UNIVERSITY OF AMSTERDAM

Group Equivariant Deep Learning

Lecture 1 - Regular group convolutions

Lecture 1.7 - Group convolutions are all you need!

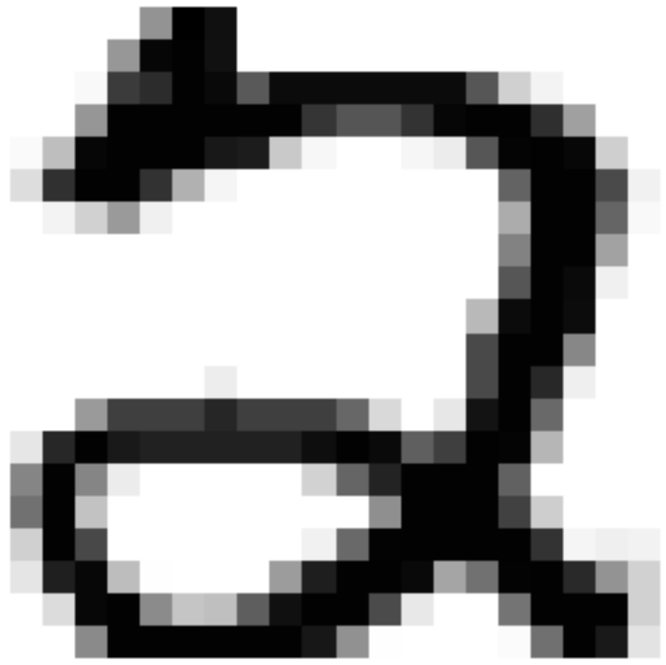
Equivariant linear layers between feature maps are group convolutions

Erik Bekkers, Amsterdam Machine Learning Lab, University of Amsterdam

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

Classical artificial neural networks

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



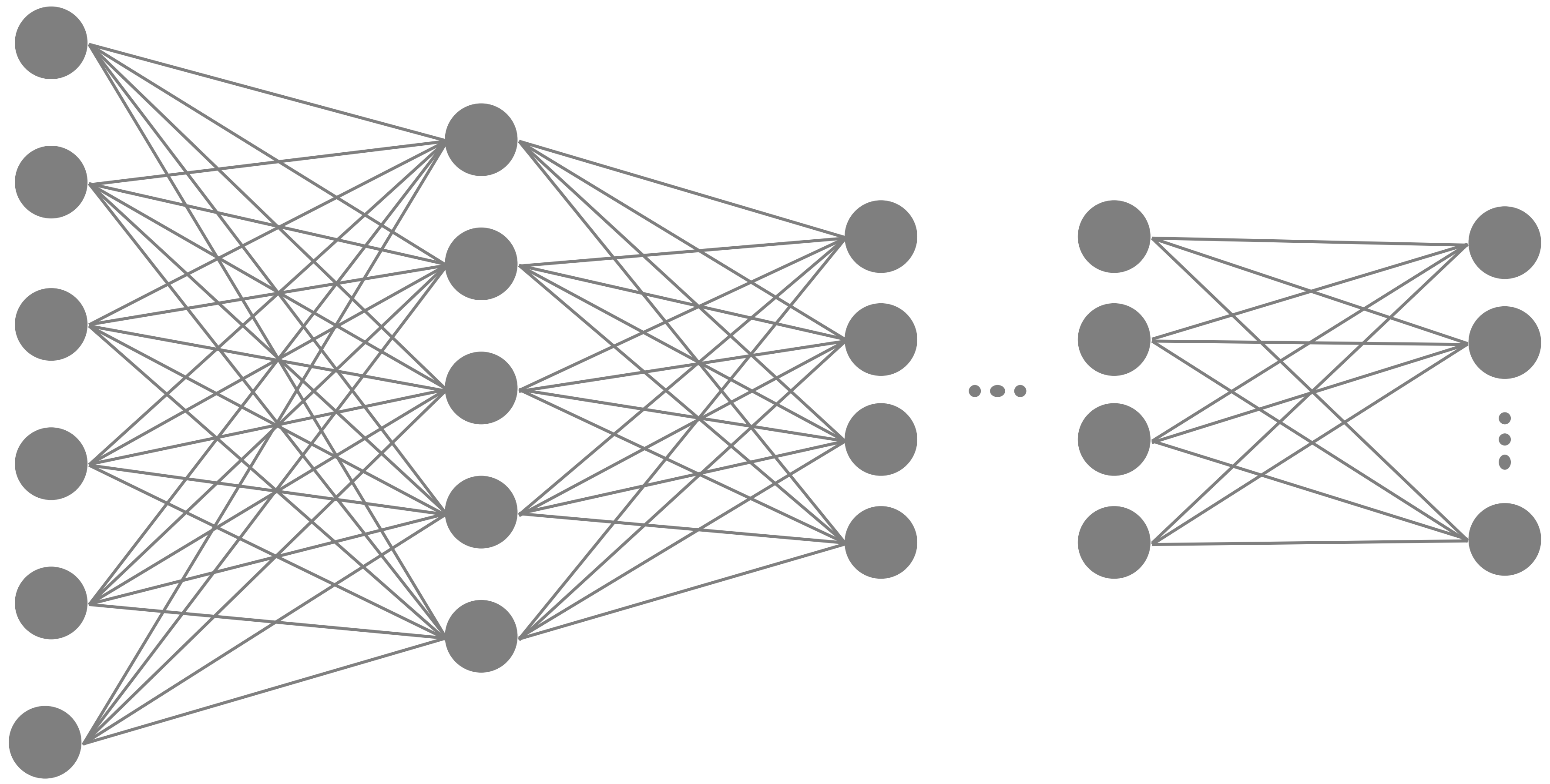


Image analyst: $\underline{x}^0 \in \mathcal{X} = \mathbb{L}_2(\mathbb{R}^2)$

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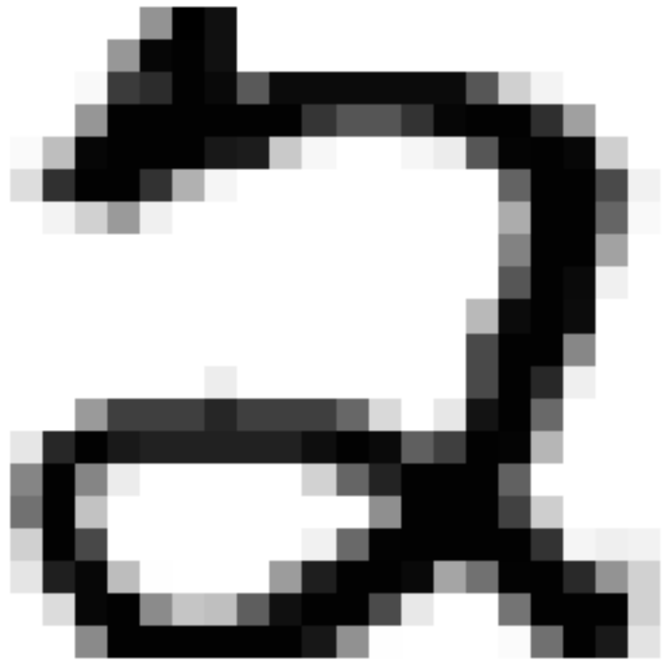
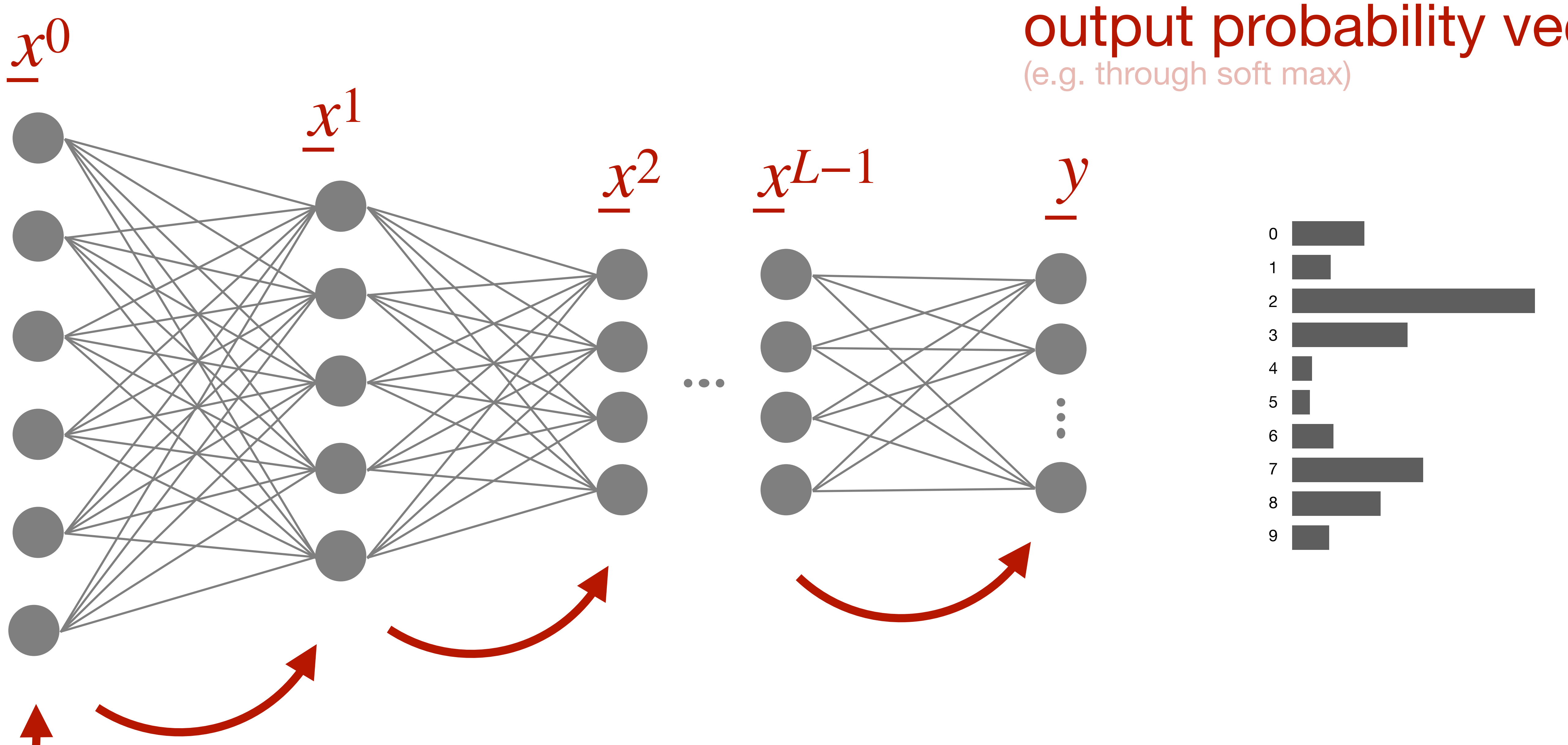


input vector

output probability vector

(e.g. through soft max)



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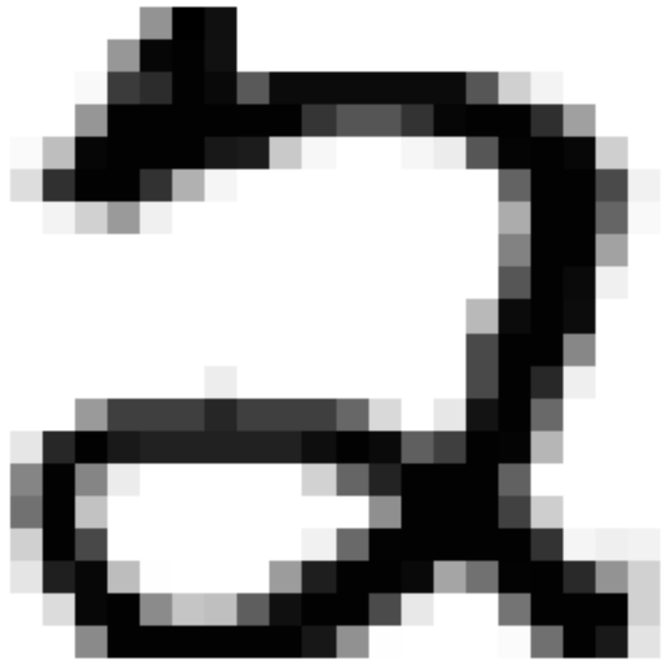

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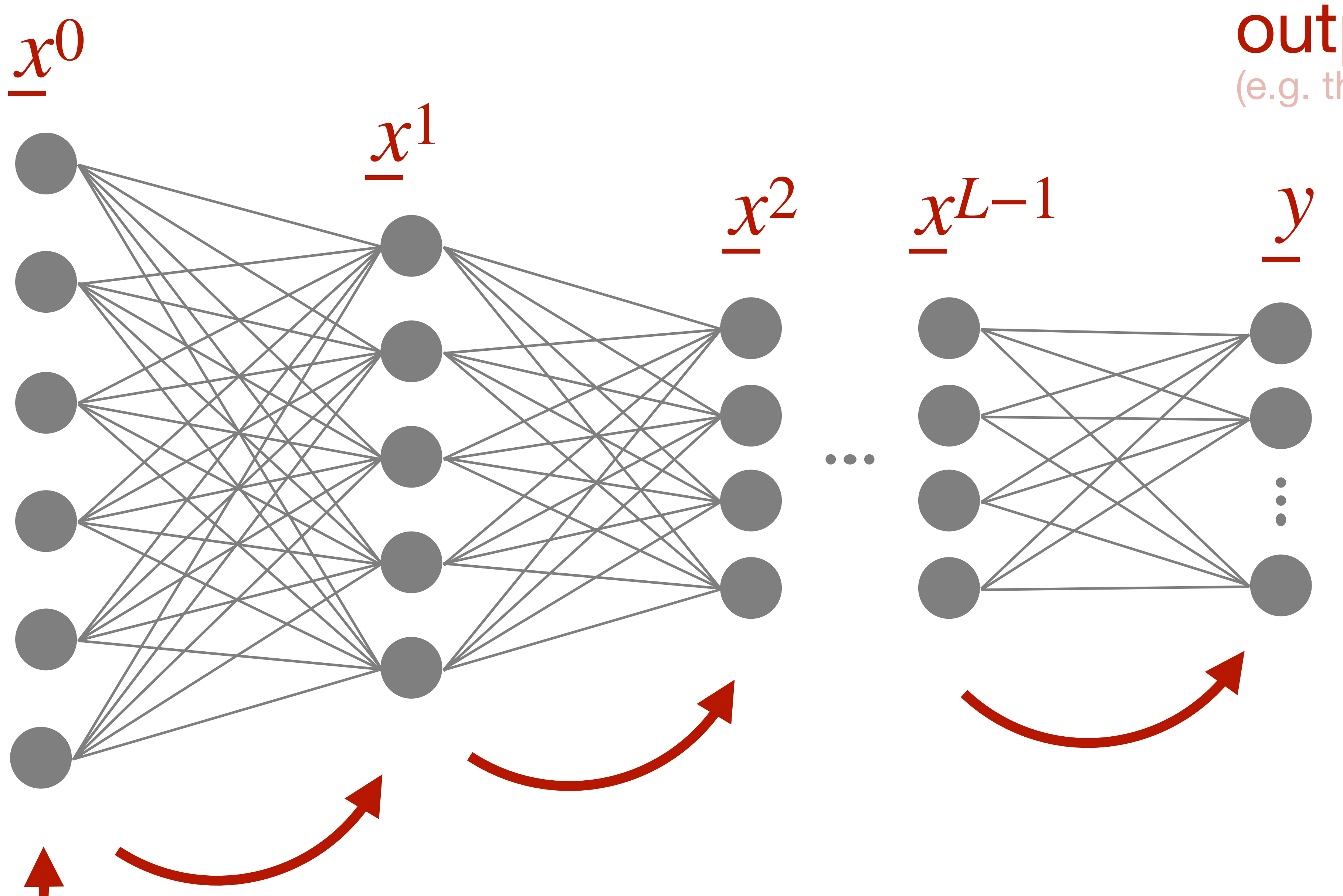

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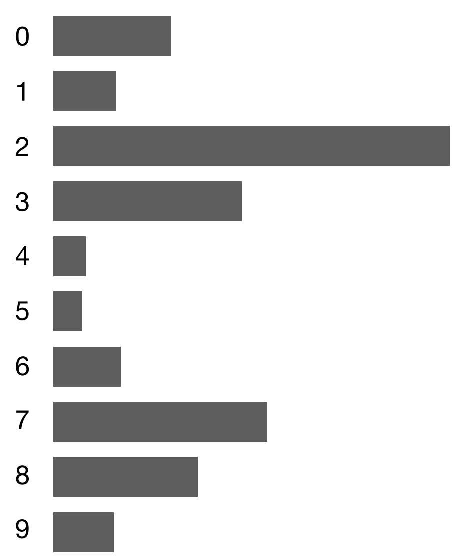

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Iteratively transform the vector via

