



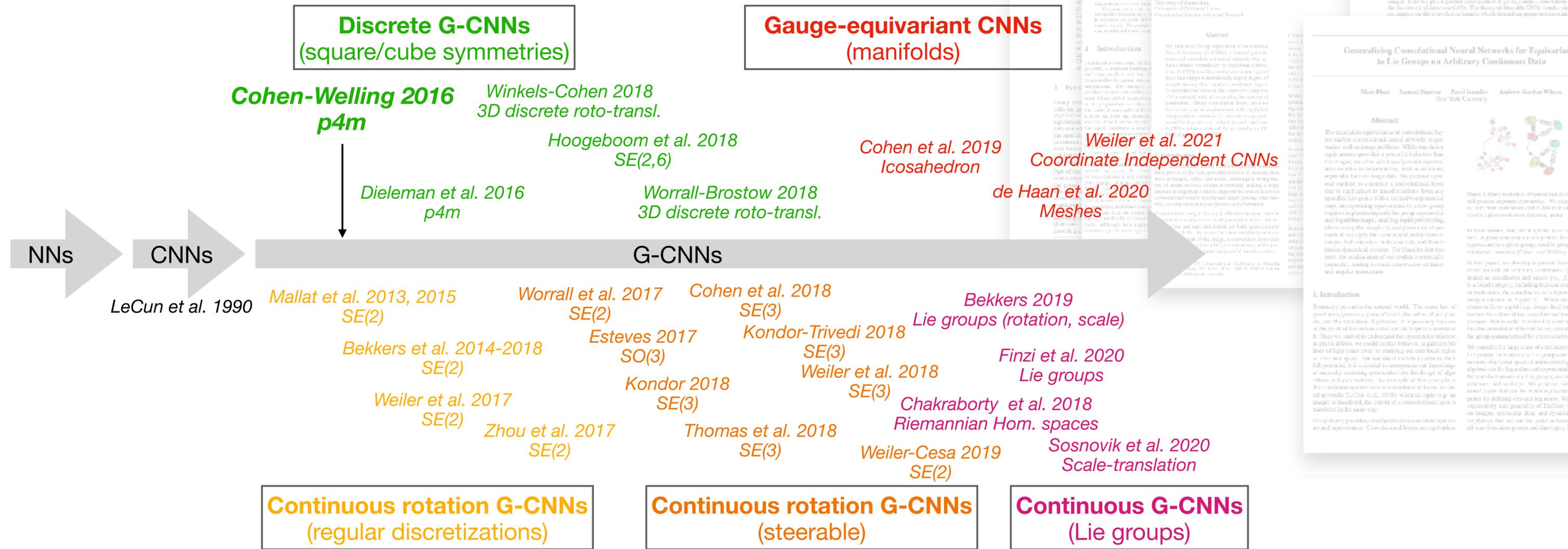
Group Equivariant Deep Learning

Lecture 3 - Equivariant graph neural networks

Lecture 3.7 - Gauge equivariant graph NNs

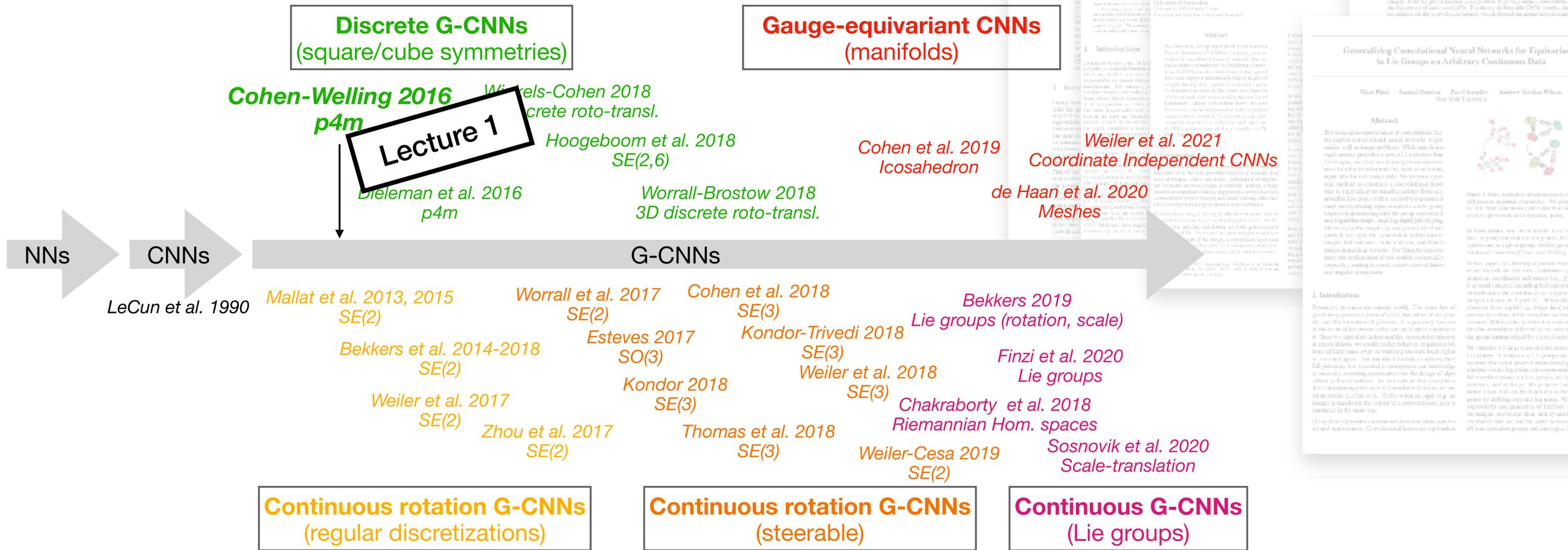
From plain NNs to Gauge-equivariant CNNs

