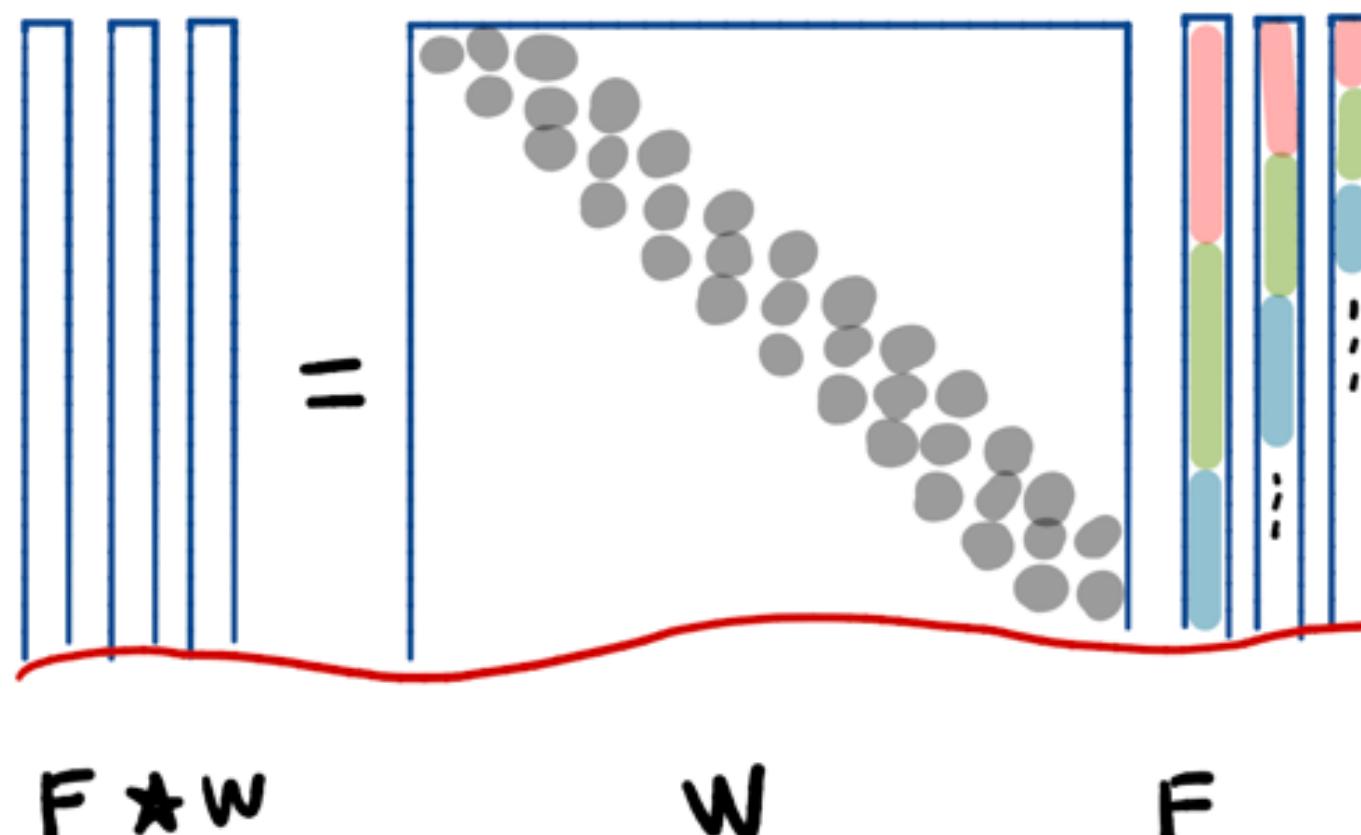


Cohen et al. (2019)