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

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

A fully connect layer as convolution on 1D signal

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

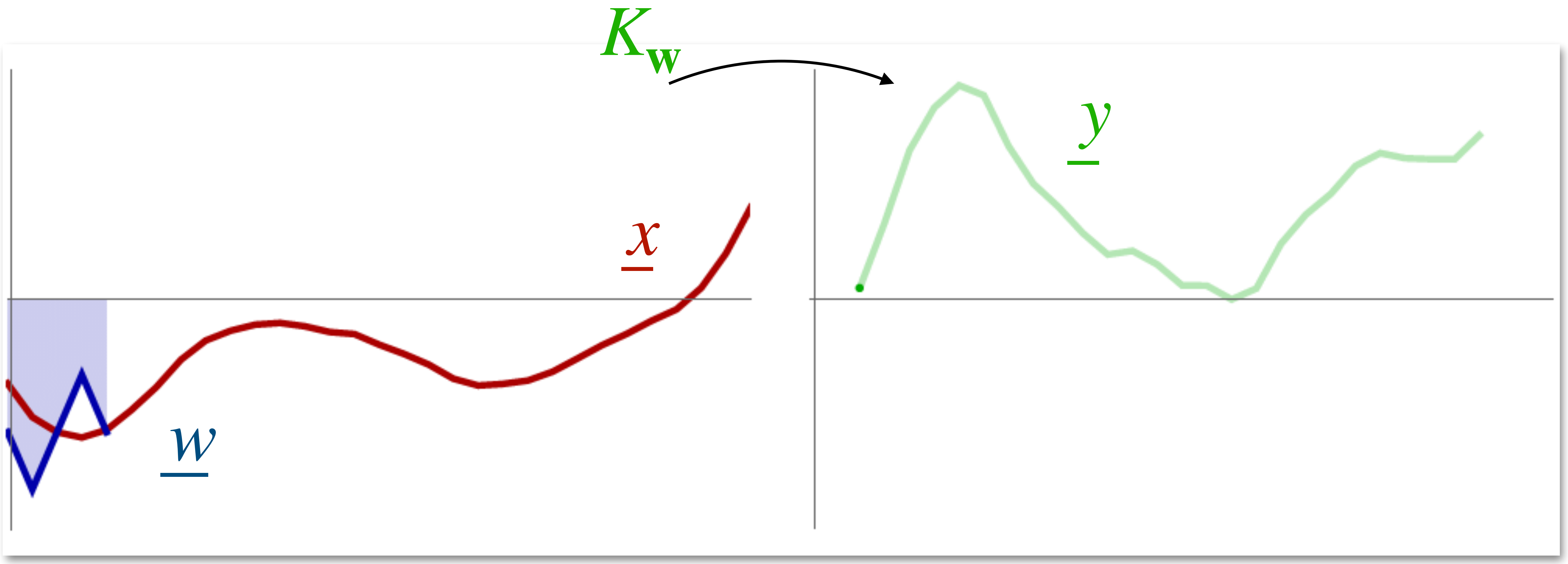
$$\underline{y} = \varphi(\quad K_{\mathbf{w}} \quad \underline{x} + \underline{b} \quad)$$

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

A fully connected layer as convolution on 1D signal

Convolution as linear operator

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



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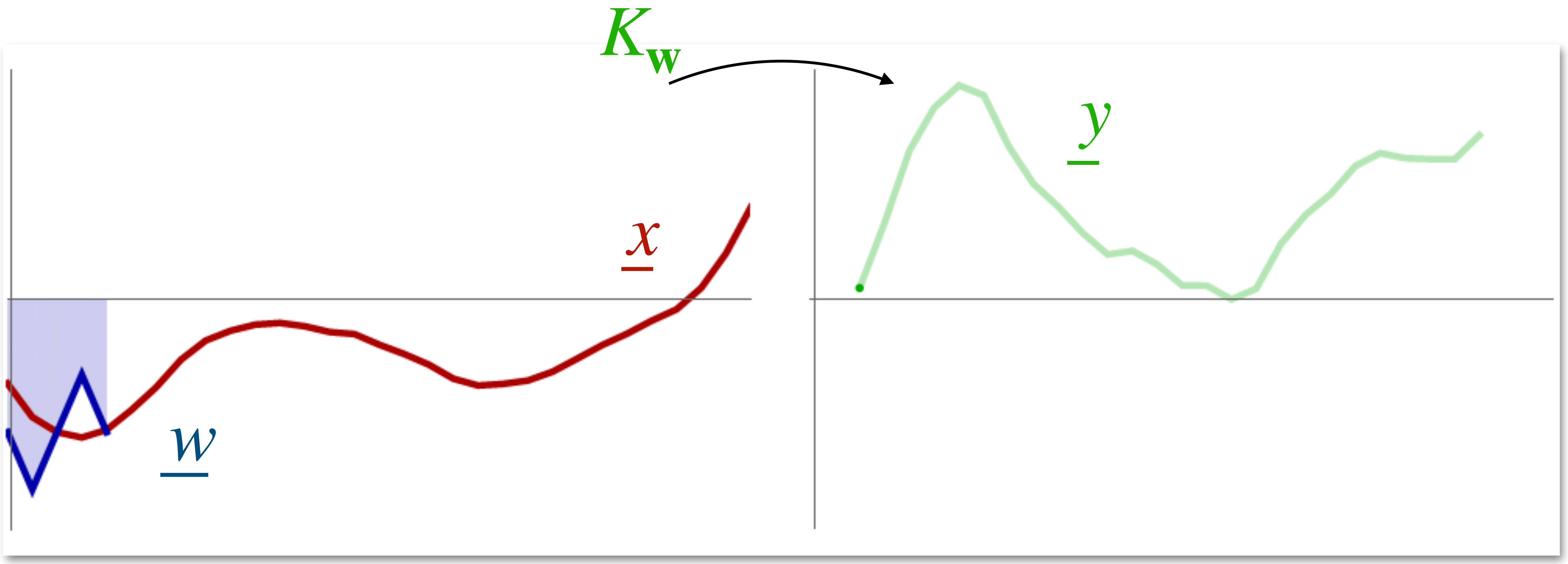

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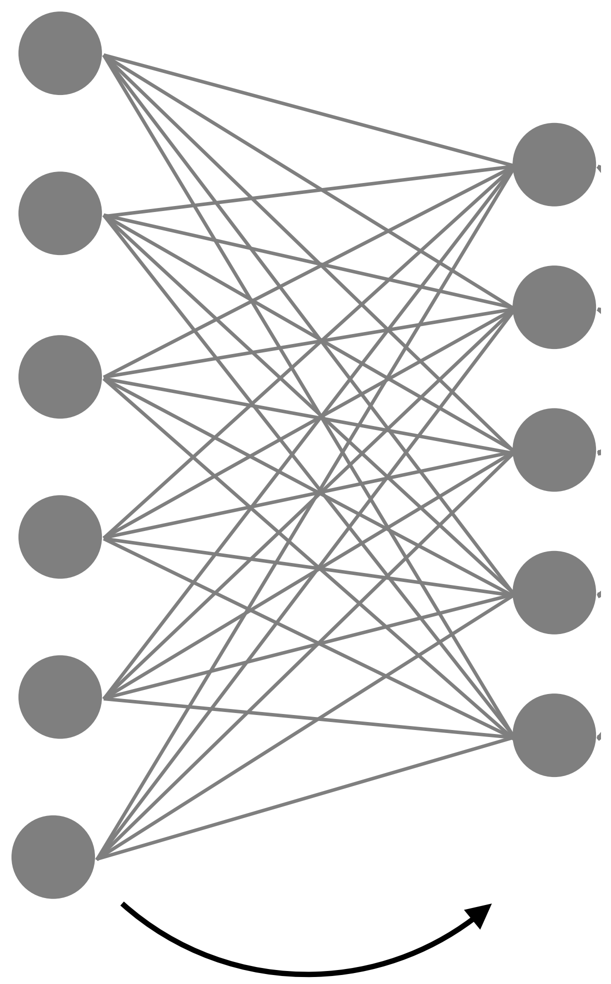
Classical artificial NNs in the continuous world

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



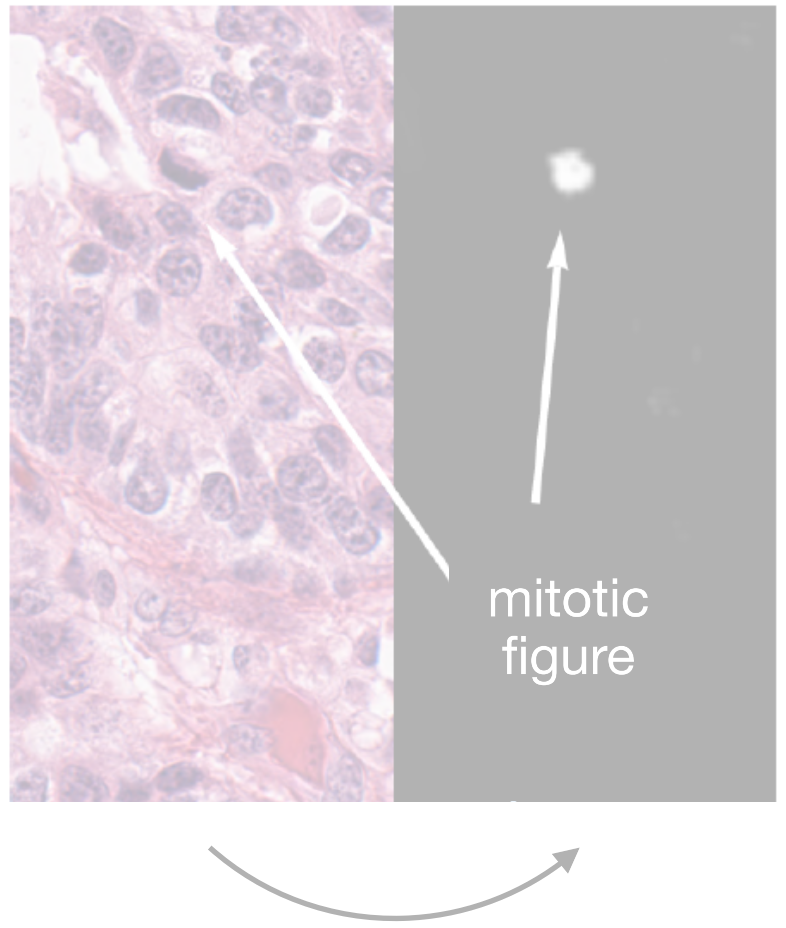
Iteratively transform the **vector** in $\mathbb{R}^{N^x}$ via

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

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

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

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



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

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

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

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

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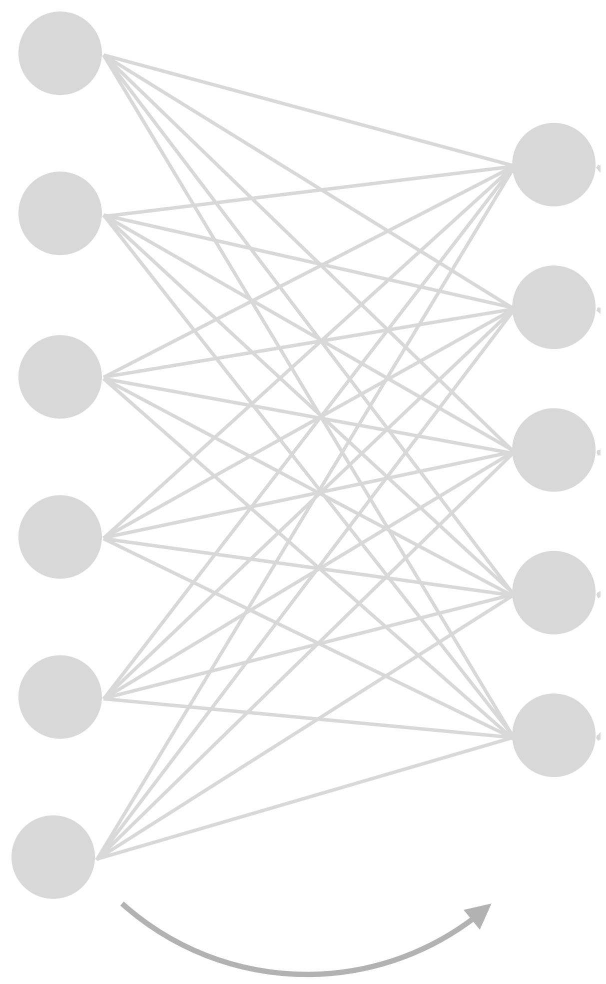

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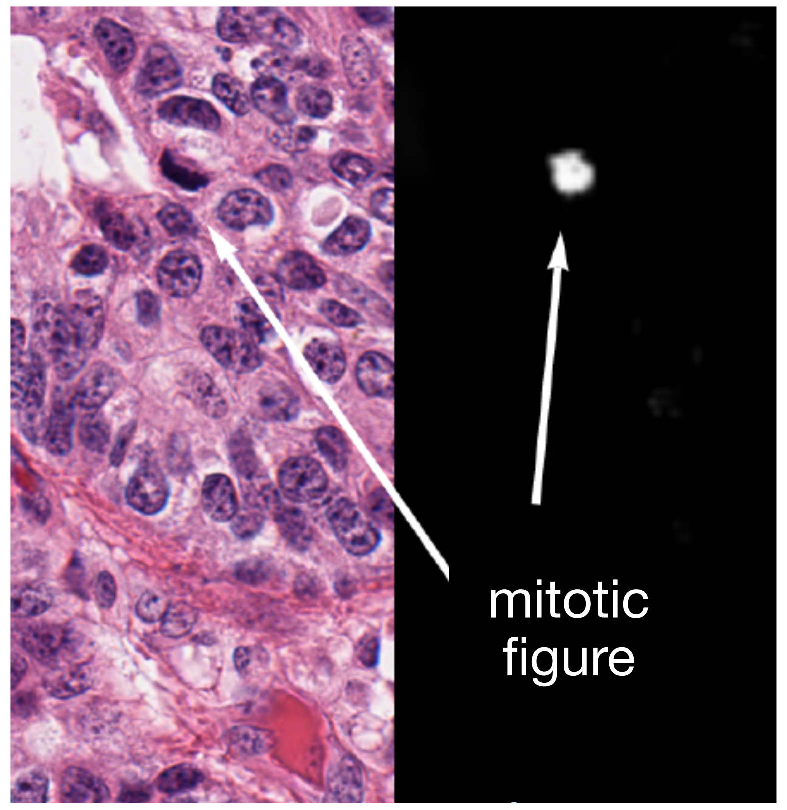

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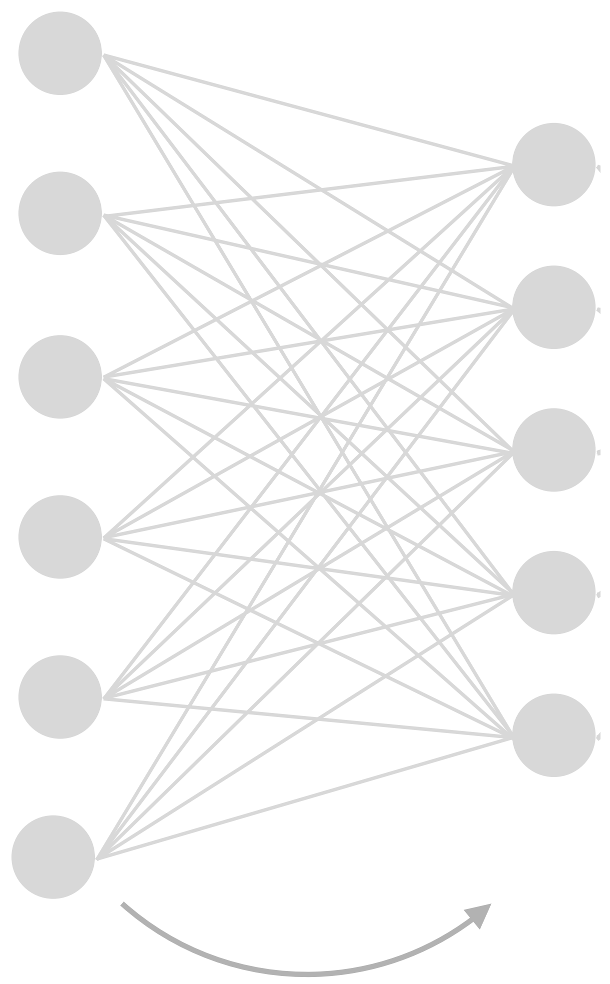

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We want K to be equivariant!