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



From plain NNs to Gauge-equivariant CNNs

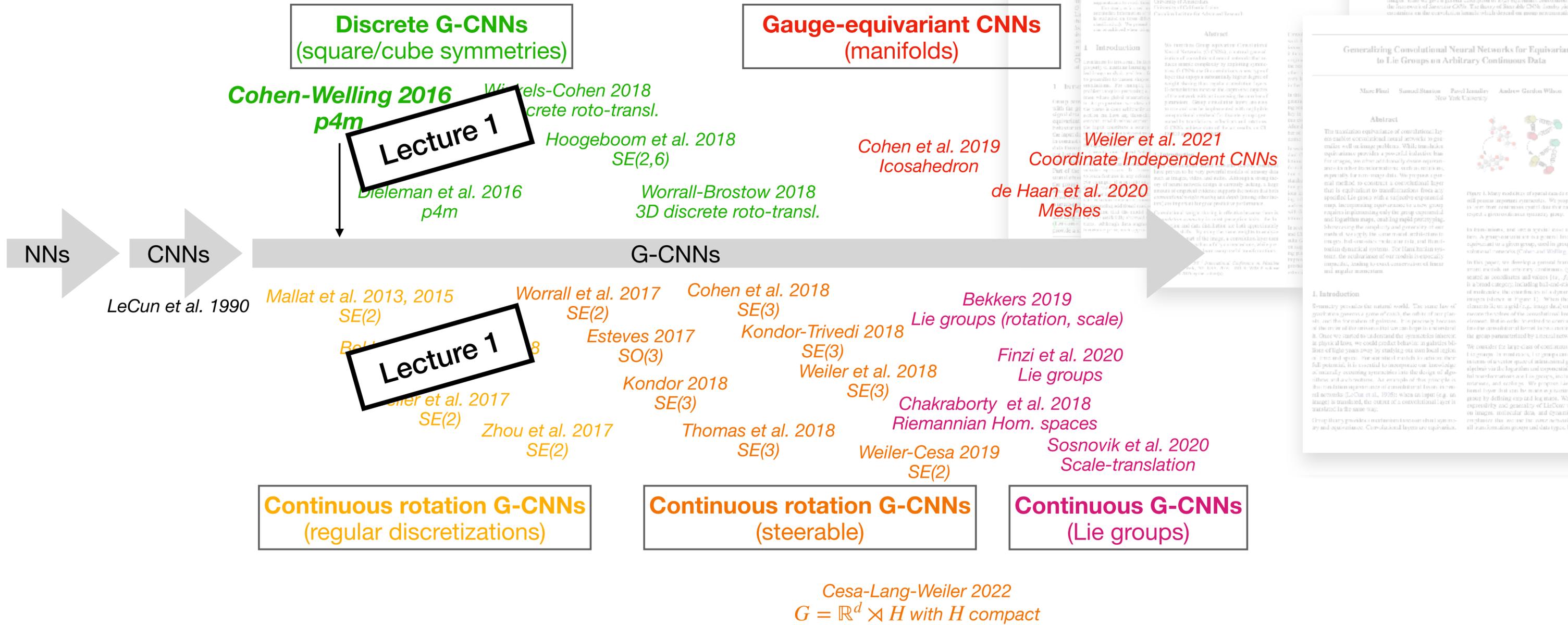
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Cesa-Lang-Weiler 2022
 $G = \mathbb{R}^d \rtimes H$ with H compact