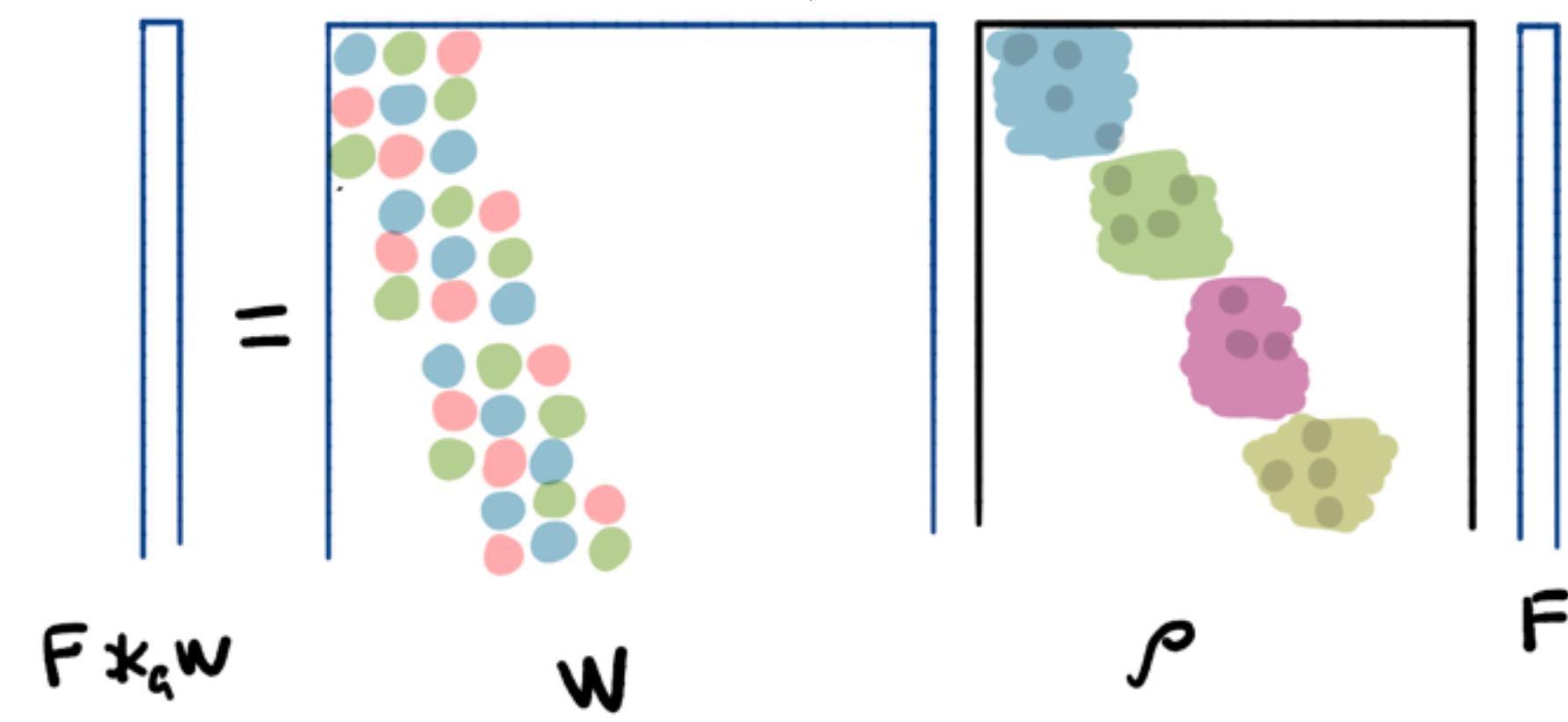


Convolutional variants

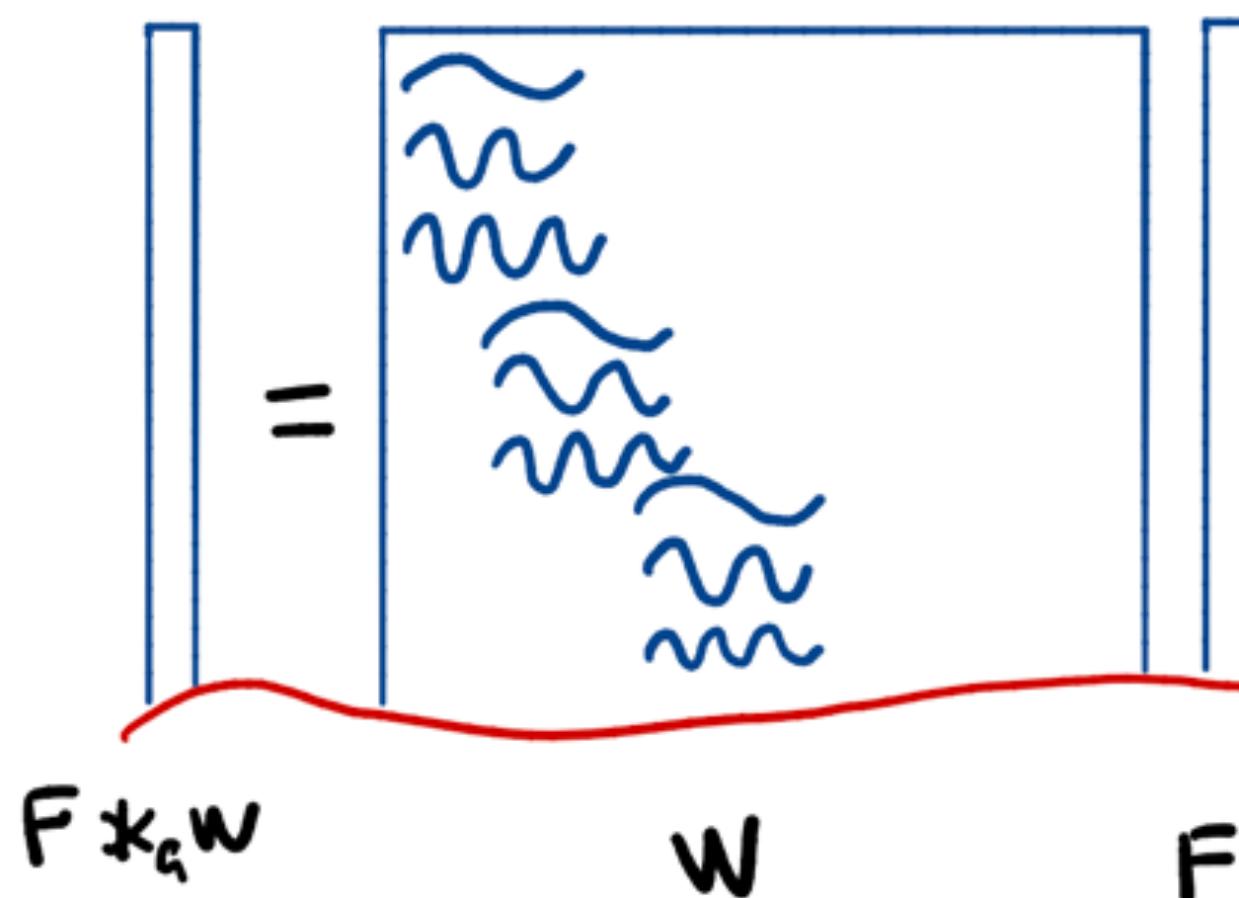
Semigroup correlation



Gauge convolution



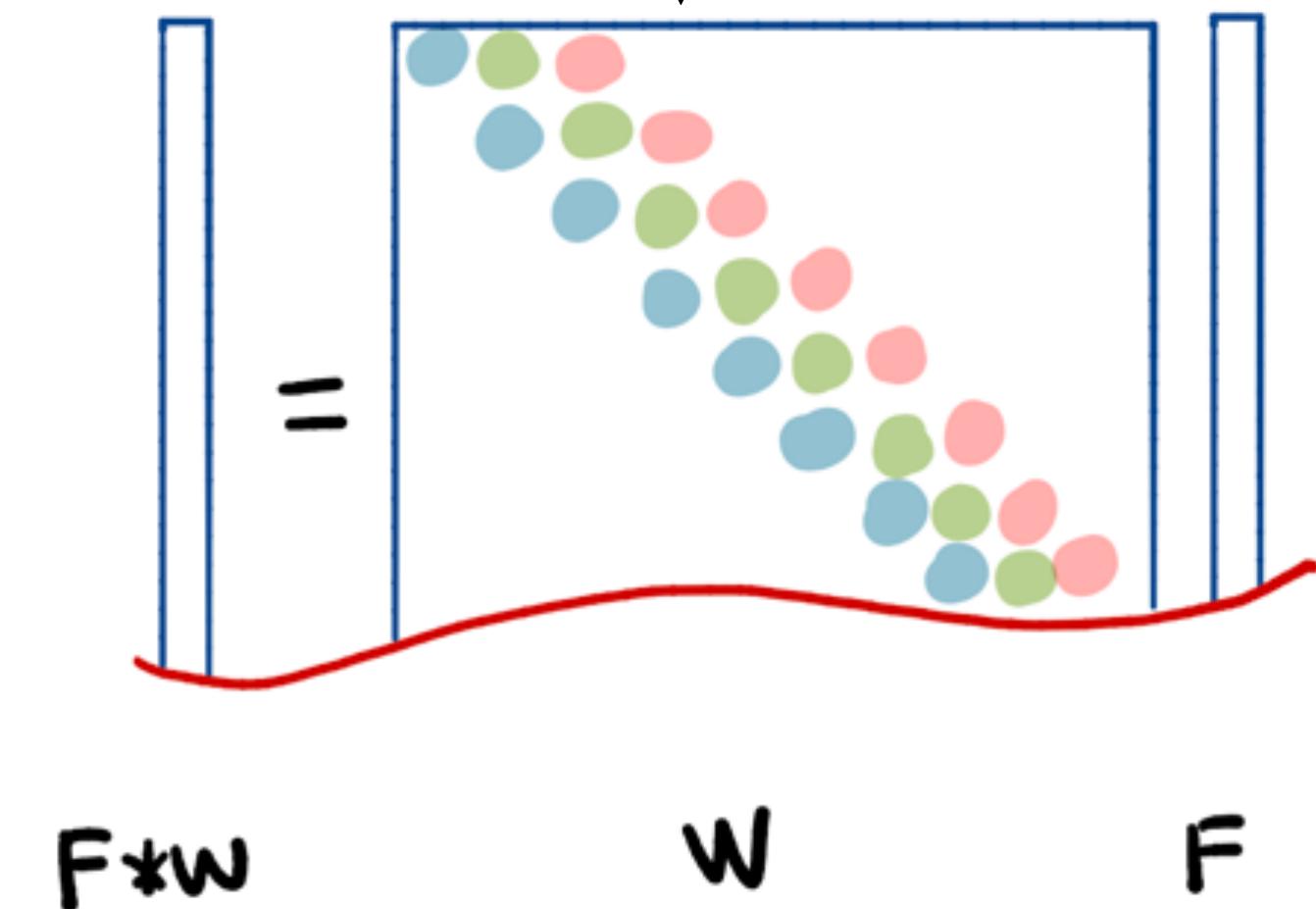
Steerable convolution

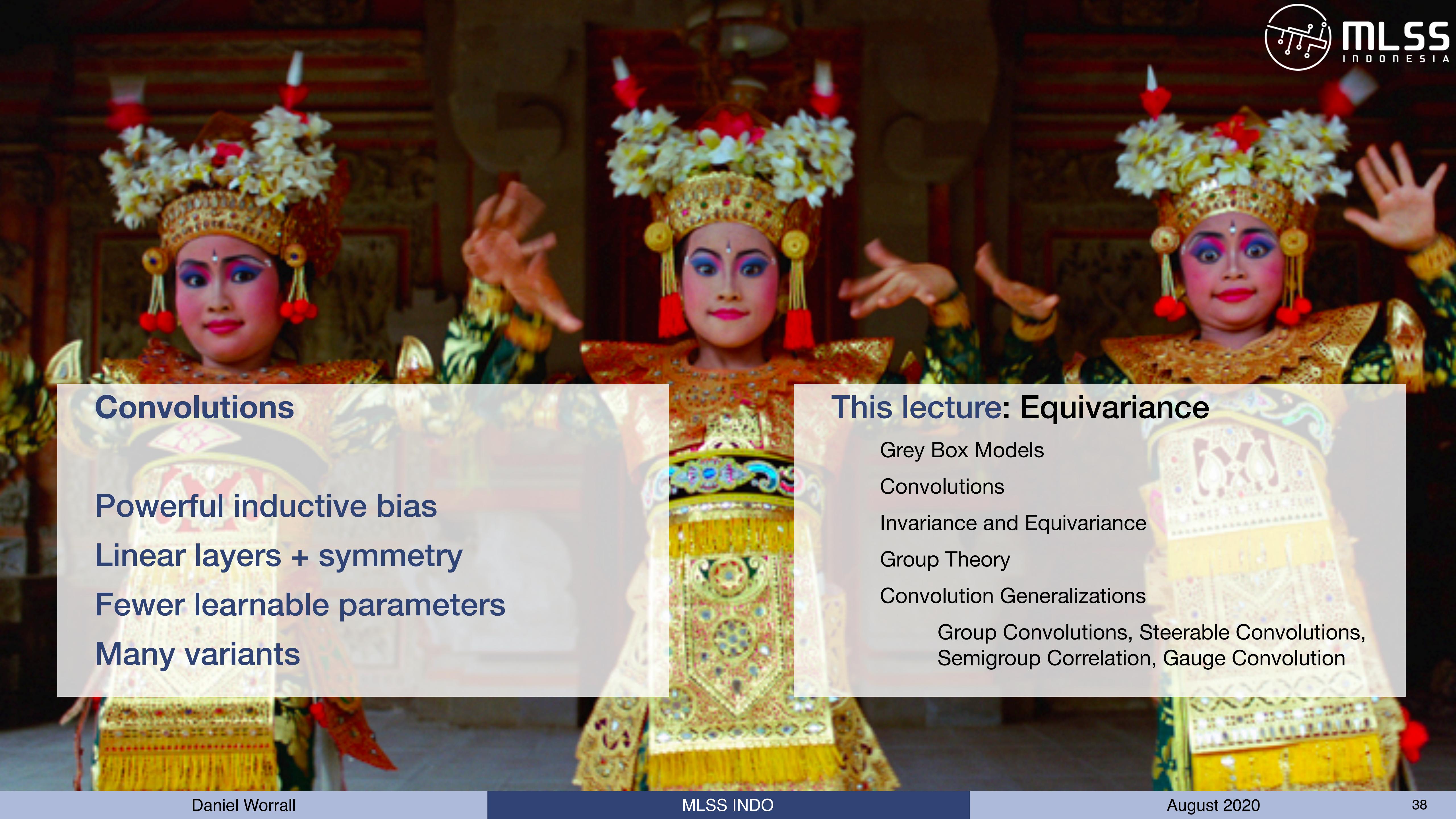


Group convolution



Regular-representation conv.





Convolutions

Powerful inductive bias

Linear layers + symmetry

Fewer learnable parameters

Many variants

This lecture: Equivariance

Grey Box Models

Convolutions

Invariance and Equivariance

Group Theory

Convolution Generalizations