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

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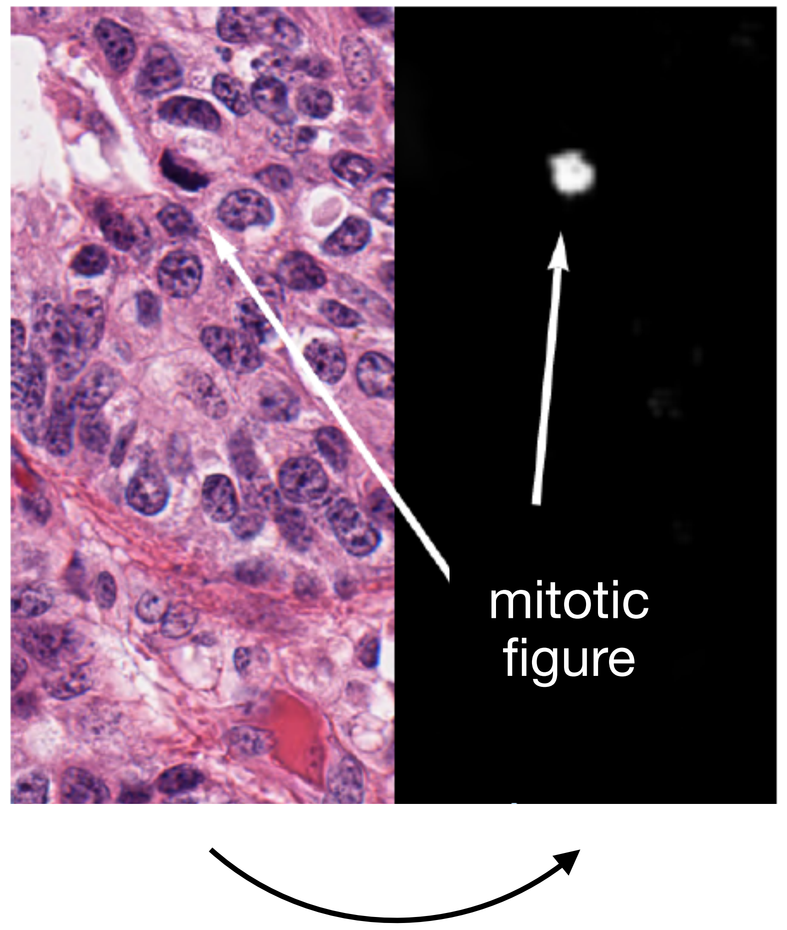

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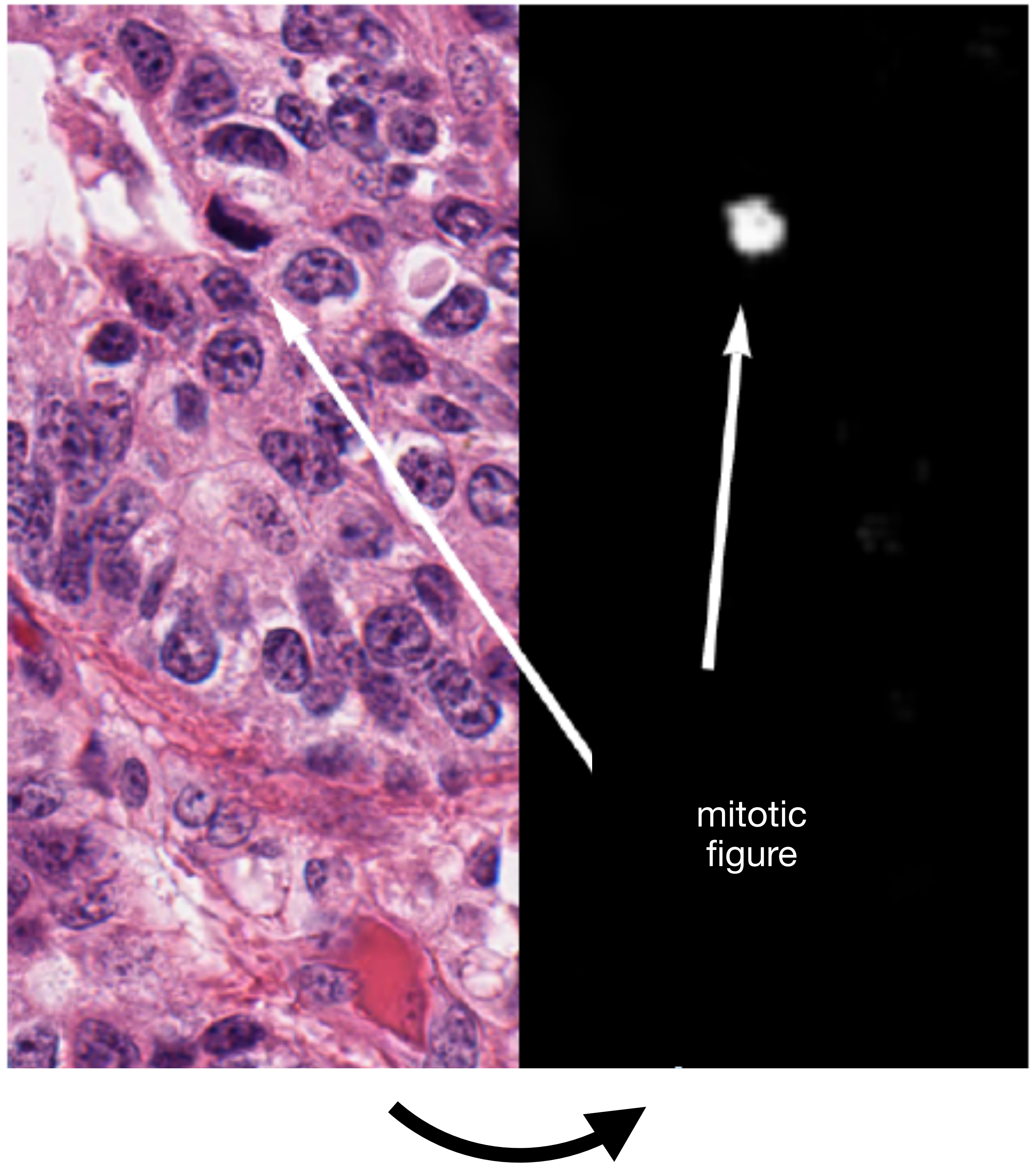
Neural Networks for Signal Data



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

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

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

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

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

Theorem (G-convs are all you need)

Bekkers ICLR 2020, Thm. 1*

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

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

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

1. It is a group convolution: $[\mathscr{K} f](y) = \int_X \frac{1}{|g_y|} k(g_y^{-1} x) f(x) \mathrm{d}x$
2. The kernel satisfies a symmetry constraint: $\forall_{h \in H}: \frac{1}{|g_y|} k(hx) = k(x)$

*Work with Remco Duits at TU/e.

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

Proof (G-convs are all you need)

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

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

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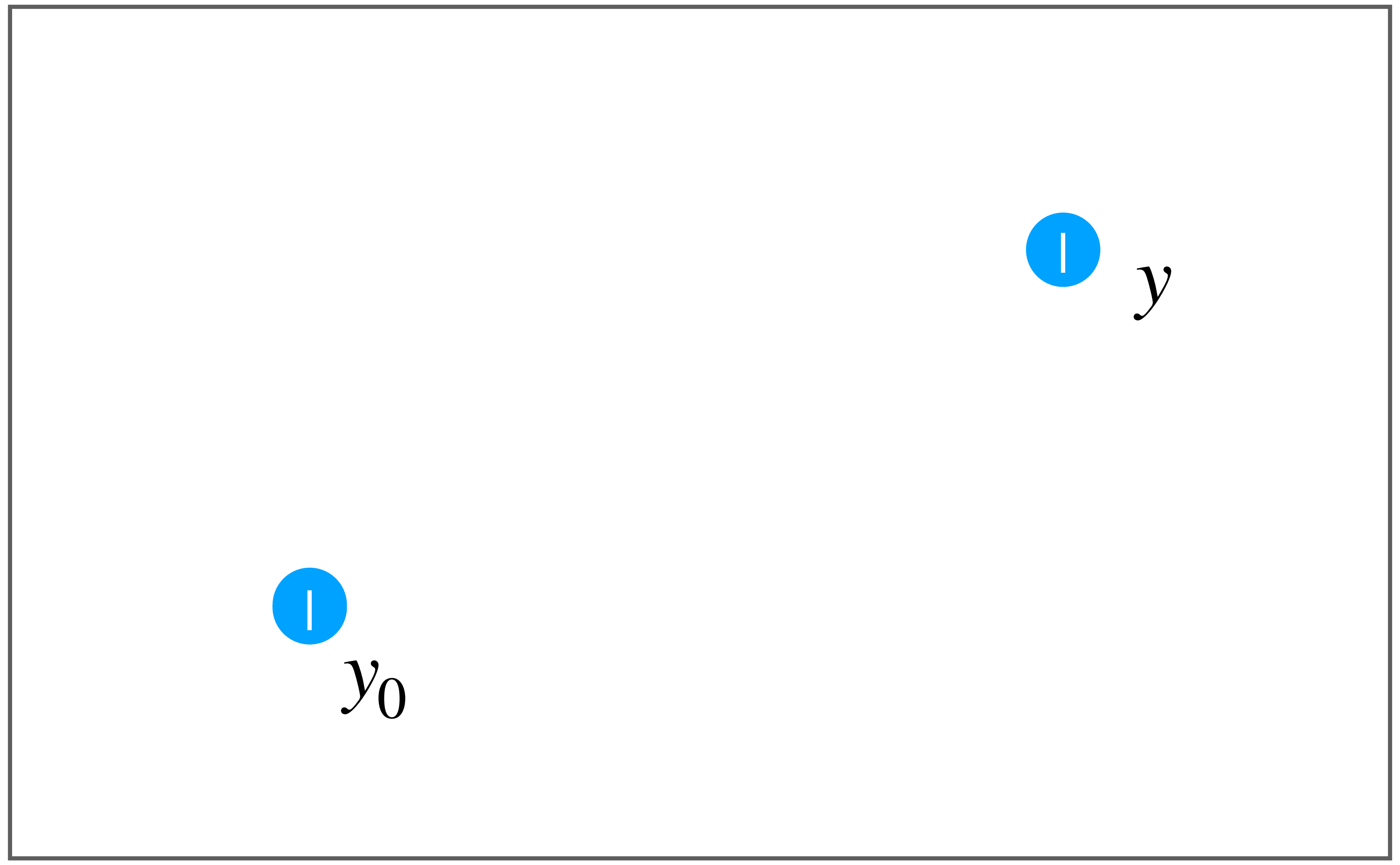
Since this should hold or all $f \in \mathbb{L}_2(X)$ we have $\forall_{g \in G}$: $\tilde{k}(y, x) = \frac{1}{|\det g|} \tilde{k}(g^{-1}y, g^{-1}x)$

Proof (G-convs are all you need)

Since G acts transitively on Y we have that $\forall_{y,y_0 \in Y} \exists_{g_y \in G}$ such that $y = g_y y_0$



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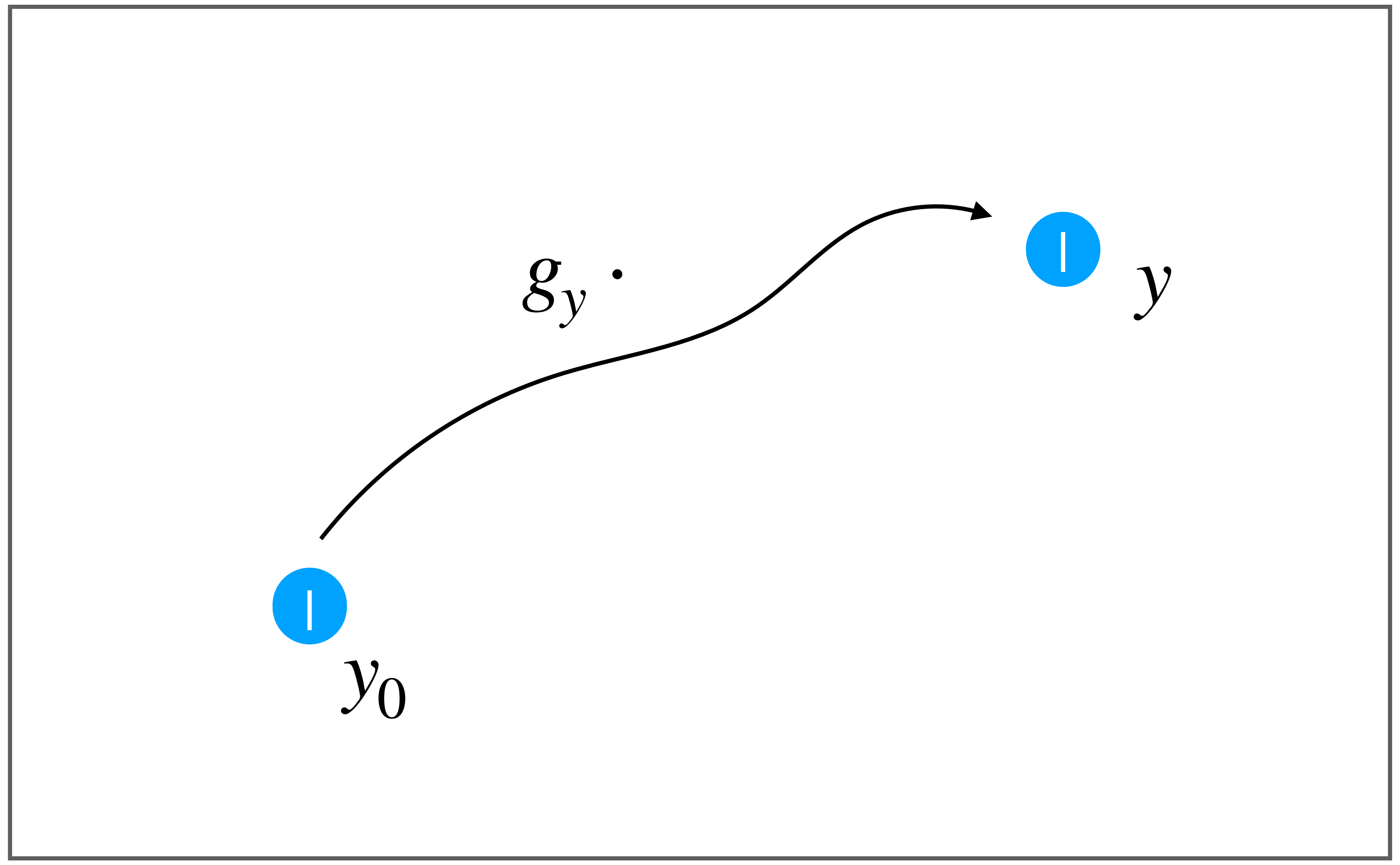

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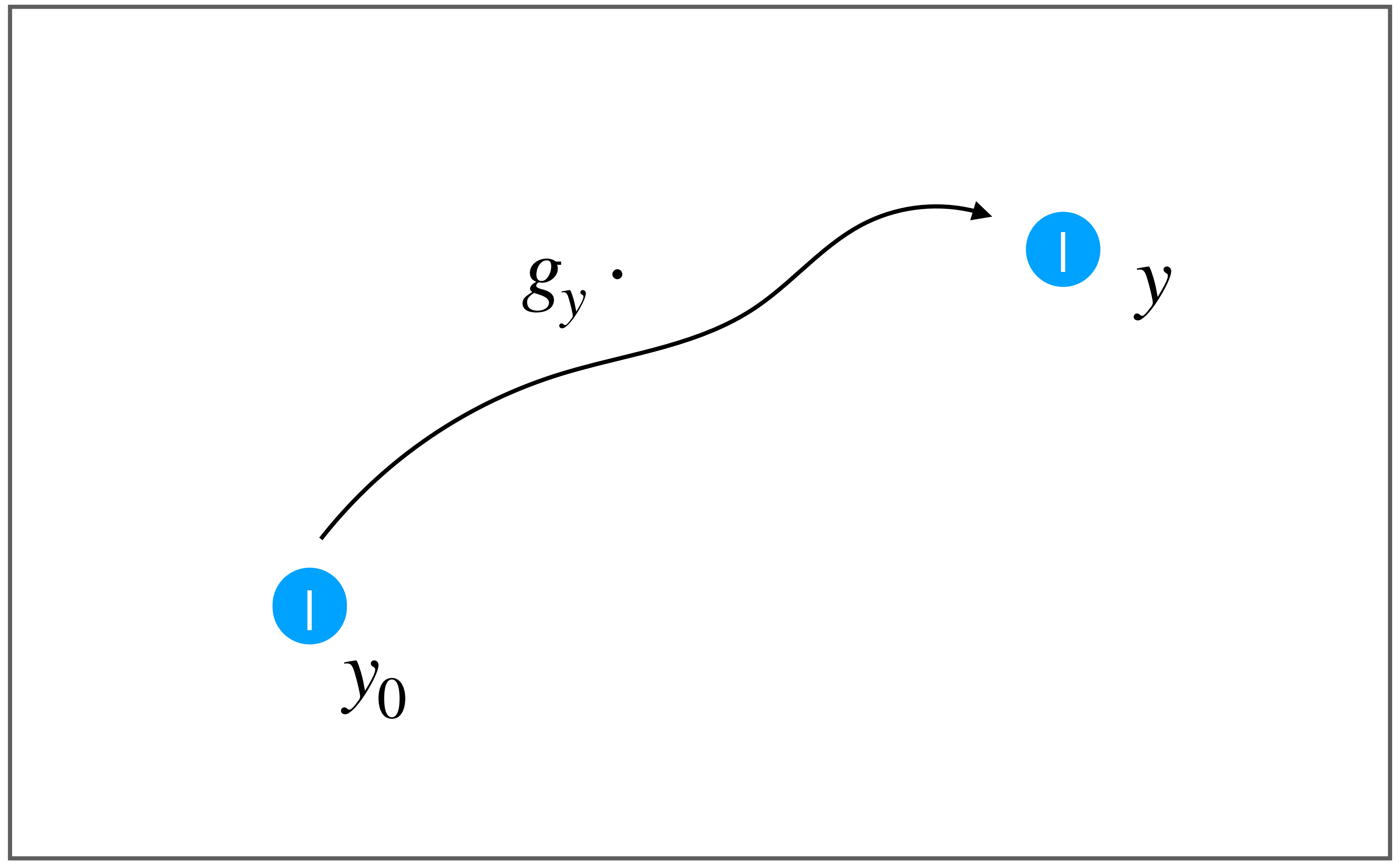