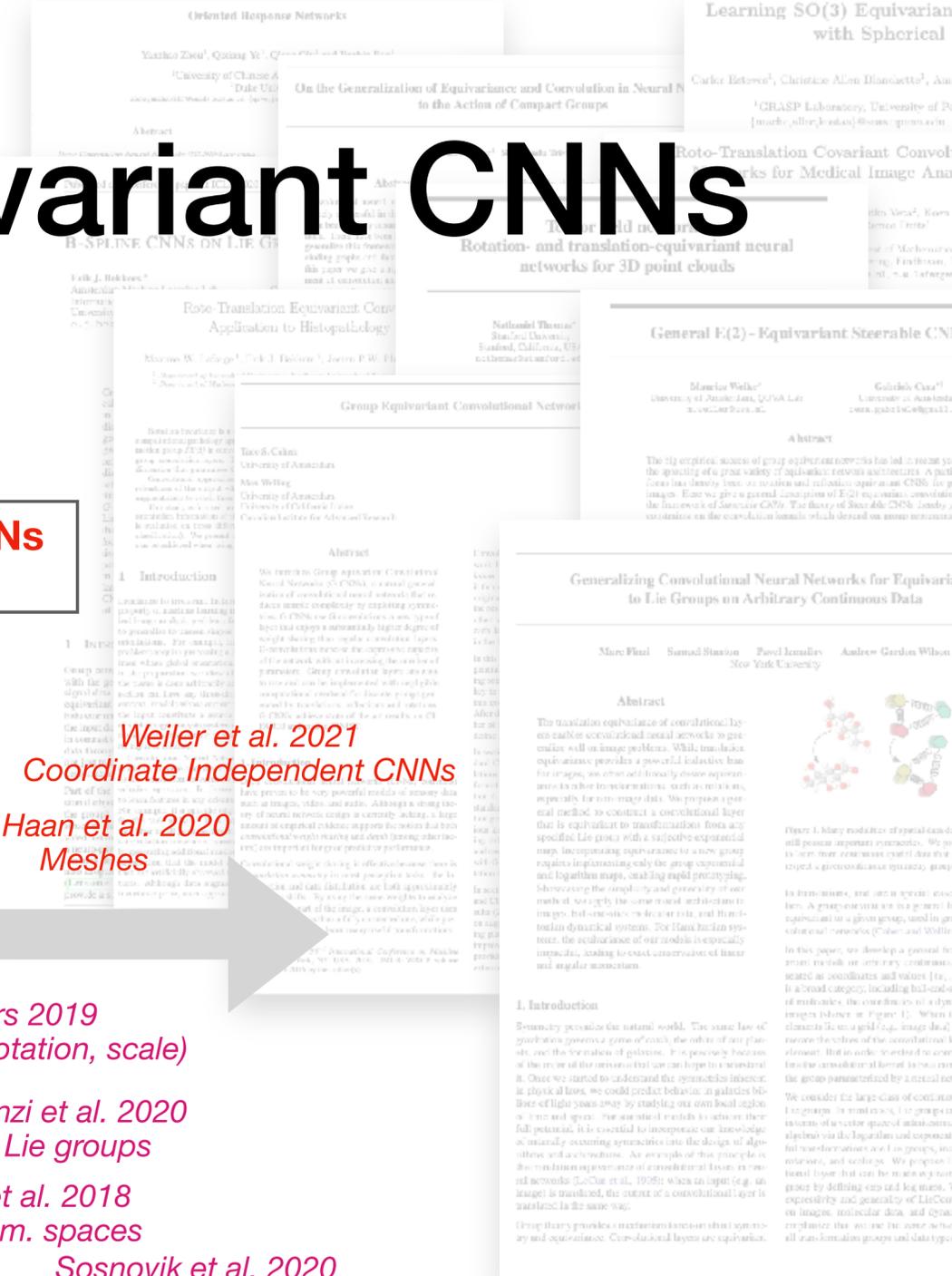
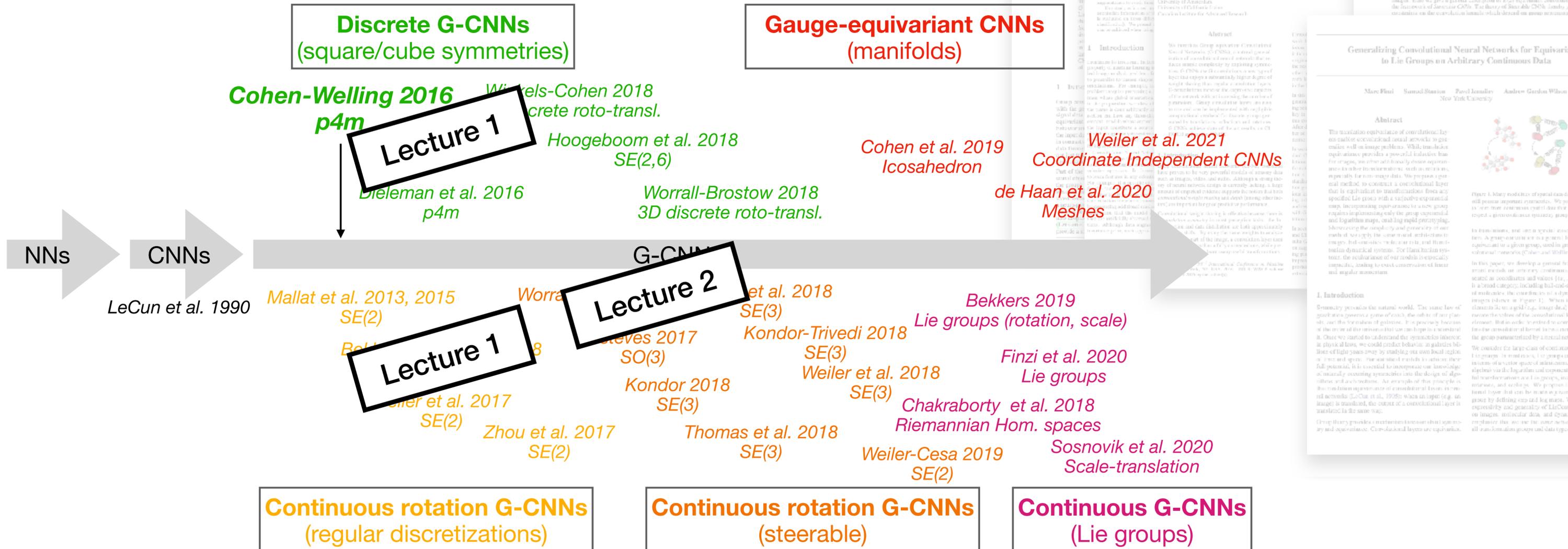
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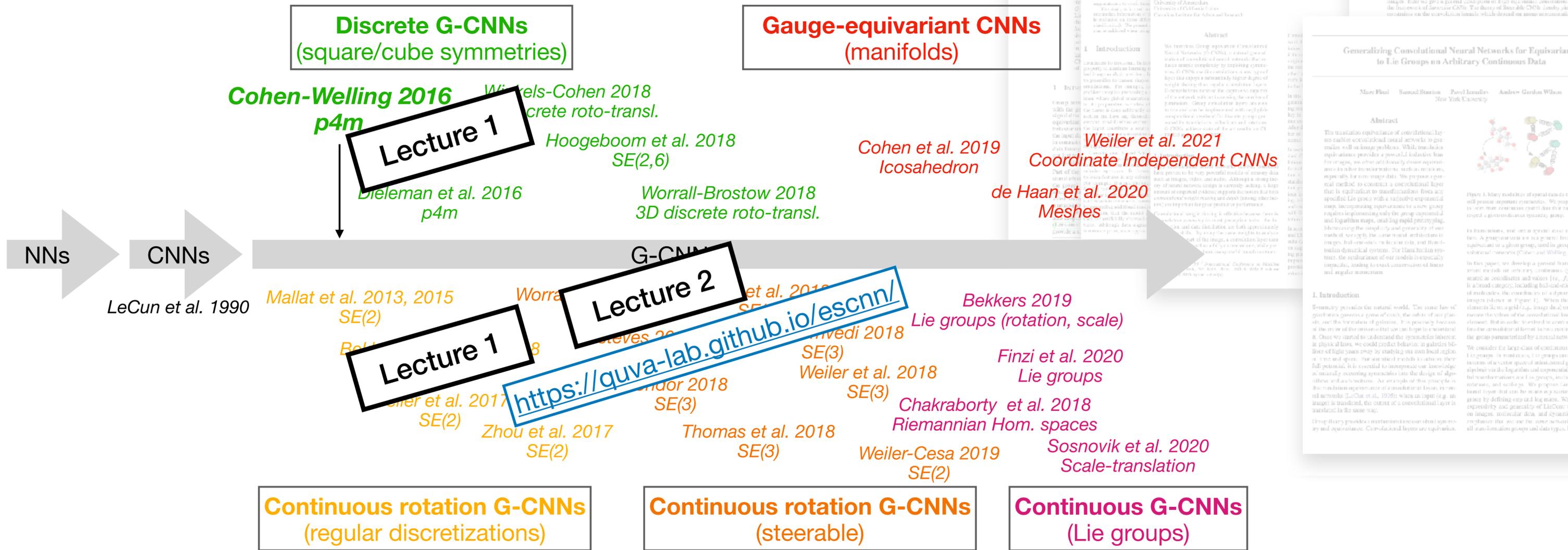
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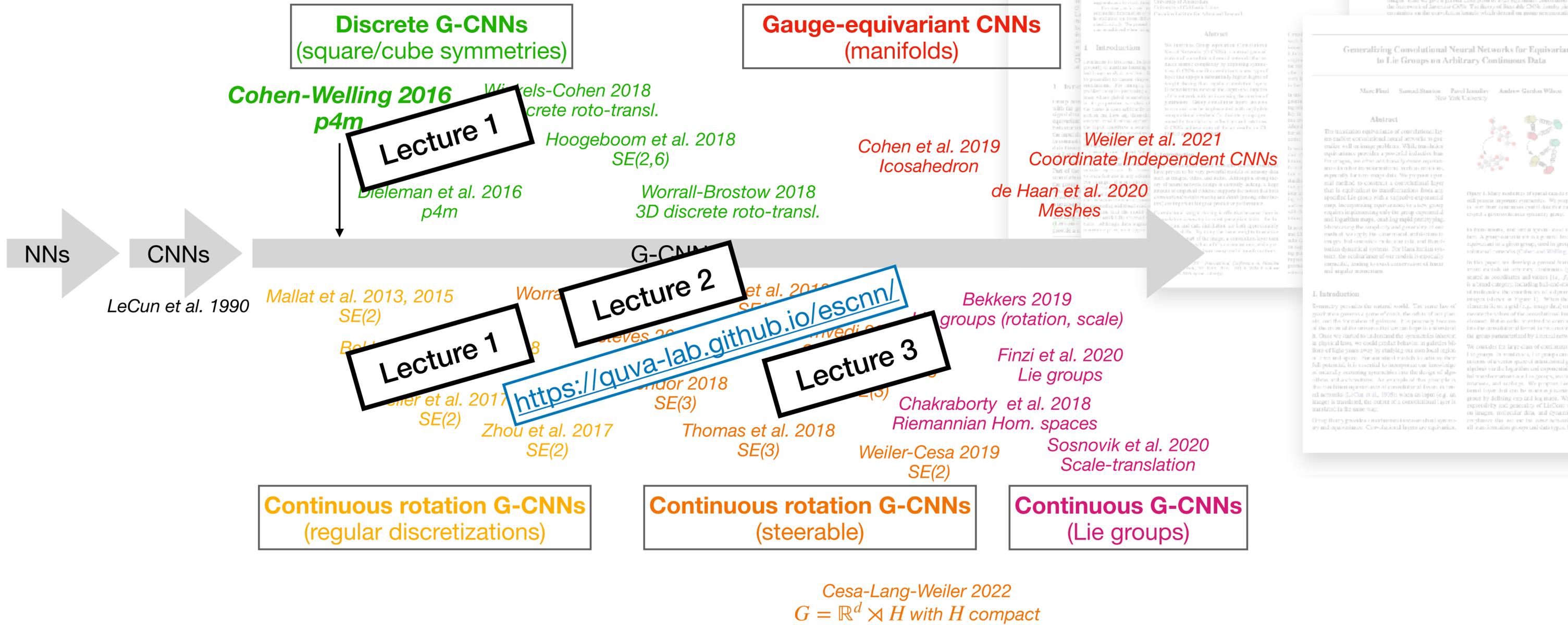