Group Convolutions, Steerable Convolutions, Semigroup Correlation, Gauge Convolution

Theory

Group CNNs - Cohen & Welling (2016)

Steerable CNNs - Cohen & Welling (2017)

On the Generalization of Equivariance and Convolution in Neural Networks to the Action of Compact Groups - Kondor & Trivedi (2018)

A General Theory of Equivariant CNNs on Homogeneous Spaces - Cohen et al. (2019)

Gauge Equivariance Convolutional Networks - Cohen*, Weiler*, Kicanaoglu* et al. (2019)

Deep Scale-spaces: Equivariance Over Scale - Worrall & Welling (2019)

\mathbb{Z}^2 - Translation

Handwritten digit recognition with a Back-Propagation network - Lecun et al. (1990)

SE(2): Full group

Harmonic Networks: Deep translation and rotation equivariance - Worrall et al. (2017)

SE(2): All subgroups

General E(2)-Equivariant Steerable CNNs - Weiler & Cesa (2019)

E(2): Discrete subgroups

Group CNNs - Cohen & Welling (2016)

Exploiting cyclic symmetry in convolutional neural networks - Dieleman et al. (2016)

Steerable CNNs - Cohen & Welling (2017)

HexaConv - Hoogeboom*, Peters* et al. (2018)

SE(2): Discrete subgroups

Learning steerable filters for rotation equivariant CNNs - Weiler et al. (2018)

Oriented response networks - Zhou et al. (2017)

Roto-translation covariant convolutions networks for medical image analysis - Bekkers et al. (2018)

Rotation equivariant vector field networks - Marcos et al. (2017)

E(3): Discrete subgroups

3D G-CNNs for pulmonary nodule detection - Winkels & Cohen (2018)

SE(3): Discrete subgroups

CubeNet: Equivariance to 3D rotation and translation - Worrall & Brostow (2018)