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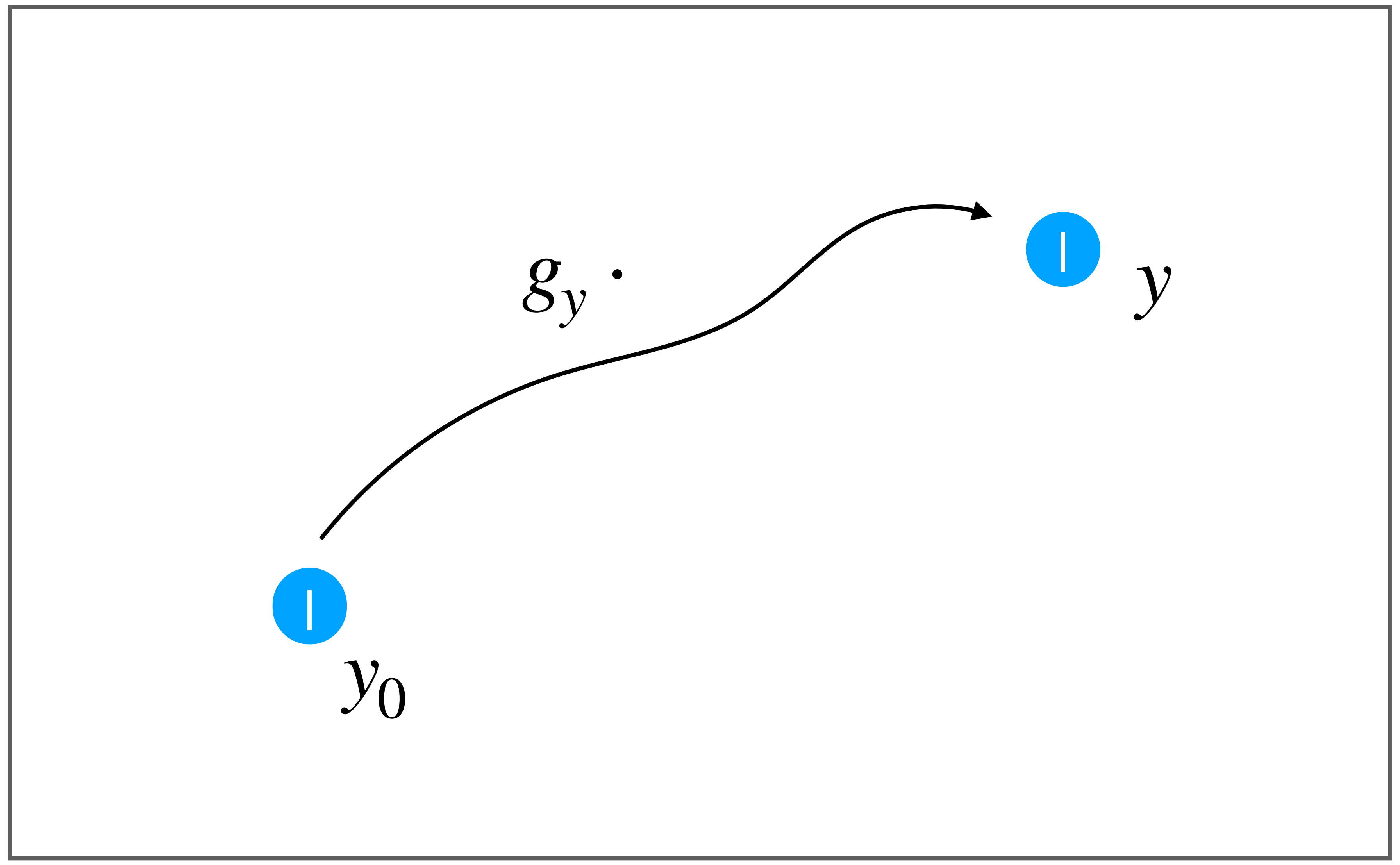

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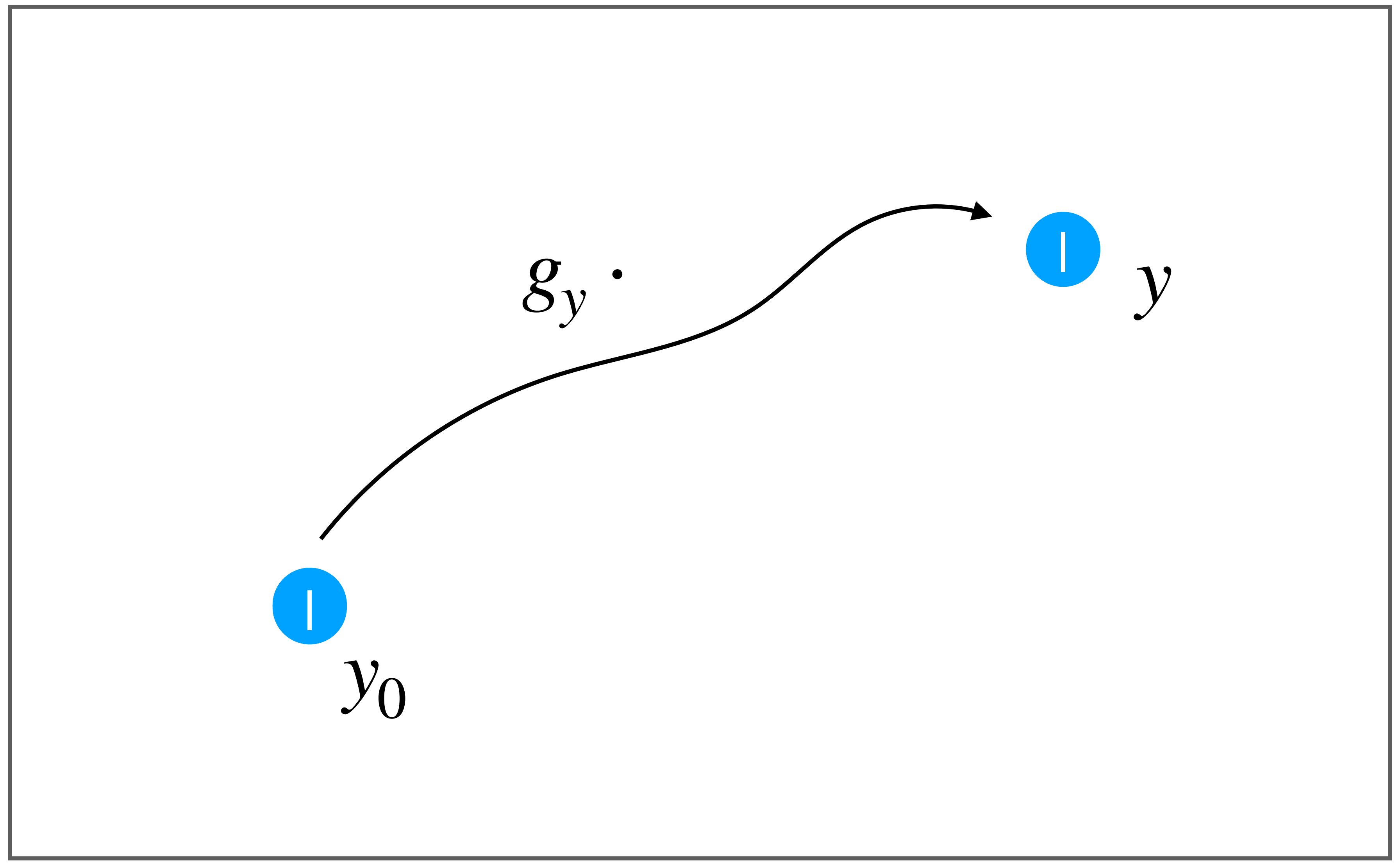

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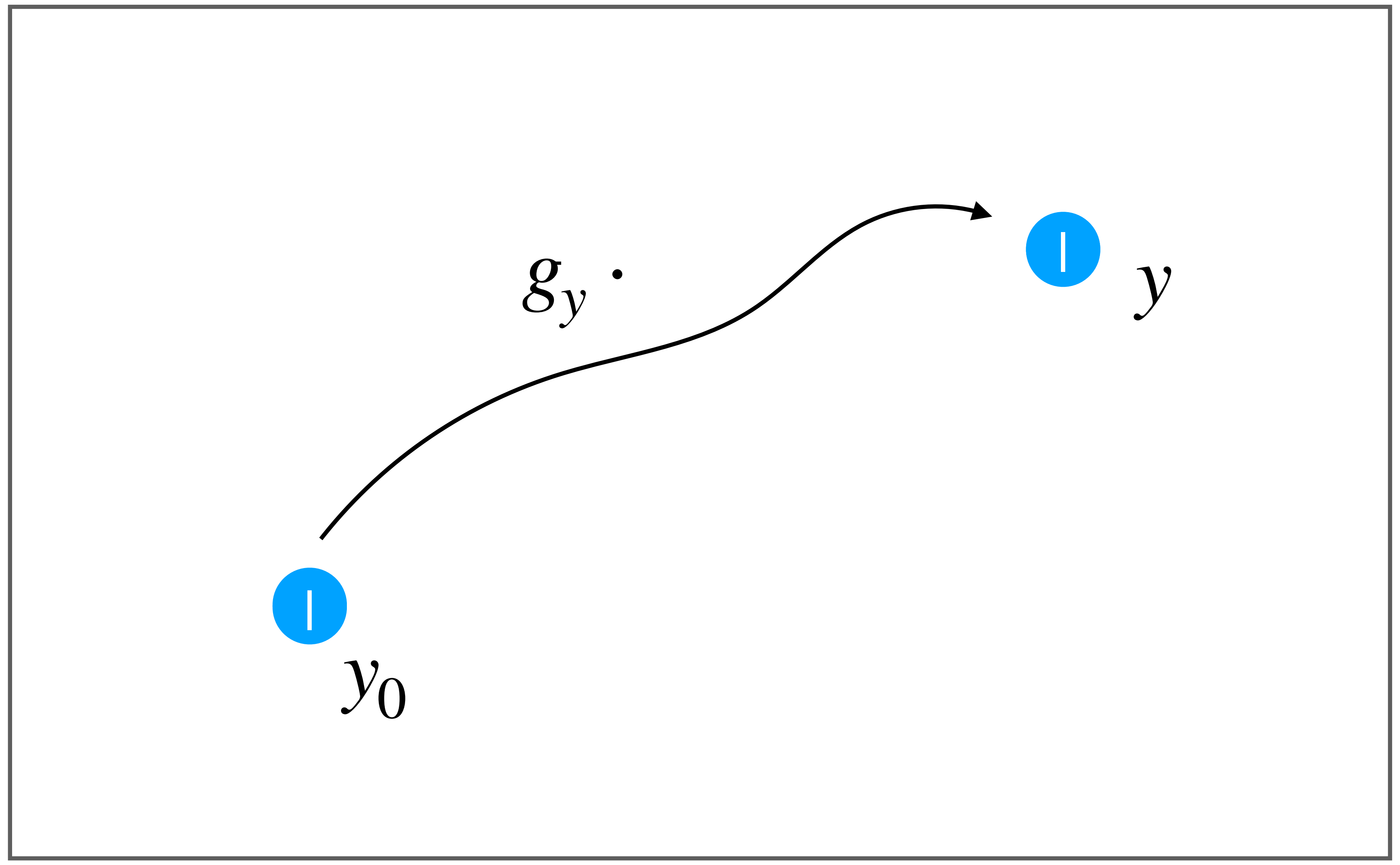

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If $Y \equiv G/H$ then there could be a whole subgroup $H = \mathrm{Stab}_G\, y_0$ that leaves y_0 invariant

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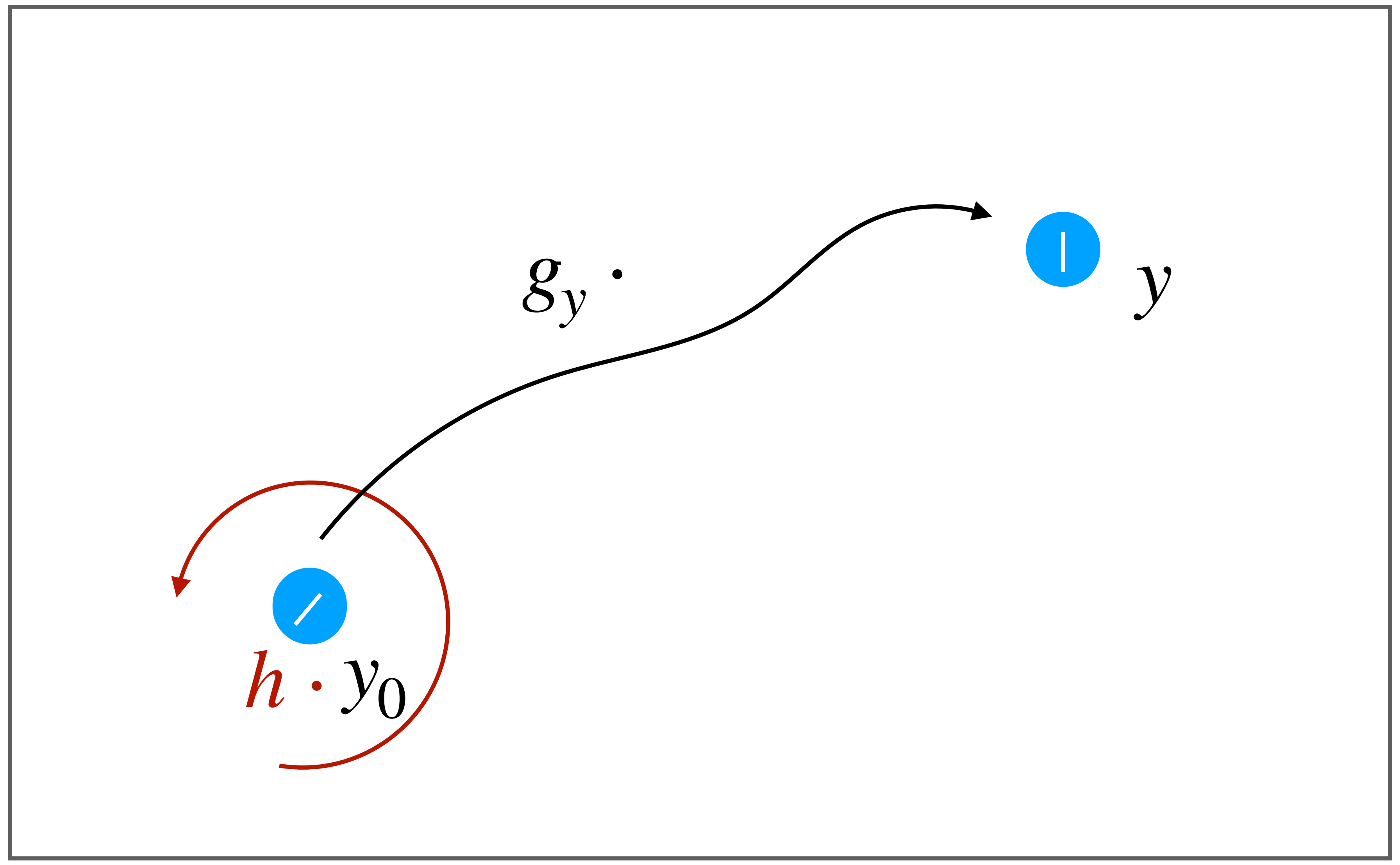