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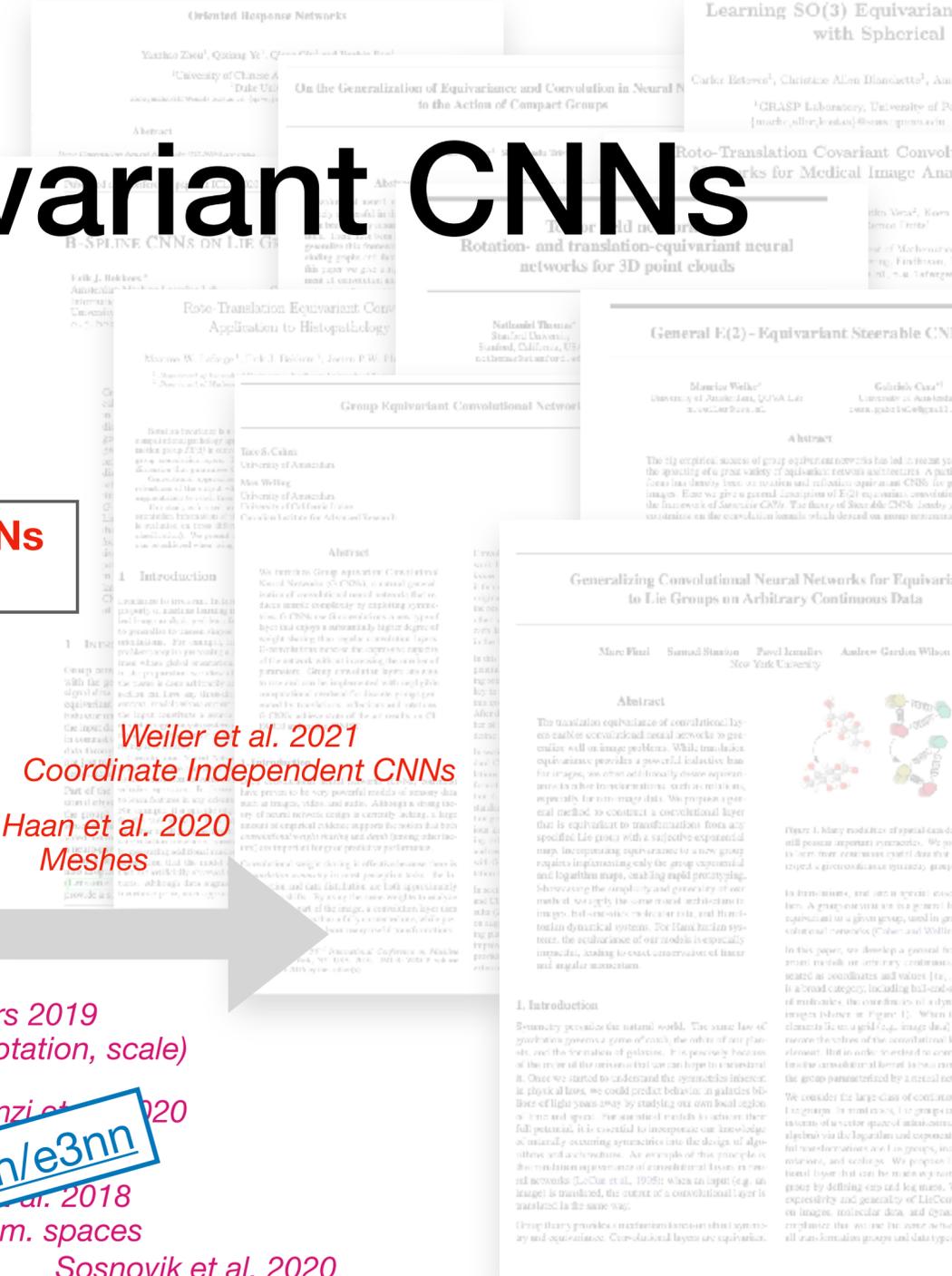
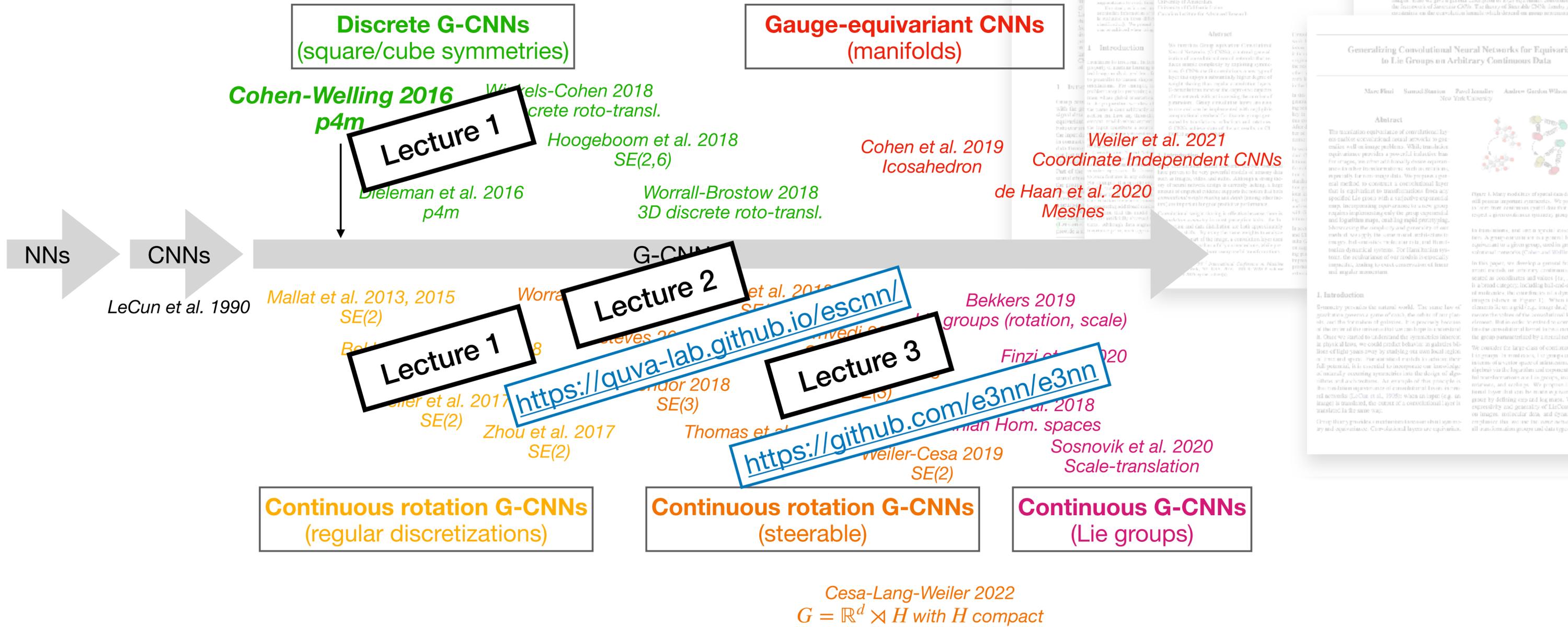
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Recall lecture 2.4