SE(3): Full group

N-body networks: a covariant hierarchical neural network architecture for learning atomic potentials - Risi (2018)

Tensor Field networks: Rotation- and translation-equivariant neural networks for 3D point clouds - Thomas, Smidt* et al. (2018)

3D Steerable CNNs: Learning Rotationally Equivariant Features in Volumetric Data - Weiler*, Geiger* et al. (2018)

Clebsch-Gordan Nets: A Fully Fourier Space Spherical Convolutional Neural Networks - Kondor et al. (2018)

Cormorant: Covariant molecular neural networks - Anderson et al. (2019)

SO(3) on the sphere: discrete subgroup

Spherical CNNs - Cohen*, Geiger*, Köhler et al. (2018)

SO(3) on the sphere: isotropic subgroup

Learning SO(3) Equivariant Representations with Spherical CNNs - Esteves et al. (2018)

DeepSphere: Efficient spherical Convolutions Neural Networks with HEALPix samplings for cosmological applications - Perraudeau et al. (2019)

SO(3) on the sphere: full group

Spherical CNNs on unstructured grids - Jiang et al. (2019)

Scale semigroup

Deep Scale-spaces: Equivariance Over Scale - Worrall & Welling (2019)

Scale group

Scale equivariance in CNNs with vector fields - Marcos et al (2018)

Scale steerable filters for locally scale-invariant neural networks - Ghosh & Gupta (2019)

Scale-equivariant steerable networks - Sosnovid & Smeulders (2020)

Lie groups:

B-Spline CNNs on Lie Groups - Bekkers (2019)

Generalizing Convolutional Neural Networks for Equivariance to Lie groups on Arbitrary Continuous Data - Finzi et al. (2020)

Reverse-complement symmetry

An equivariant Bayesian convolutional network predicts recombination hotspots and accurately resolves binding motifs - Brown & Lunter (2019)

PDEs

PDE-based Group Equivariant Convolutional Neural Networks - Smets et al. (2020)

Incorporating Symmetry into Deep Dynamics Models for Improved Generalization - Wang*,
Walters* et al. (2020)

Attention

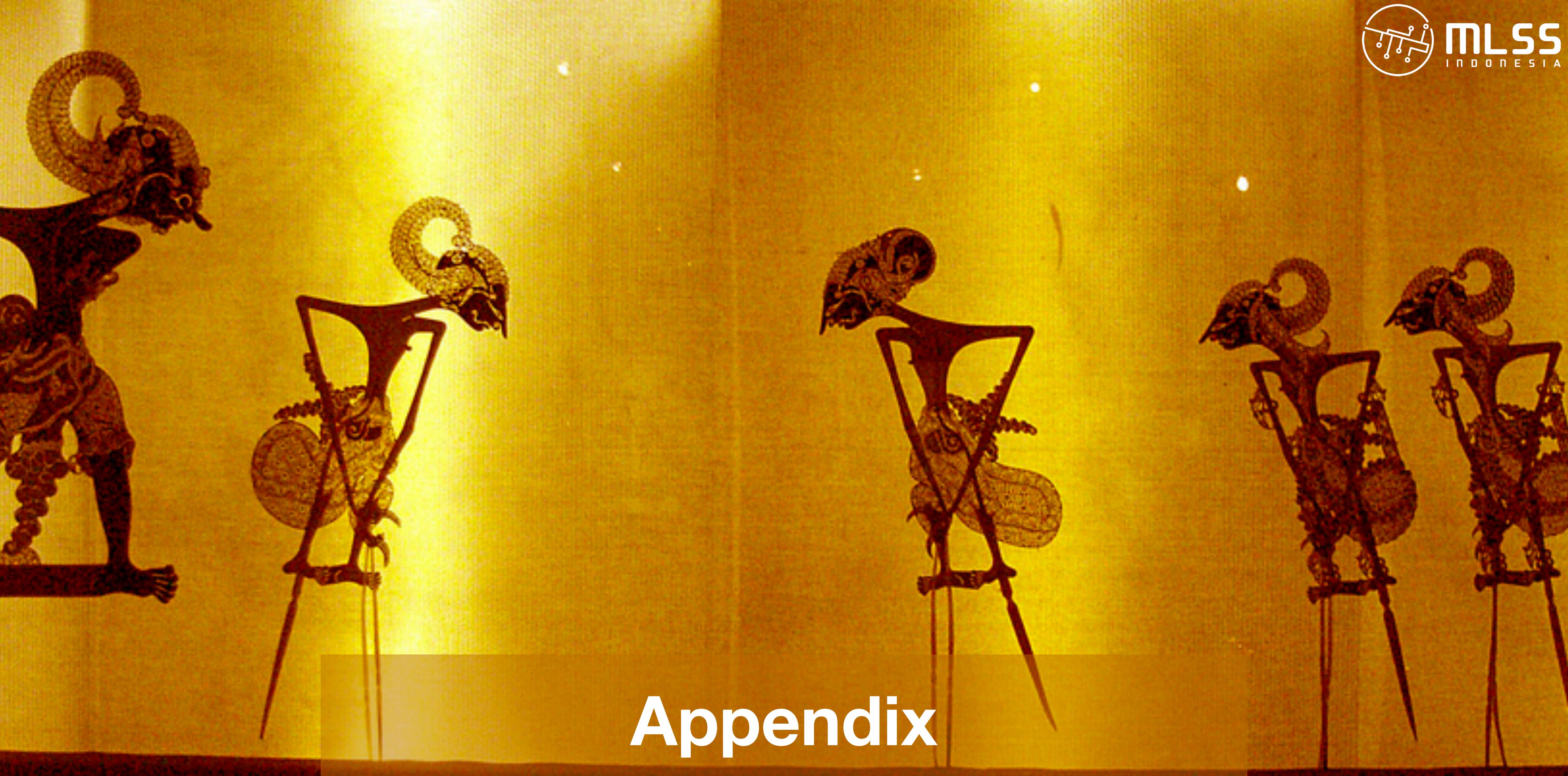
Affine Self Convolution - Diaconu & Worrall, (2019)