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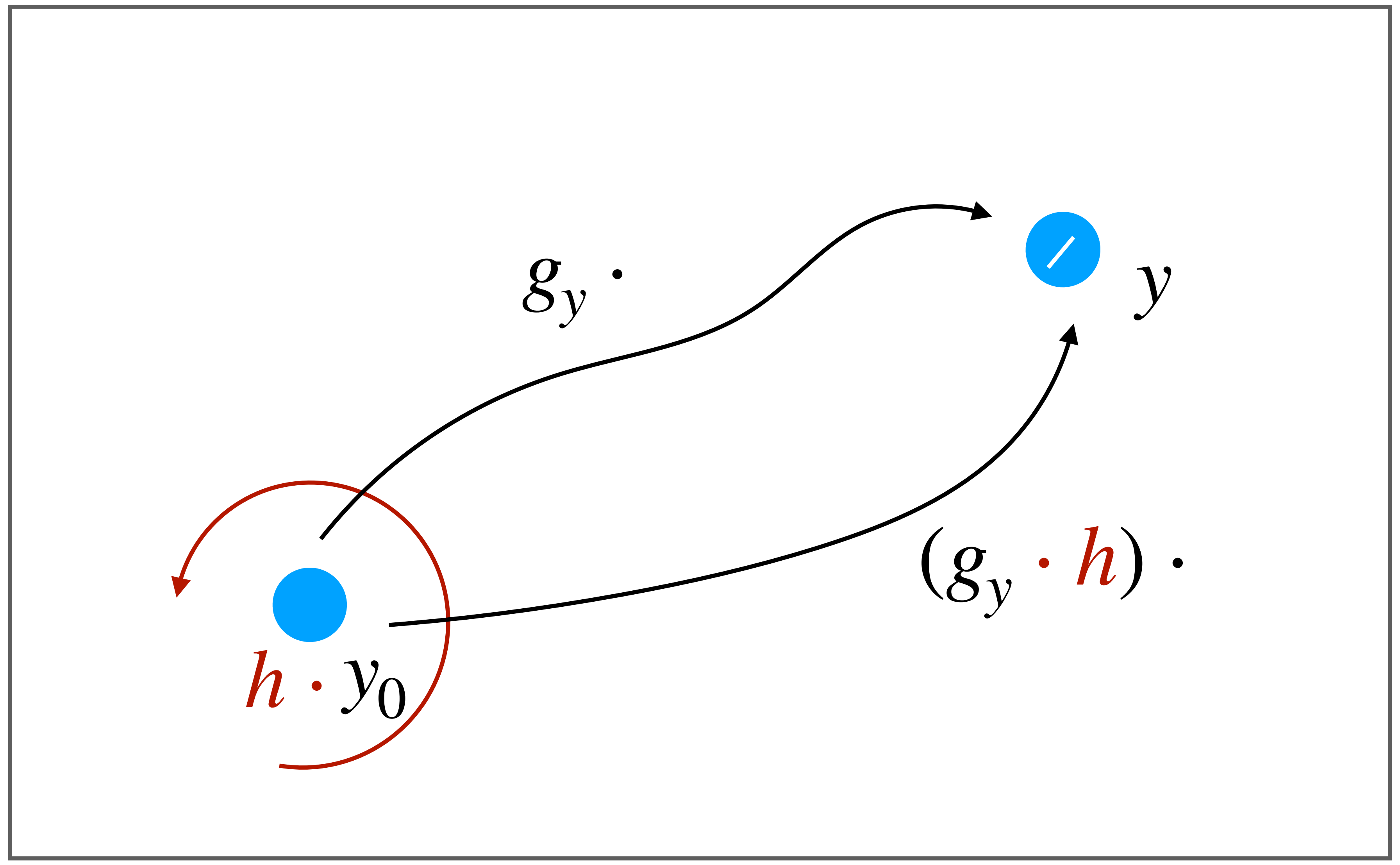

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$\forall_{h \in H}: \quad \tilde{k}(h\, y_0, x) = \tilde{k}(y_0, x)$

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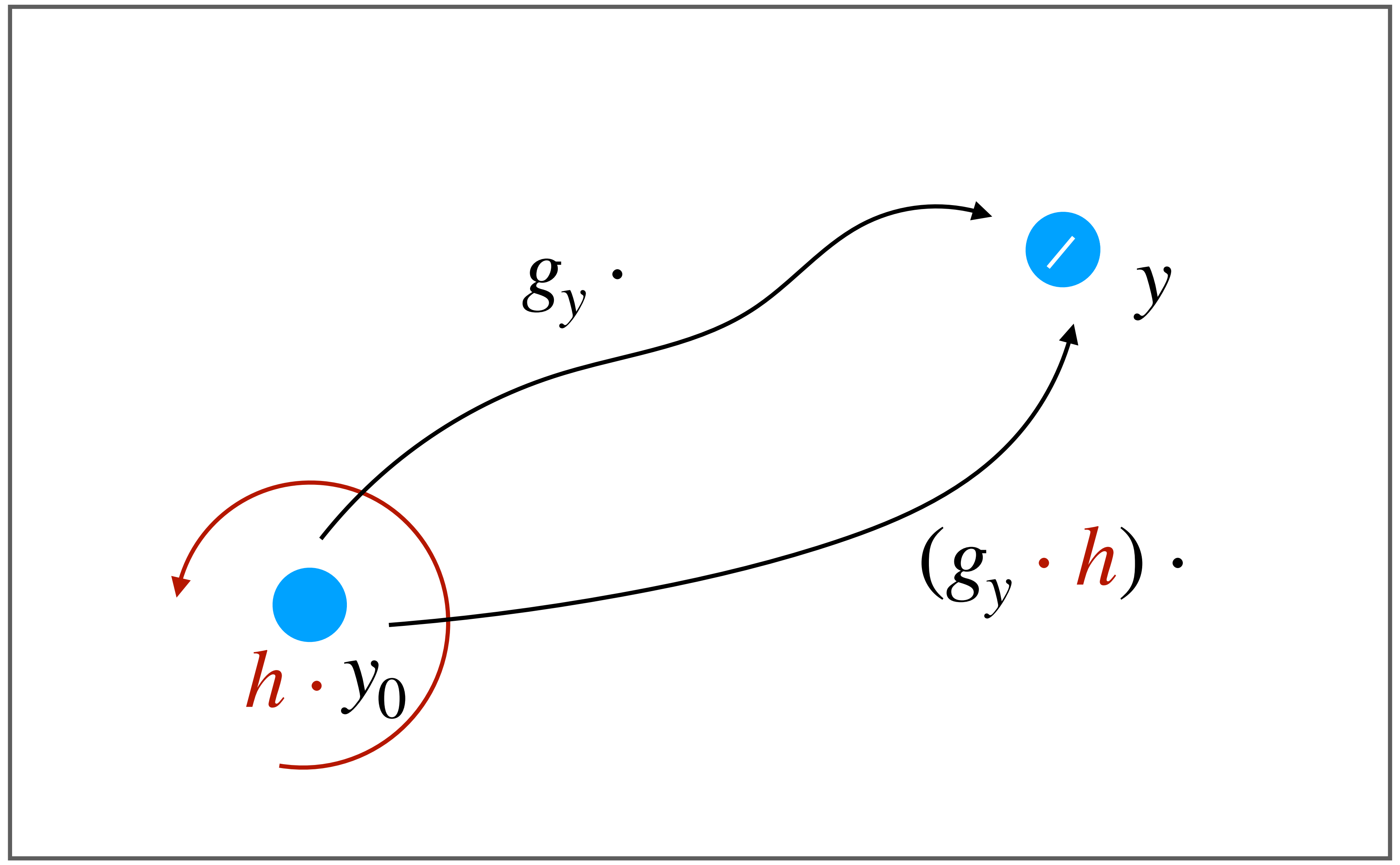

Thus $\tilde{k}(y,x) = \tilde{k}(g_y\, y_0, x)$

(since $\tilde{k}(y,x) = \frac{1}{|\det g|}\tilde{k}(g^{-1}y, g^{-1}x)$)

$$= \frac{1}{|\det g_y|}\tilde{k}(y_0, g_y^{-1}\, x)$$

$$= \frac{1}{|\det g_y|}k(g_y^{-1}\, x)$$

If $Y \equiv G/H$ then there could be a whole subgroup $H = \mathrm{Stab}_G\, y_0$ that leaves y_0 invariant

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

Theorem (G-convs are all you need)

Bekkers ICLR 2020, Thm. 1*

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

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

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

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

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

*Work with Remco Duits at TU/e.

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

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

$(X = Y = G/H)$

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

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

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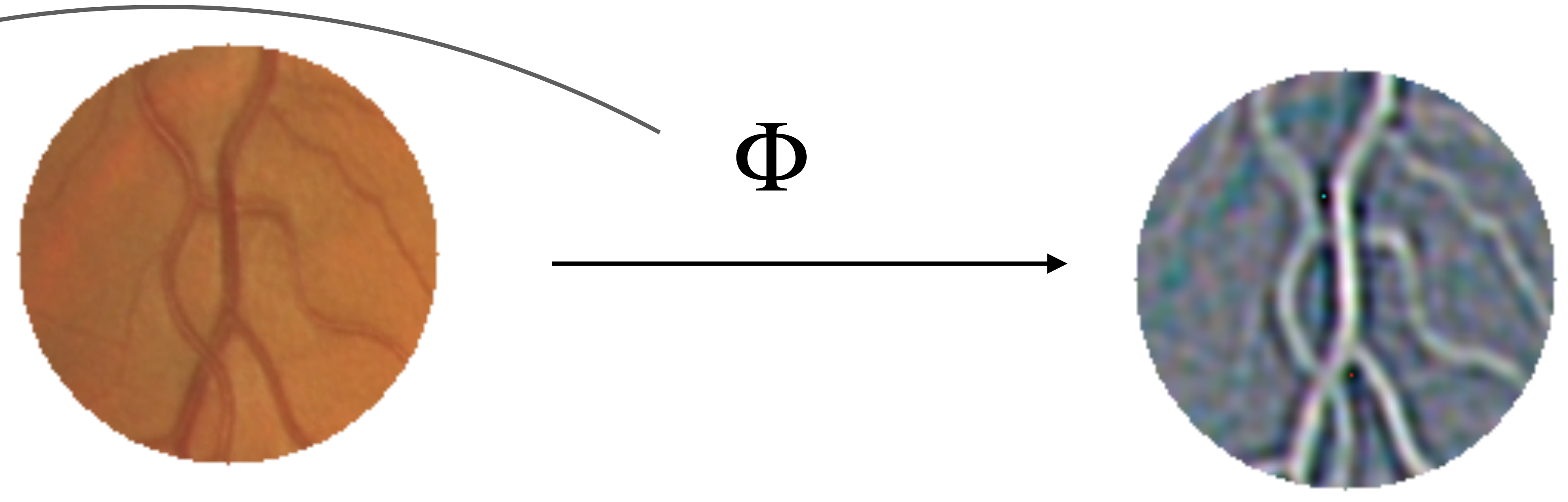
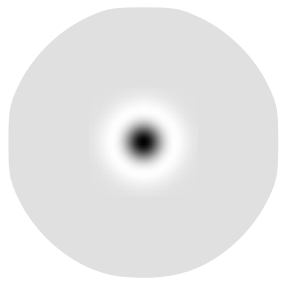


Conv2D(input , )

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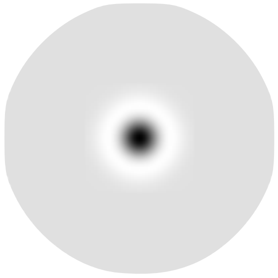
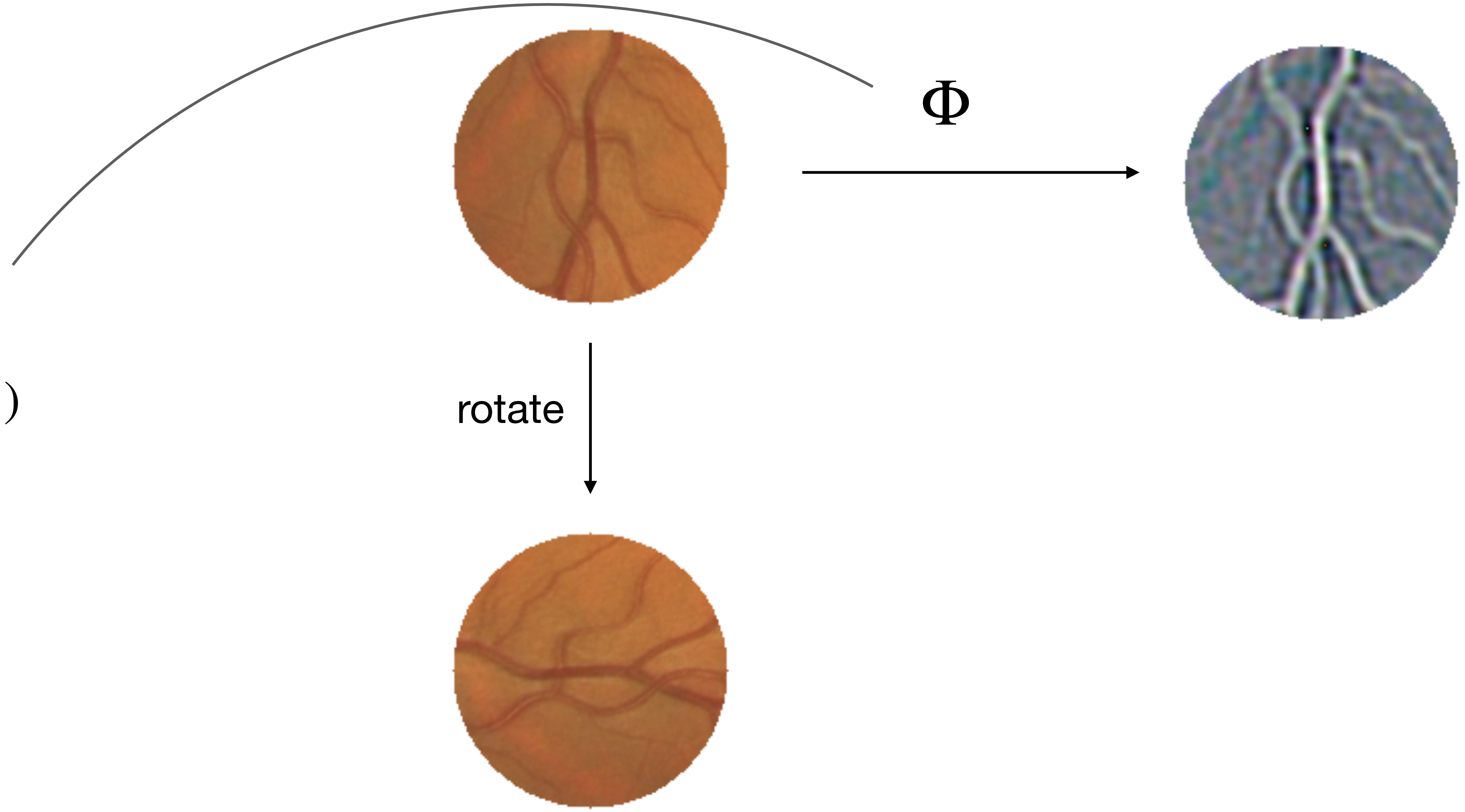
Conv2D(input , )



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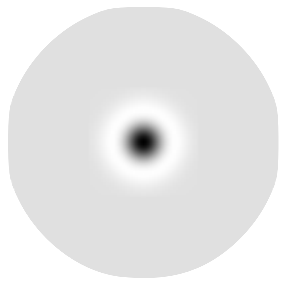
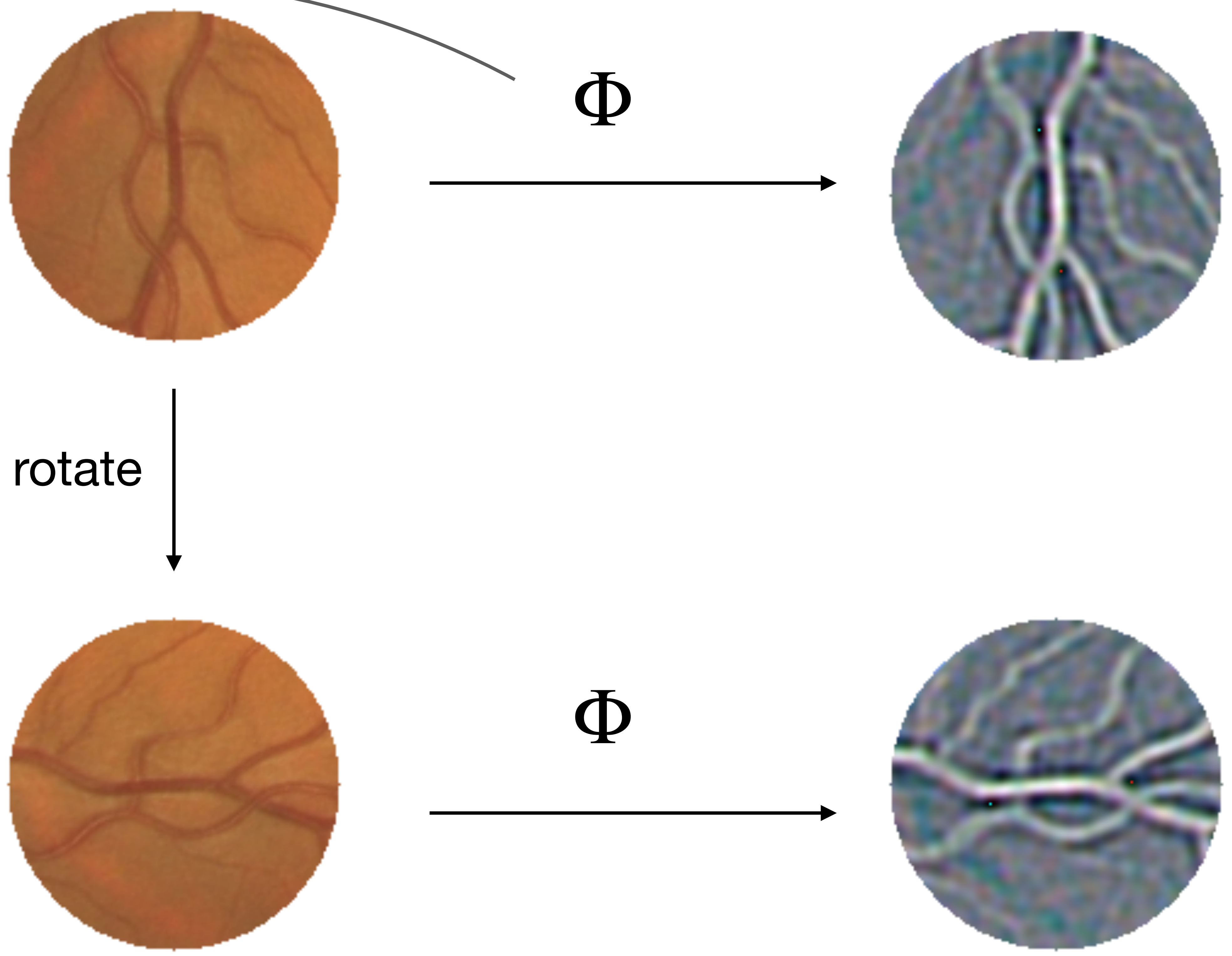
Conv2D(input , )