Feature field and induced representation

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

<i>codomain</i>	transforms via a representation	$\rho(h)$	of H
<i>domain</i>	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**

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

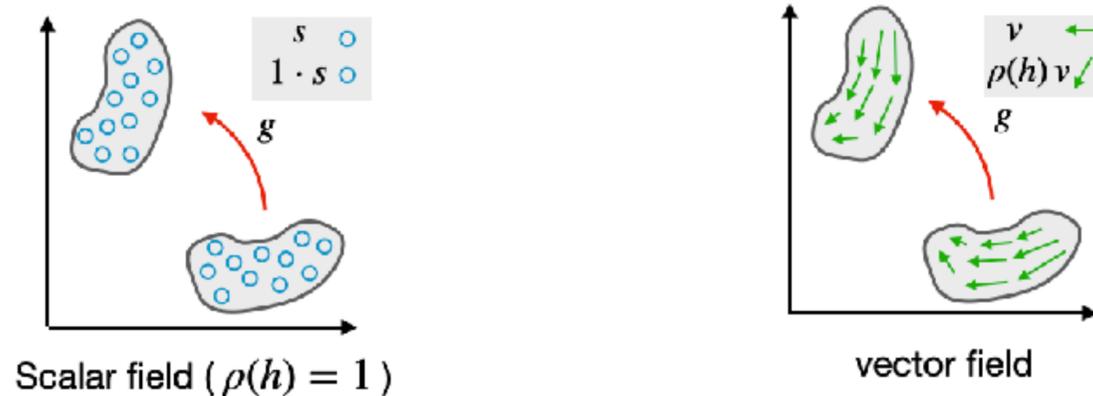


Figure adapted from: Weiler, M., & Cesa, G. (2019). General e (2)-equivariant steerable cnns. NeurIPS. See also <https://github.com/QUVA-Lab/e2cnn>

2

Recall lecture 2.4

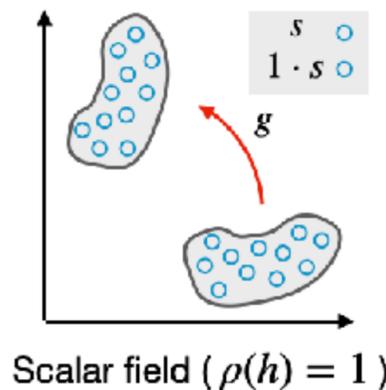
Feature field and induced representation

We call $\hat{f}: \mathbb{R}^d \rightarrow \mathbb{R}^{d_\rho}$ a feature vector field, ρ

codomain transforms via a representation
domain transforms via the action

Representation ρ defines the **type** of the field
induced representation

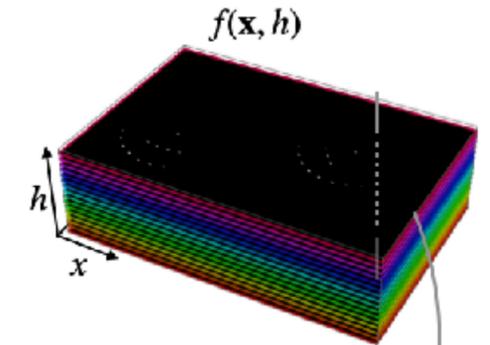
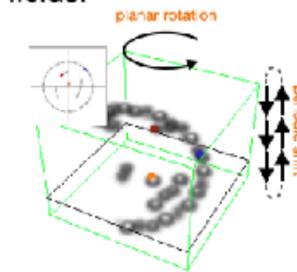
$$\left(\text{Ind}_H^G[\rho](\mathbf{x}, h) \right)$$



Feature field and induced representation

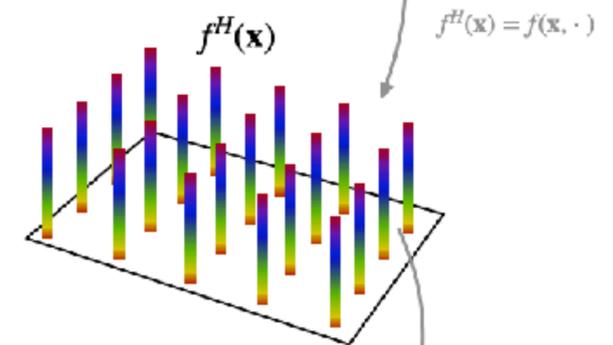
Regular G feature maps: $f(\mathbf{x}, h)$ considered so far can be considered feature fields.

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



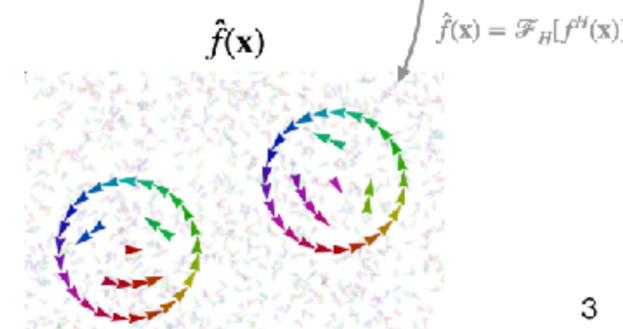
Regular H feature fields: Let $f^H(\mathbf{x}) = f(\mathbf{x}, \cdot)$ be the field of functions $f^H(\mathbf{x}) : H \rightarrow \mathbb{R}$ on the subgroup H , then the functions (**fibers**) transform via the regular representation \mathcal{L}_h^H (recall. $\mathcal{L}_h^H f(h') = f(h^{-1}h')$)

$$(\mathcal{L}_g f)(\mathbf{x}', h') \iff \left(\text{Ind}_H^G[\mathcal{L}_h^H](\mathbf{x}, h) f^H(\mathbf{x}') \right)$$



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

$$(\mathcal{L}_g f)(\mathbf{x}', h') \iff \left(\text{Ind}_H^G[\mathcal{L}_h^H](\mathbf{x}, h) \hat{f} \right)(\mathbf{x}') \iff \left(\text{Ind}_H^G[\rho(h)](\mathbf{x}, h) \hat{f} \right)(\mathbf{x}')$$



Recall lecture 2.4

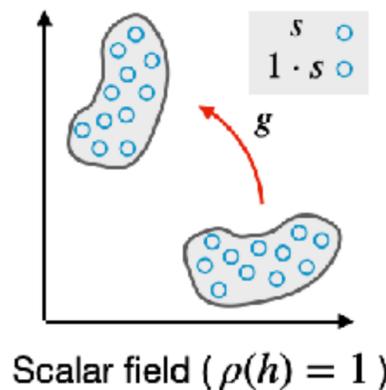
Feature field and induced representation

We call $\hat{f} : \mathbb{R}^d \rightarrow \mathbb{R}^{d_\rho}$ a feature vector field, c

codomain transforms via a represent
domain transforms via the action

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induced representation

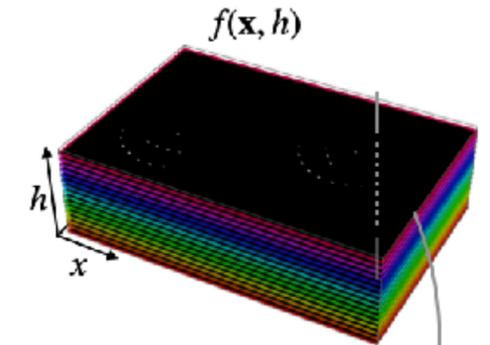
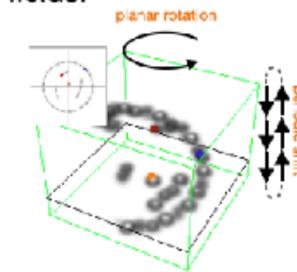
$$\left(\text{Ind}_H^G[\rho](\mathbf{x}, h) \right)$$