Attentive Group Equivariant Convolution Networks - Romero et al., (2020)

SE(3)-Transformers: 3D Roto-Translation Equivariant Attention Networks - Fuchs et al. (2020)

Reinforcement Learning

MDP Homomorphic Networks: Group Symmetries in Reinforcement Learning - van der Pol et al. (2020)



Appendix

Wayang Kulit Show

Group Equivariance Proof

$$[\mathcal{T}_z[F] * W](x) = \sum_{y \in \mathcal{Y}} \mathcal{T}_z[F](y) W(\mathcal{T}_x^{-1}[y])$$

Write out convolution in full

$$= \sum_{y \in \mathcal{Y}} F(\mathcal{T}_{z^{-1}}[y]) W(\mathcal{T}_{x^{-1}}[y])$$

Expand transformation operator

$$= \sum_{y' \in \mathcal{Y}} F(y') W(\mathcal{T}_x^{-1}[\mathcal{T}_z[y']])$$

Change of variables
 $y' = \mathcal{T}_{z^{-1}}[y] \iff y = \mathcal{T}_z[y']$

$$= \sum_{y' \in \mathcal{Y}} F(y') W(\mathcal{T}_{x^{-1}z}[y'])$$

Rewriting: use the hints

$$= \sum_{y' \in \mathcal{Y}} F(y') W(\mathcal{T}_{z^{-1}x}^{-1}[y']) = [F * W](z^{-1}x) = \mathcal{T}_z[F * W](x)$$

It's a convolution!

Hints

Homomorphism property

$$\mathcal{T}_{z^{-1}}[y] = \mathcal{T}_z^{-1}[y]$$

Inversion

$$(xy)^{-1} = y^{-1}x^{-1}$$

Composition

$$\mathcal{T}_x \mathcal{T}_y = \mathcal{T}_{xy}$$

Semigroup Equivariance Proof

$$[\mathcal{T}_z[F] \star W](x) = \sum_{y \in \mathcal{Y}} \mathcal{T}_x[\mathcal{T}_z[F]](y) W(y)$$

Write out convolution in full

$$= \sum_{y \in \mathcal{Y}} \mathcal{T}_{xz}[F](y) W(y)$$

Semigroup composition

$$= [F \star W](xz) = \mathcal{T}_z[F \star W](x)$$

Define this as left action on activations

It's a convolution!