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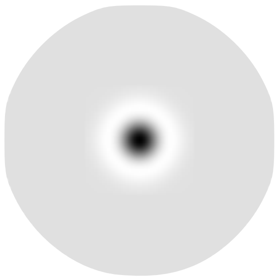
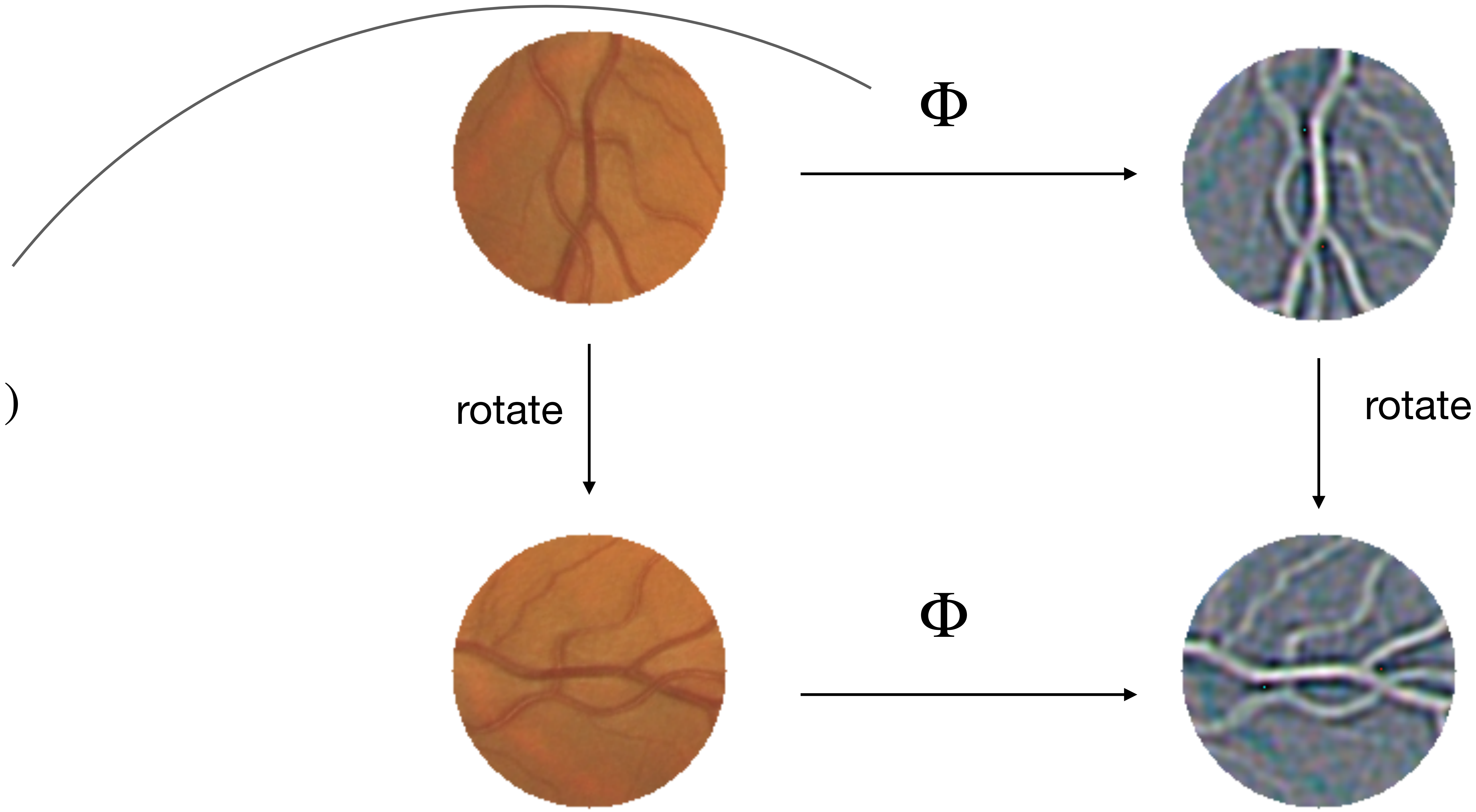
Conv2D(input , )



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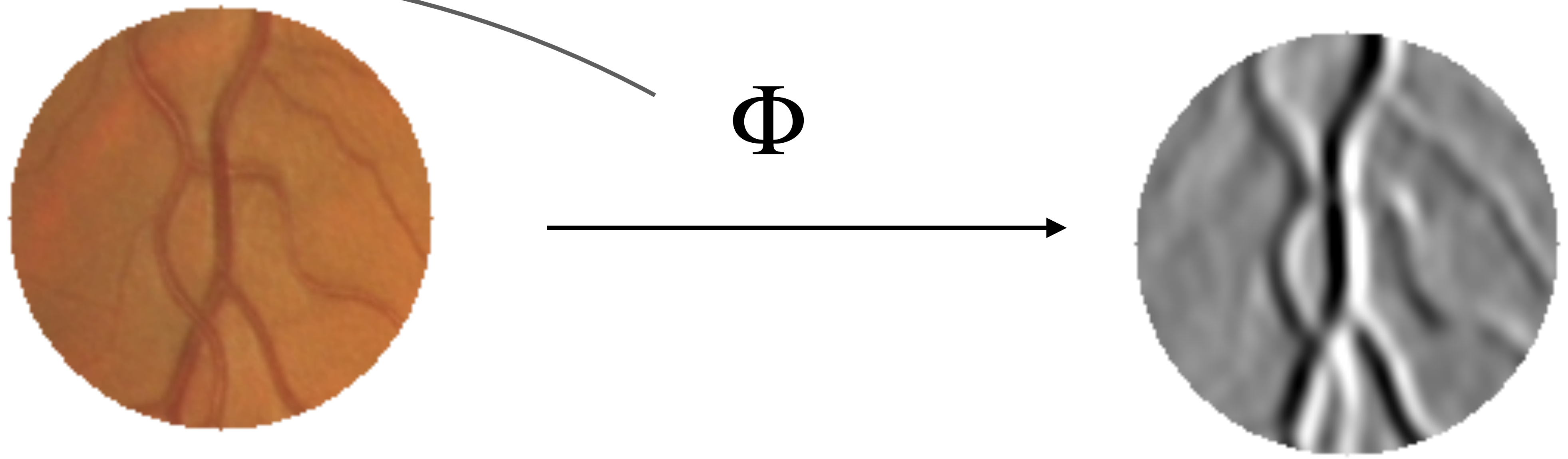
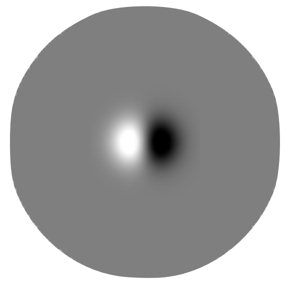


Conv2D(input , )

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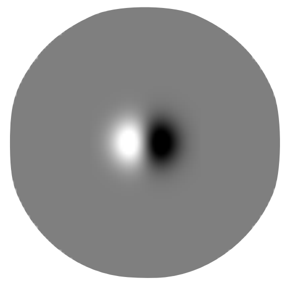
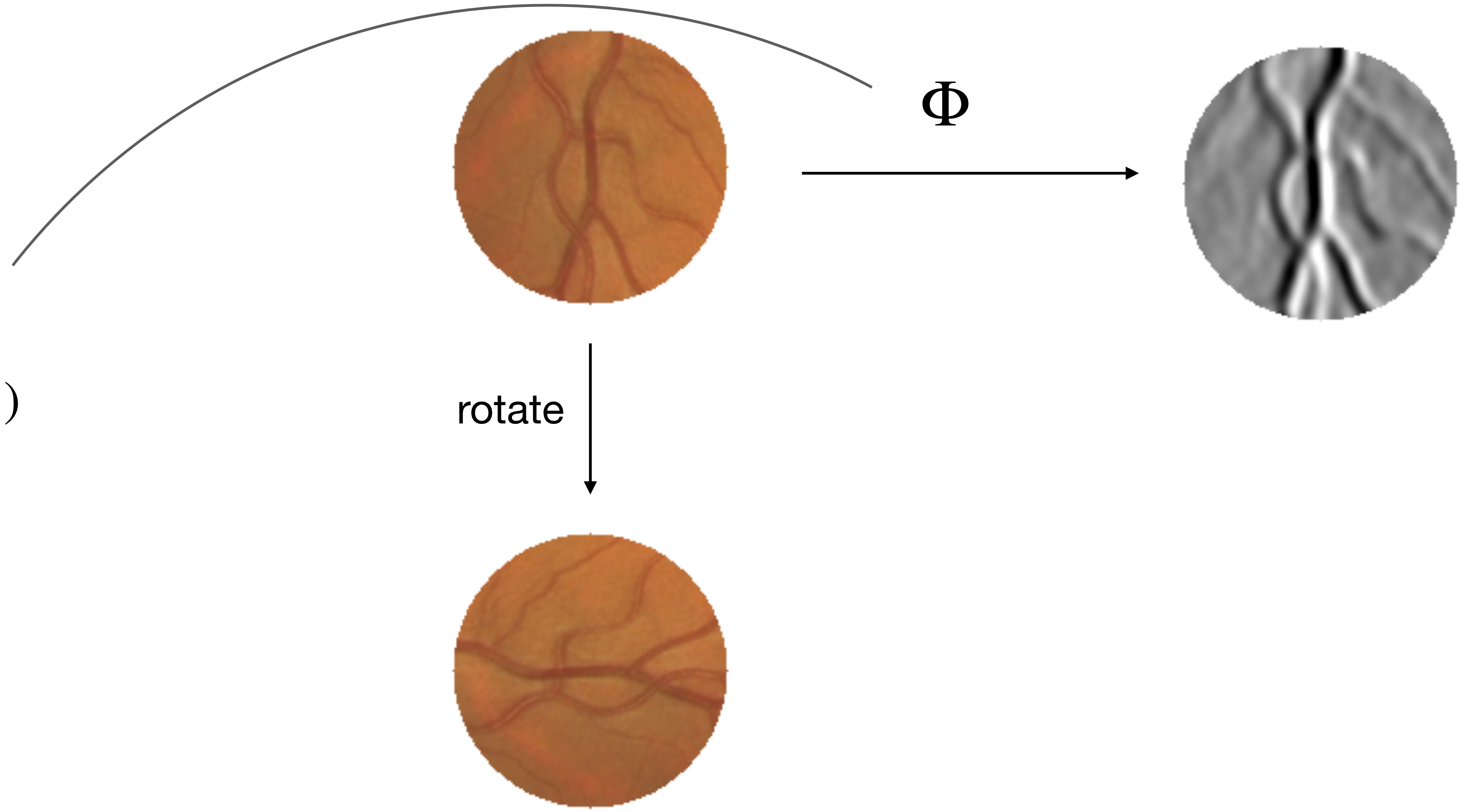
Conv2D(input , )



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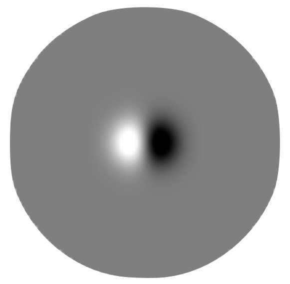
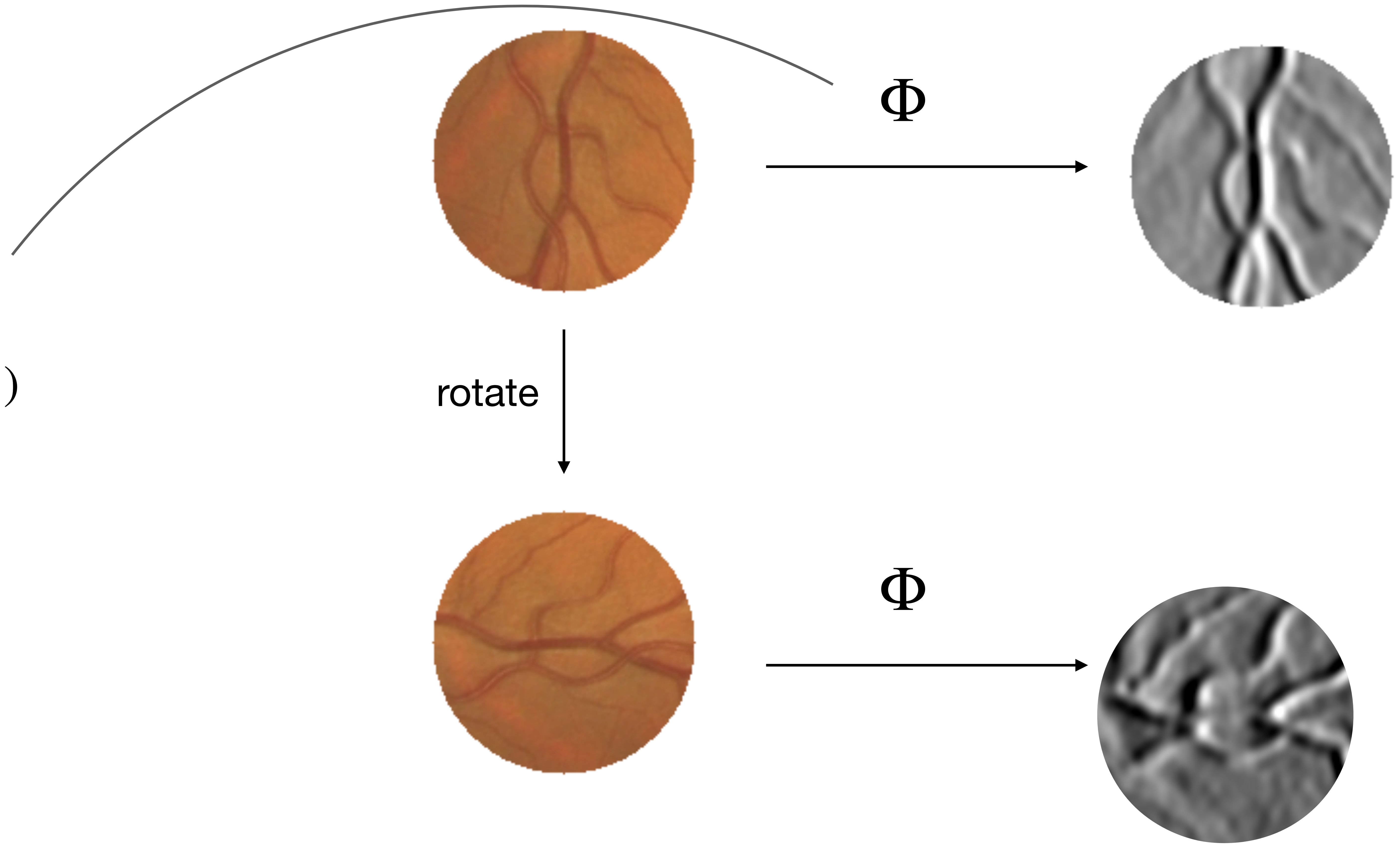
Conv2D(input , )