Feature field and induced representation

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

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



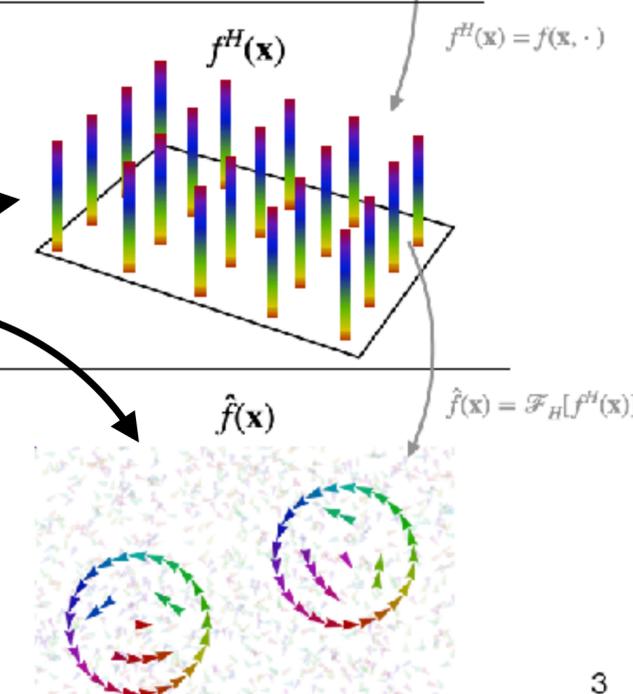
Regular H feature fields: Let $f^H(\mathbf{x}) = f(\mathbf{x}, \cdot)$ be the field of functions $f^H(\mathbf{x}) : H \rightarrow \mathbb{R}$ on the subgroup H , then the functions (**fibers**) transform via the regular representation \mathcal{L}_h^H (recall. $\mathcal{L}_h^H f(h) = f(h^{-1}h)$)

$$(\mathcal{L}_g f)(\mathbf{x}', h') = \mathcal{L}_h^H(\mathbf{x}, h) f^H(\mathbf{x}')$$

Fibers (with oriented features) given relative to globally shared reference frame

Steerable H feature fields: Since the fibers $f^H(\mathbf{x})$ are functions on H , their coefficients $\hat{f}(\mathbf{x}) = \mathcal{F}_H[f^H(\mathbf{x})]$. These vectors of coefficients transform via irreps $\rho(h)$

$$(\mathcal{L}_g f)(\mathbf{x}', h') \iff \left(\text{Ind}_H^G[\mathcal{L}_h^H](\mathbf{x}, h) \hat{f} \right)(\mathbf{x}') \iff \left(\text{Ind}_H^G[\rho(h)](\mathbf{x}, h) \hat{f} \right)(\mathbf{x}')$$



COORDINATE INDEPENDENT CONVOLUTIONAL NETWORKS

ISOMETRY AND GAUGE EQUIVARIANT CONVOLUTIONS ON RIEMANNIAN MANIFOLDS

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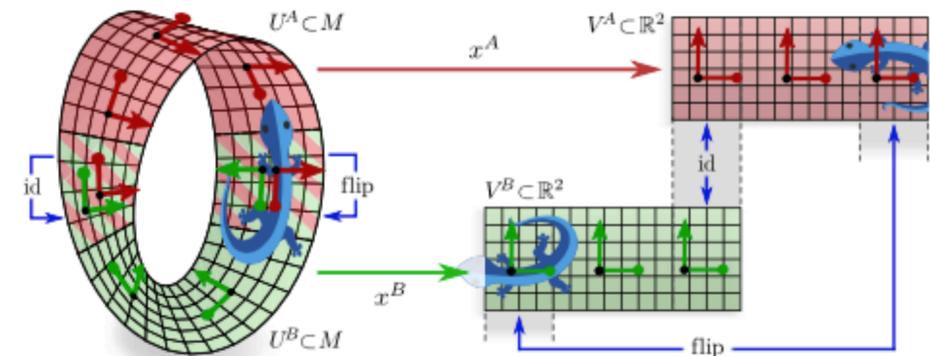
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ABSTRACT

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



Gauge Equivariant Convolutional Networks and the Icosahedral CNN

Taco S. Cohen^{*1} Maurice Weiler^{*2} Berkay Kicanaoglu^{*2} Max Welling¹

Abstract

The principle of *equivariance to symmetry transformations* enables a theoretically grounded approach to neural network architecture design. Equivariant networks have shown excellent performance and data efficiency on vision and medical imaging problems that exhibit symmetries. Here we show how this principle can be extended beyond global symmetries to local gauge transformations. This enables the development of a very general class of convolutional neural networks on manifolds that depend only on the intrinsic geometry, and which includes many popular methods from equivariant and geometric deep learning.

We implement gauge equivariant CNNs for signals defined on the surface of the icosahedron, which provides a reasonable approximation of the sphere. By choosing to work with this very regular manifold, we are able to implement the gauge equivariant convolution using a single `conv2d` call, making it a highly scalable and practical alternative to Spherical CNNs. Using this method, we demonstrate substantial improvements over previous methods on the task of segmenting omnidirectional images and global climate patterns.

1. Introduction

By and large, progress in deep learning has been achieved through intuition-guided experimentation. This approach is indispensable and has led to many successes, but has not produced a deep understanding of *why and when* certain architectures work well. As a result, every new application requires an extensive architecture search, which comes at a significant labor and energy cost.

^{*}Equal contribution ¹Qualcomm AI Research, Amsterdam, NL. ²Qualcomm-University of Amsterdam (QUVA) Lab. Theory co-developed by Cohen & Weiler. Correspondence to: Taco S. Cohen <taco.cohen@gmail.com>, Maurice Weiler <m.weiler@uva.nl>.

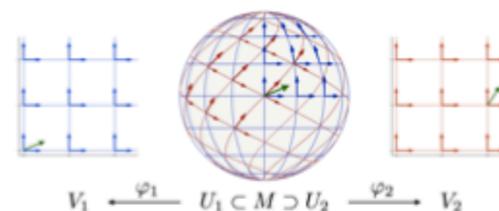


Figure 1. A gauge is a smoothly varying choice of tangent frame on a subset U of a manifold M . A gauge is needed to represent geometrical quantities such as convolutional filters and feature maps (i.e. fields), but the choice of gauge is ultimately arbitrary. Hence, the network should be equivariant to gauge transformations, such as the change between red and blue gauge pictured here.

Although a theory that tells us which architecture to use for any given problem is clearly out of reach, we can nevertheless come up with *general principles* to guide architecture search. One such rational design principle that has met with substantial empirical success (Winkels & Cohen, 2018; Zaher et al., 2017; Lunter & Brown, 2018) maintains that network architectures should be equivariant to symmetries.

Besides the ubiquitous translation equivariant CNN, equivariant networks have been developed for sets, graphs, and homogeneous spaces like the sphere (see Sec. 3). In each case, the network is made equivariant to the global symmetries of the underlying space. However, manifolds do not in general have global symmetries, and so it is not obvious how one might develop equivariant CNNs for them.

General manifolds do however have *local gauge symmetries*, and as we will show in this paper, taking these into account is not just useful but *necessary* if one wishes to build manifold CNNs that depend only on the intrinsic geometry. To this end, we define a convolution-like operation on general manifolds M that is equivariant to local gauge transformations (Fig. 1). This *gauge equivariant convolution* takes as input a number of *feature fields* on M of various types (analogous to matter fields in physics), and produces as output new feature fields. Each field is represented by a number of feature maps, whose activations are interpreted as the coefficients of a geometrical object (e.g. scalar, vector, tensor, etc.) relative to a spatially varying frame (i.e. gauge). The network is constructed such that if the gauge is changed,

GAUGE EQUIVARIANT MESH CNNs

ANISOTROPIC CONVOLUTIONS ON GEOMETRIC GRAPHS

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Max Welling
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ABSTRACT

A common approach to define convolutions on meshes is to interpret them as a graph and apply graph convolutional networks (GCNs). Such GCNs utilize *isotropic* kernels and are therefore insensitive to the relative orientation of vertices and thus to the geometry of the mesh as a whole. We propose Gauge Equivariant Mesh CNNs which generalize GCNs to apply *anisotropic* gauge equivariant kernels. Since the resulting features carry orientation information, we introduce a geometric message passing scheme defined by parallel transporting features over mesh edges. Our experiments validate the significantly improved expressivity of the proposed model over conventional GCNs and other methods.

1 INTRODUCTION

Convolutional neural networks (CNNs) have been established as the default method for many machine learning tasks like speech recognition or planar and volumetric image classification and segmentation. Most CNNs are restricted to flat or spherical geometries, where convolutions are easily defined and optimized implementations are available. The empirical success of CNNs on such spaces has generated interest to generalize convolutions to more general spaces like graphs or Riemannian manifolds, creating a field now known as geometric deep learning (Bronstein et al., 2017).

A case of specific interest is convolution on *meshes*, the discrete analog of 2-dimensional embedded Riemannian manifolds. Mesh CNNs can be applied to tasks such as detecting shapes, registering different poses of the same shape and shape segmentation. If we forget the positions of vertices, and which vertices form faces, a mesh M can be represented by a graph \mathcal{G} . This allows for the application of *graph convolutional networks* (GCNs) to processing signals on meshes.

^{*}Equal Contribution

[†]Qualcomm AI Research is an initiative of Qualcomm Technologies, Inc.

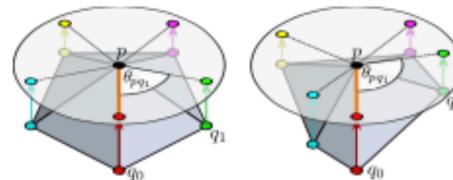


Figure 1: Two local neighbourhoods around vertices p and their representations in the tangent planes $T_p M$. The distinct geometry of the neighbourhoods is reflected in the different angles θ_{pq_i} of incident edges from neighbours q_i . Graph convolutional networks apply isotropic kernels and can therefore not distinguish both neighbourhoods. Gauge Equivariant Mesh CNNs apply anisotropic kernels and are therefore sensitive to orientations. The arbitrariness of reference orientations, determined by a choice of neighbour q_0 , is accounted for by the gauge equivariance of the model.

COORDINATE INDEPENDENT CONVOLUTIONAL NETWORKS

ISOMETRY AND GAUGE EQUIVARIANT CONVOLUTIONS ON RIEMANNIAN MANIFOLDS

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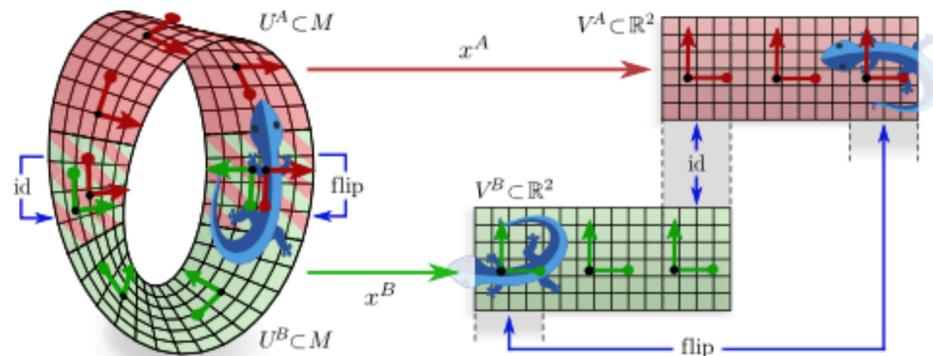
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ABSTRACT

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



COORDINATE INDEPENDENT CONVOLUTIONAL NETWORKS

ISOMETRY AND GAUGE EQUIVARIANT CONVOLUTIONS

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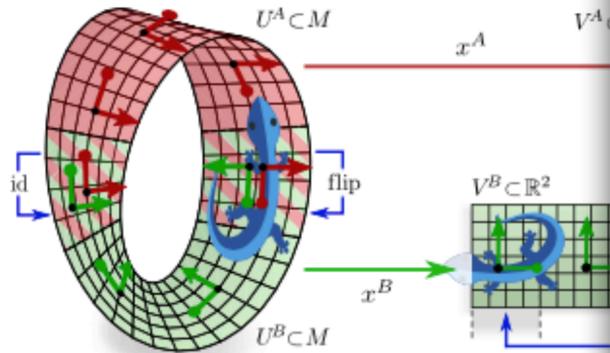
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ABSTRACT

Motivated by the vast success of deep convolutional networks generalizing convolutions to non-Euclidean manifolds. A comparison to flat spaces is that it is unclear in which alignment a filter is applied on a manifold. The underlying reason for this ambiguity do not come with a canonical choice of reference frames (they therefore have to be expressed relative to *arbitrary coordinate frames*). A particular choice of coordinatization should not affect a network's *coordinate independent*. A simultaneous demand for coordinate sharing is shown to result in a requirement on the network's *gauge transformations* (changes of local reference frames) depends thereby on the *G-structure* of the manifold. The theory of gauge equivariance is prescribed by the corresponding symmetries of the *G-structure*. The resulting theory is formulated in terms of fiber bundles. To exemplify the design of coordinate independent convolutions are proven to be equivariant w.r.t. the symmetries of the *G-structure*. The resulting theory is formulated in terms of fiber bundles. To exemplify the design of coordinate independent convolutions we implement a convolutional network on the Möbius strip. An essential geometric formulation of convolutional networks is given in a literature review which explains a large number of Euclidean CNNs on general surfaces as specific instances of coordinate independent CNNs.