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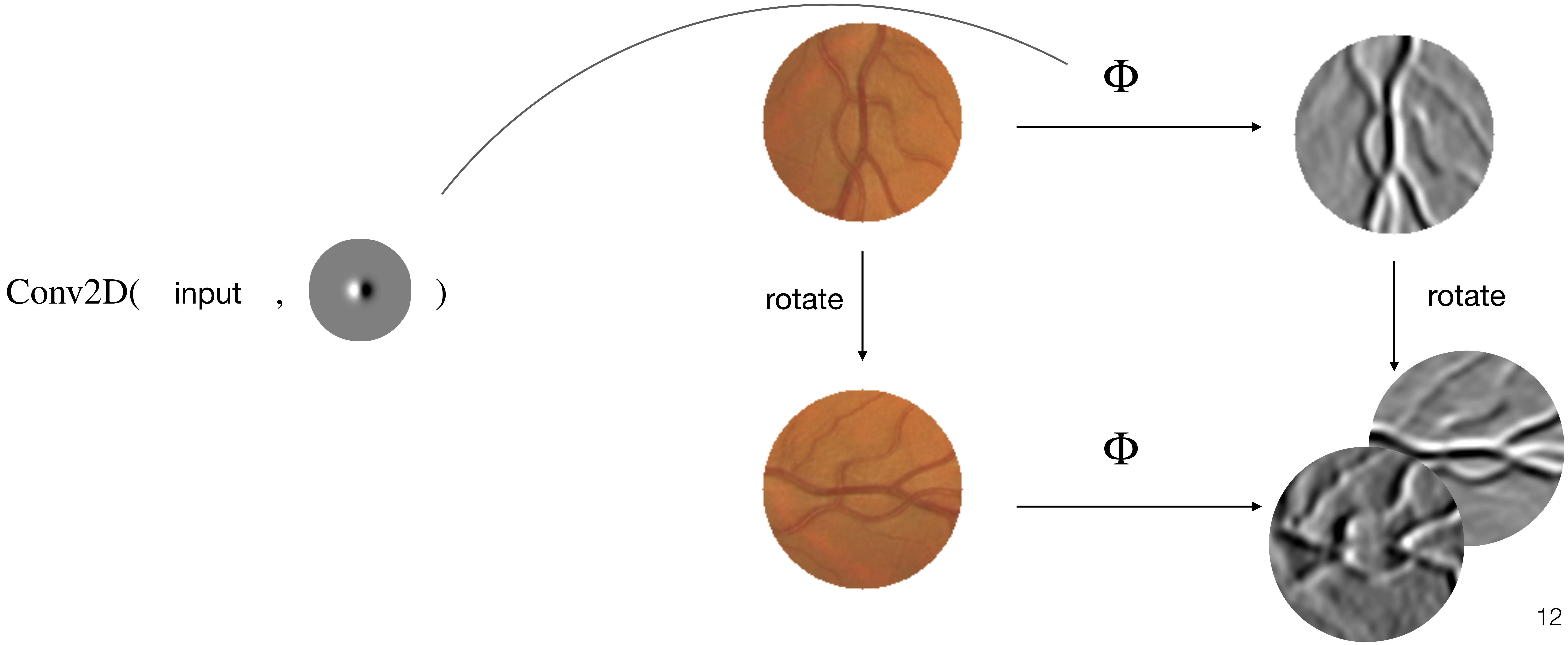

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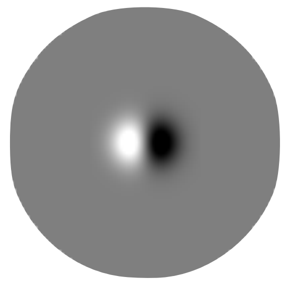
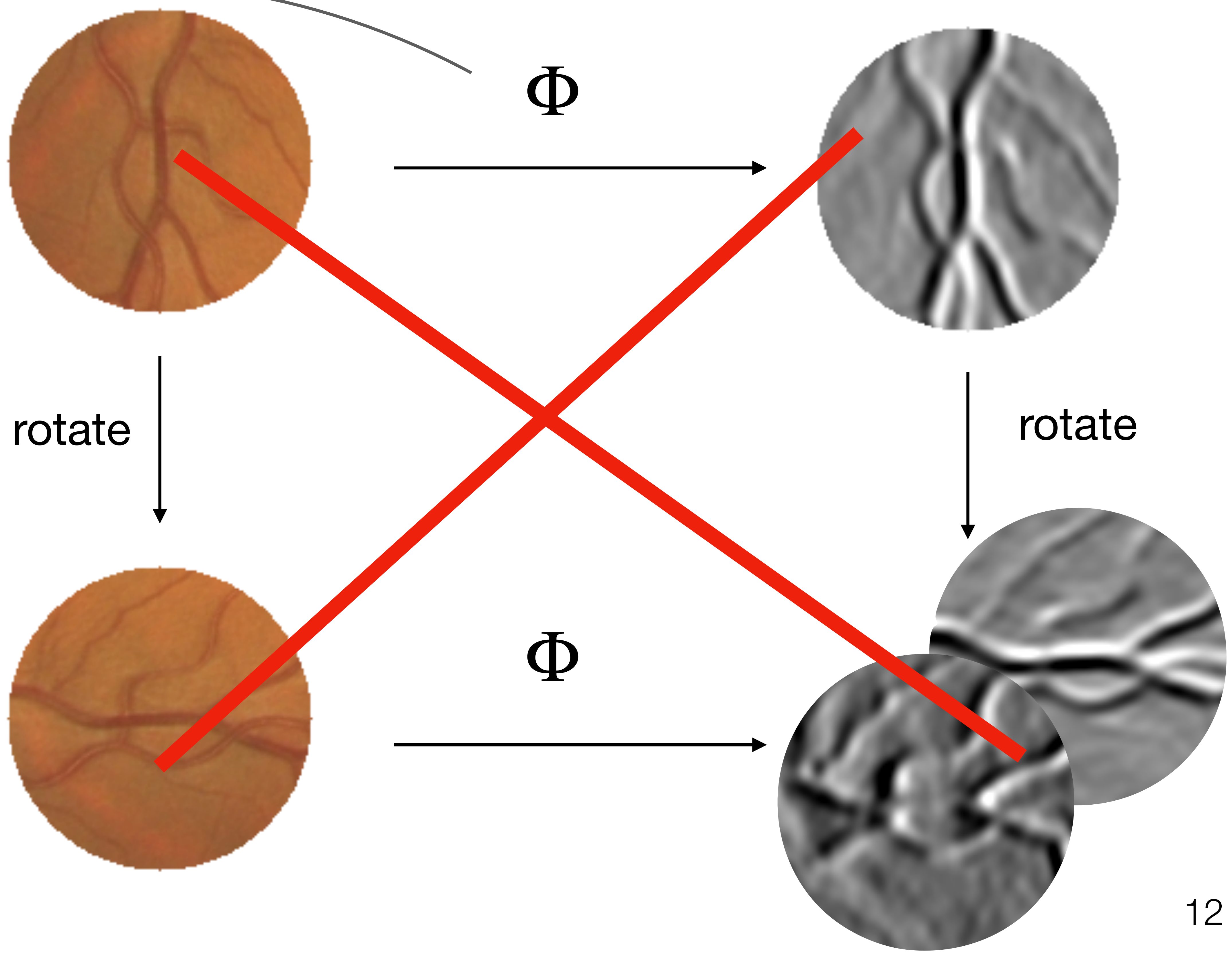
Conv2D(input , )



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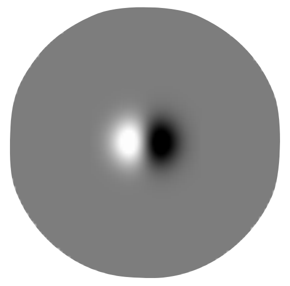
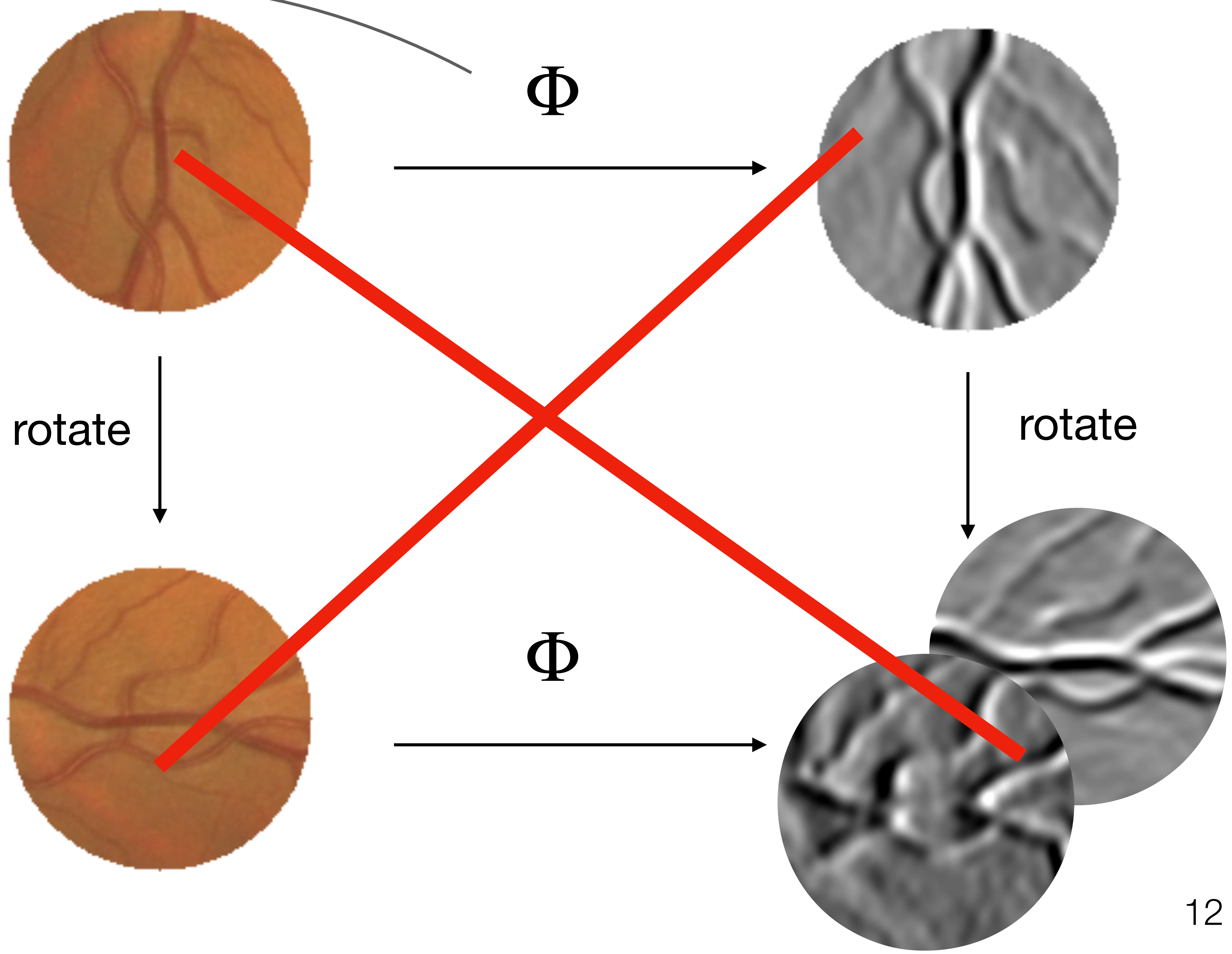
Conv2D(input , )



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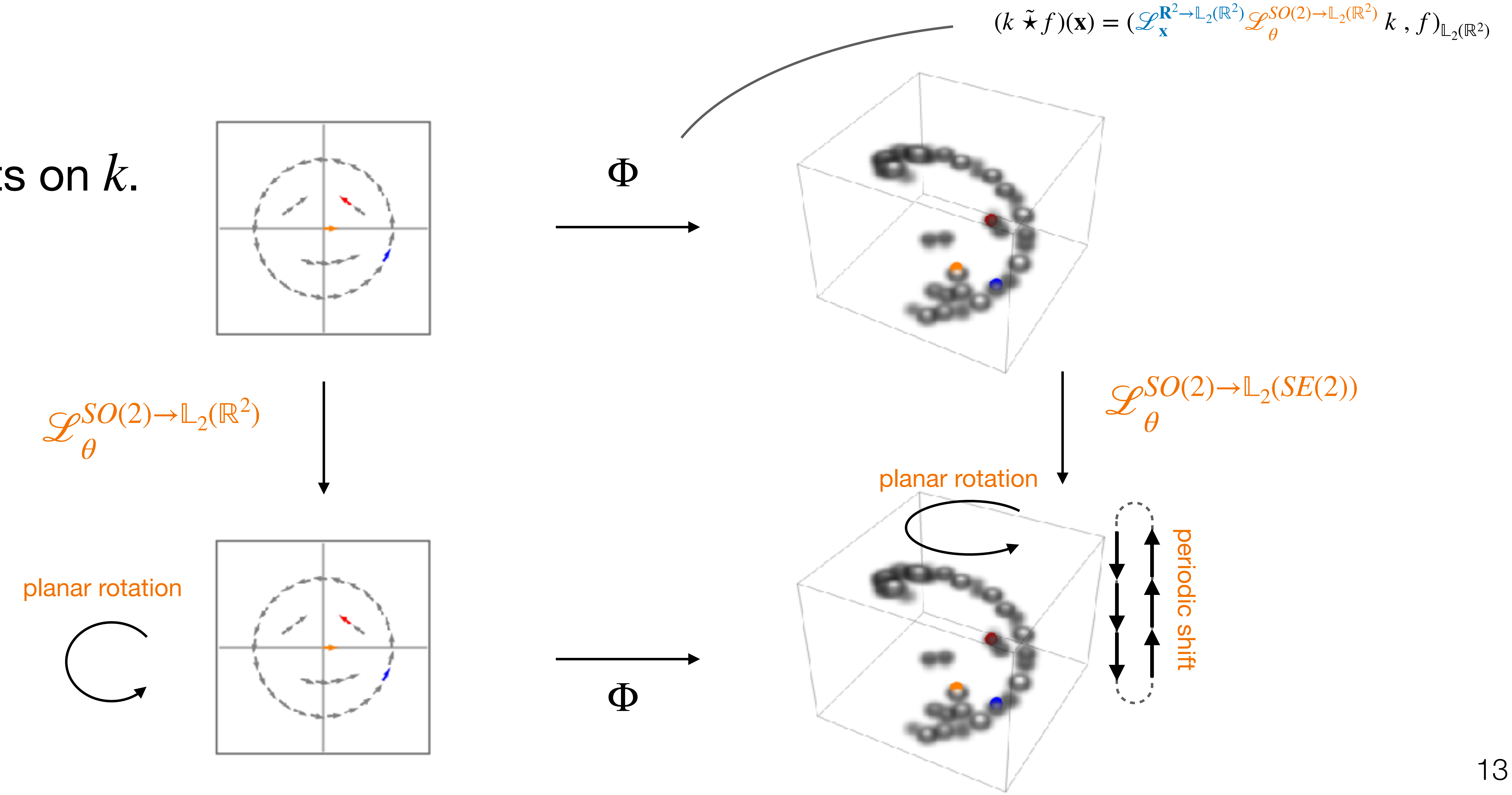
$(X = G/H, Y = G)$

Lifting convolution. No constraints on k.



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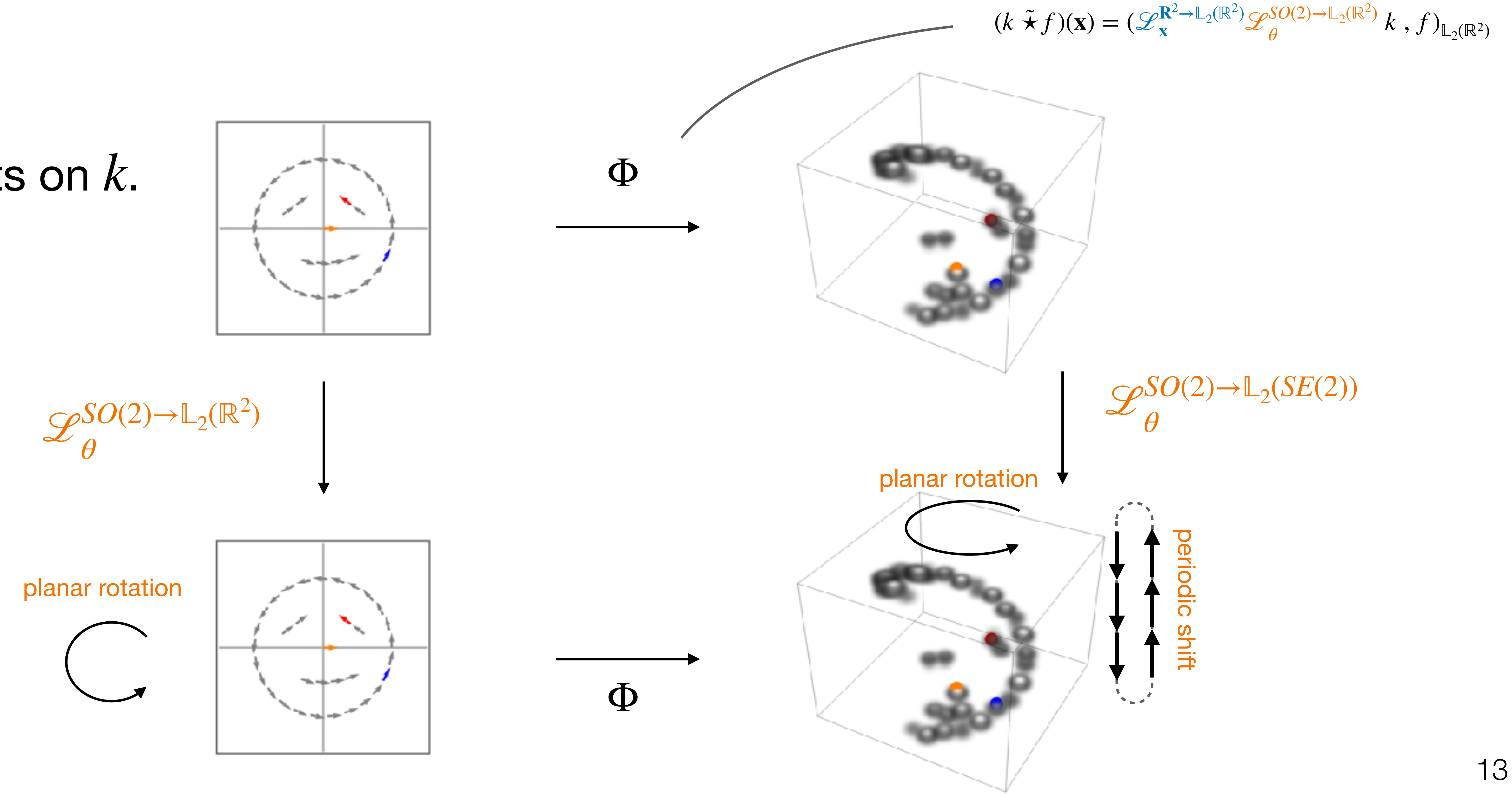

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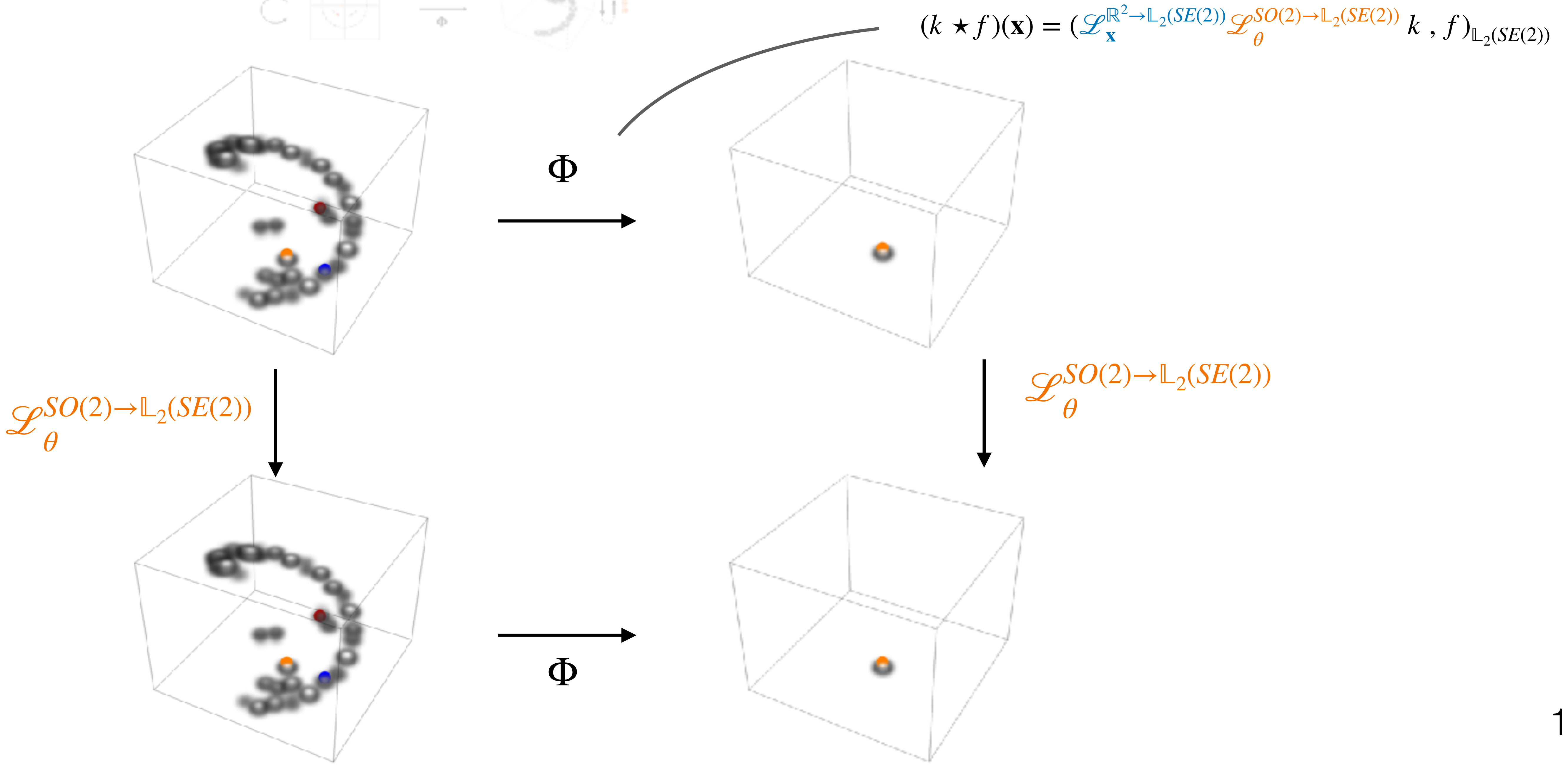

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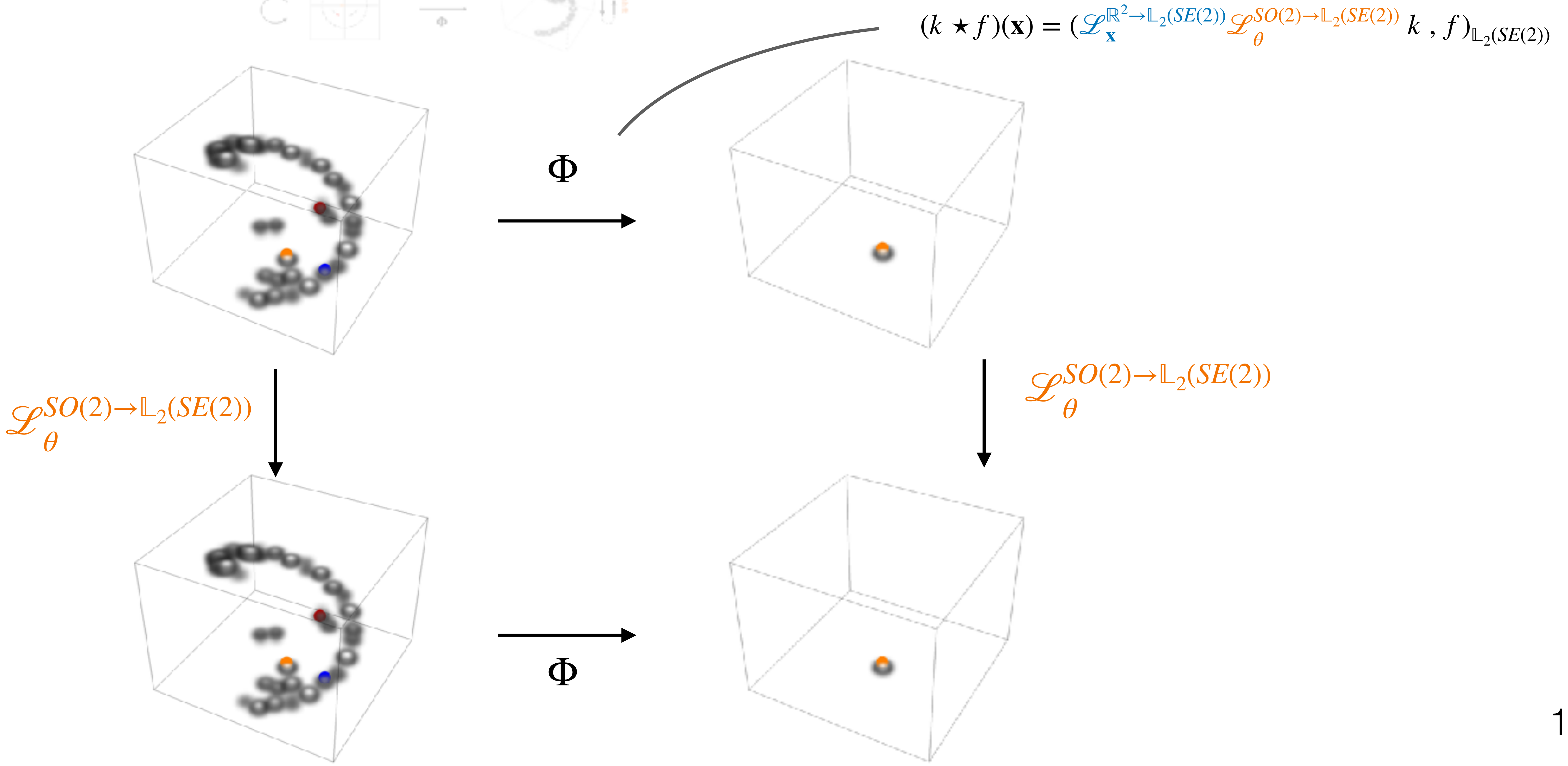

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$(X = G, Y = G/H)$

Projection layer. Mean pooling over H.

Types of layers

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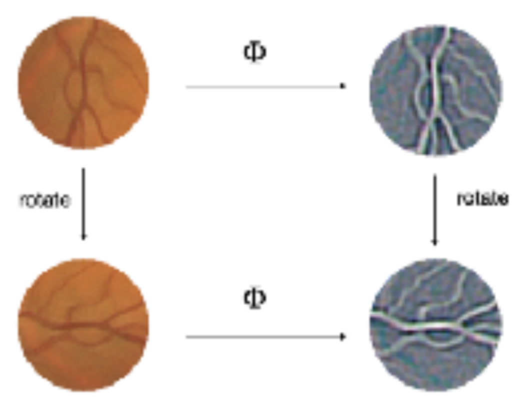

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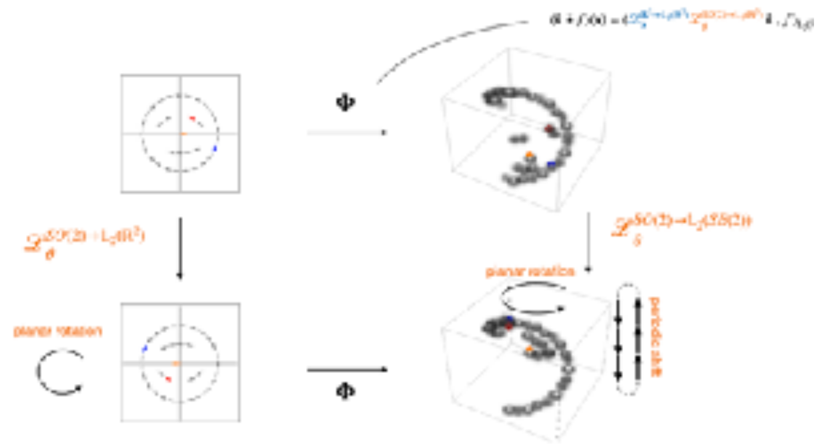

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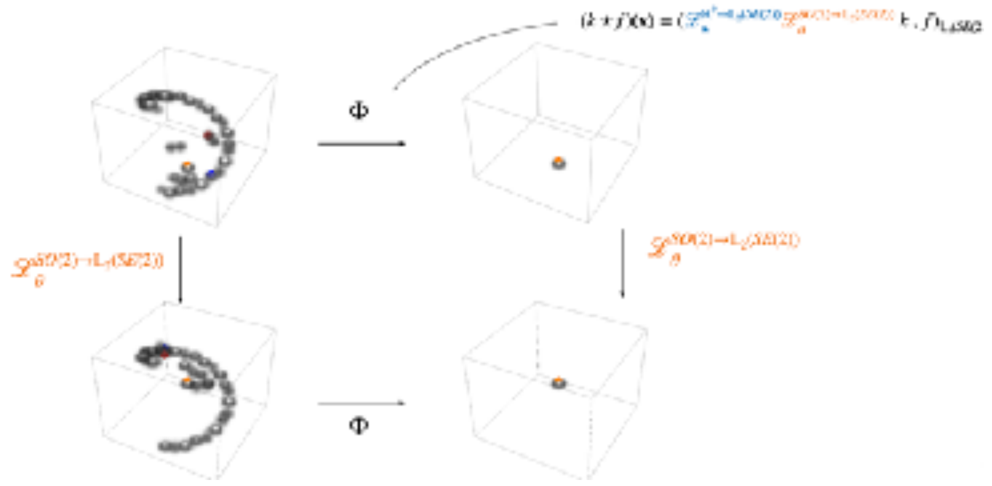

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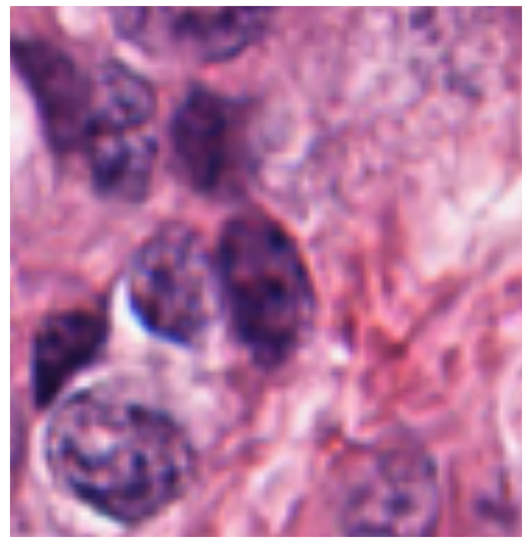
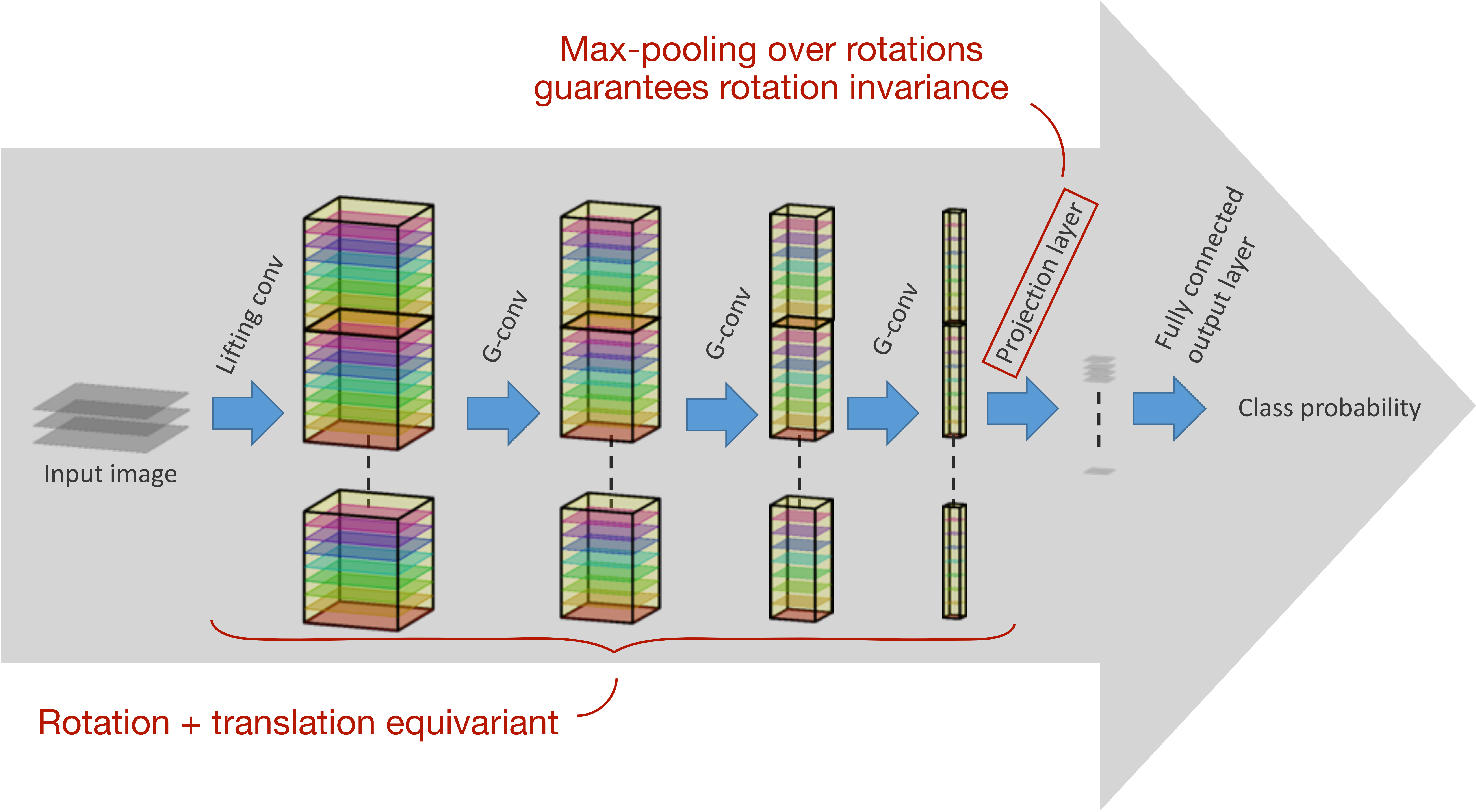
Projection layer. Mean pooling over H.

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

General group equivariant architecture





“normal” (0)
vs
“mitotic” (1)

Conclusion

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

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Group convolutions are all you need!