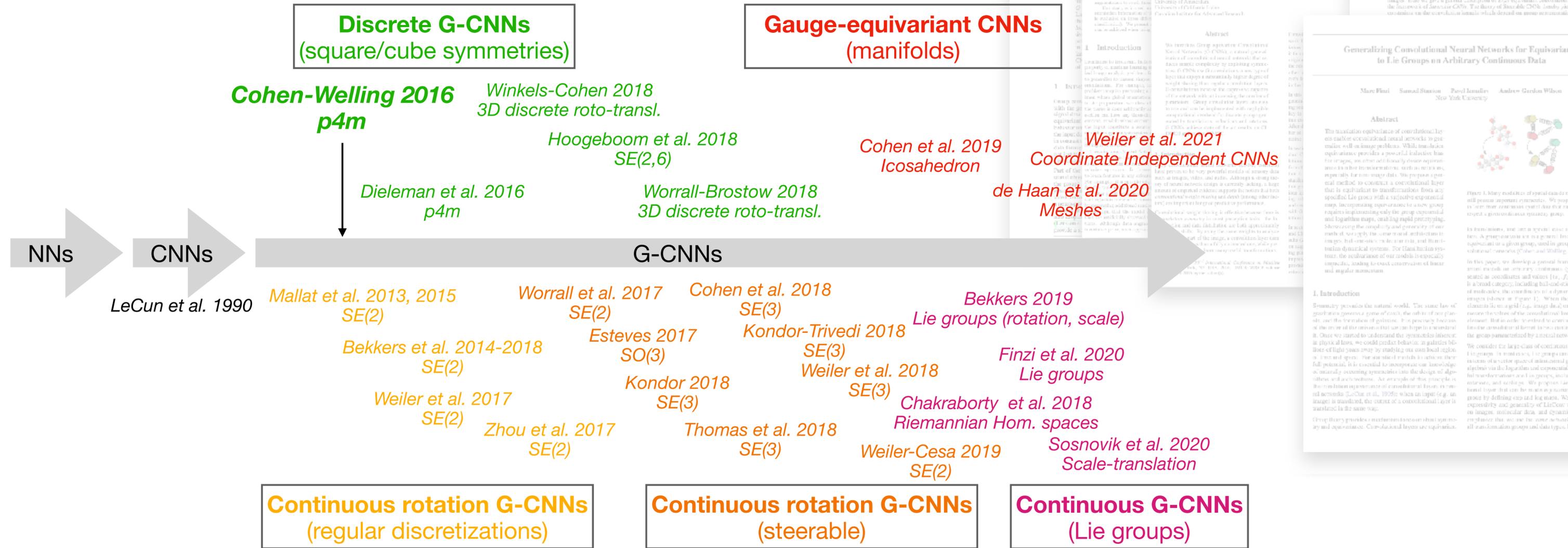


	manifold M	structure group G	global symmetry Aff_{GM} or Isom_{GM}	representation ρ	citation
1	\mathbb{E}_d	$\{e\}$	\mathcal{T}_d	trivial	[130] [253] + any conventional CNN
2	\mathbb{E}_1	\mathcal{S}	$\mathcal{T}_1 \times \mathcal{S}$	regular	[186]
3		\mathcal{R}	$\mathcal{T}_2 \times \mathcal{R}$	regular	[234]
4				irreps	[244] [234] [231]
5		$\text{SO}(2)$	$\text{SE}(2)$	regular	[51] [33] [257] [34] [236] [8] [93] [192] [234] [79] [125] [210] [232] [185] [158] [201] [7] [67] [227] [83] [159] [231] [92] [50] [206] [19] [207] [208] [164] [29] [86]
6				quotients	[34] [234]
7				regular $\xrightarrow{\text{poor}}$ trivial	[33] [143] [234]
8				regular $\xrightarrow{\text{poor}}$ vector	[144] [234]
9	\mathbb{E}_2			trivial	[110] [234]
10				irreps	[234]
11		$\text{O}(2)$	$\text{E}(2)$	regular	[51] [33] [93] [34] [234] [159] [79] [201]
12				quotients	[34]
13				regular $\xrightarrow{\text{poor}}$ trivial	[234]
14				induced $\text{SO}(2)$ -irreps	[234]
15		\mathcal{S}	$\mathcal{T}_2 \times \mathcal{S}$	regular	[243] [212] [7] [258]
16				regular $\xrightarrow{\text{poor}}$ trivial	[77]
17				irreps	[235] [224] [156] [120] [2] [6]
18		$\text{SO}(3)$	$\text{SE}(3)$	quaternion	[250]
19				regular	[67] [241] [242]
20				regular $\xrightarrow{\text{poor}}$ trivial	[3]
21				regular	[241]
22	\mathbb{E}_3	$\text{O}(3)$	$\text{E}(3)$	quotient $\text{O}(3)/\text{O}(2)$	[103]
23				irrep $\xrightarrow{\text{nom}}$ trivial	[174]
24		C_4	$\mathcal{T}_3 \times C_4$	regular	[219]
25		D_4	$\mathcal{T}_3 \times D_4$	regular	[219]
26	$\mathbb{E}_{d-1,1}$	$\text{SO}(d-1,1)$	$\mathcal{T}_d \times \text{SO}(d-1,1)$	irreps	[205]
27	$\mathbb{E}_2 \setminus \{0\}$	$\{e\}$	$\text{SO}(2)$	trivial	[30] [67]
28			$\text{SO}(2) \times \mathcal{S}$	trivial	[62] [67]
29	$\mathbb{E}_3 \setminus \{0\}$	$\text{O}(2)$	$\text{O}(3)$	trivial	[178]
30		$\{e\}$	$\{e\}$	trivial	[13]
31	S^2	$\text{SO}(2)$	$\text{SO}(3)$	irreps	[122] [64]
32				regular	[35] [111]
33		$\text{O}(2)$	$\text{O}(3)$	trivial	[61] [169] [245] [39] [222] [254] [149] [105] [217] [218] [55] [131]
34	$S^2 \setminus \text{poles}$	$\{e\}$	$\text{SO}(2)$	trivial	[38]
35	icosahedron	C_5	$\text{I} (\approx \text{SO}(3))$	regular	[251] [139]
36	ico \ poles	$\{e\}$	$C_5 (\approx \text{SO}(2))$	trivial	[238]
37				irreps	[238]
38	surface ($d=2$)	$\text{SO}(2)$	$\text{Isom}_+(M)$	regular	[173] [220] [246] [48]
39	(e.g. meshes)			regular $\xrightarrow{\text{poor}}$ trivial	[150] [151] [160] [220]
40		D_4	Isom_{D_4M}	trivial	[98]
41		$\{e\}$	$\text{Isom}_{\{e\}M}$	trivial	[160] [194] [106] [221] [133]
42	Möbius strip	\mathcal{R}	$\text{SO}(2)$	irreps	Section 5
43				regular	Section 5

Table 6: Classification of convolutional networks in the literature from the viewpoint of coordinate independent CNNs. Bold lines separate different geometries. The affine group equivariant convolutions on Euclidean spaces \mathbb{E}_d (rows 1-26) are reviewed in Section 9. Section 10 discusses GM -convolutions on punctured Euclidean spaces $\mathbb{E}_d \setminus \{0\} \cong S^{d-1} \times \mathbb{R}^+$ (rows 27-30). Details on spherical CNNs (rows 31-36) are found in Section 11. The models in rows (37-41) operate on general surfaces, mostly represented by triangle meshes; see Section 12. The last two lines list our Möbius convolutions from Section 5. \mathcal{T}_d , \mathcal{R} and \mathcal{S} denote the translation, reflection and scaling group, respectively, while C_N and D_N are cyclic and dihedral groups. Infinite-dimensional representations are in implementations discretized or sampled. For instance, the regular representations of $\text{SO}(2)$ or $\text{O}(2)$ are typically approximated by the regular representations of cyclic or dihedral groups C_N or D_N .

From plain NNs to Gauge-equivariant CNNs

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

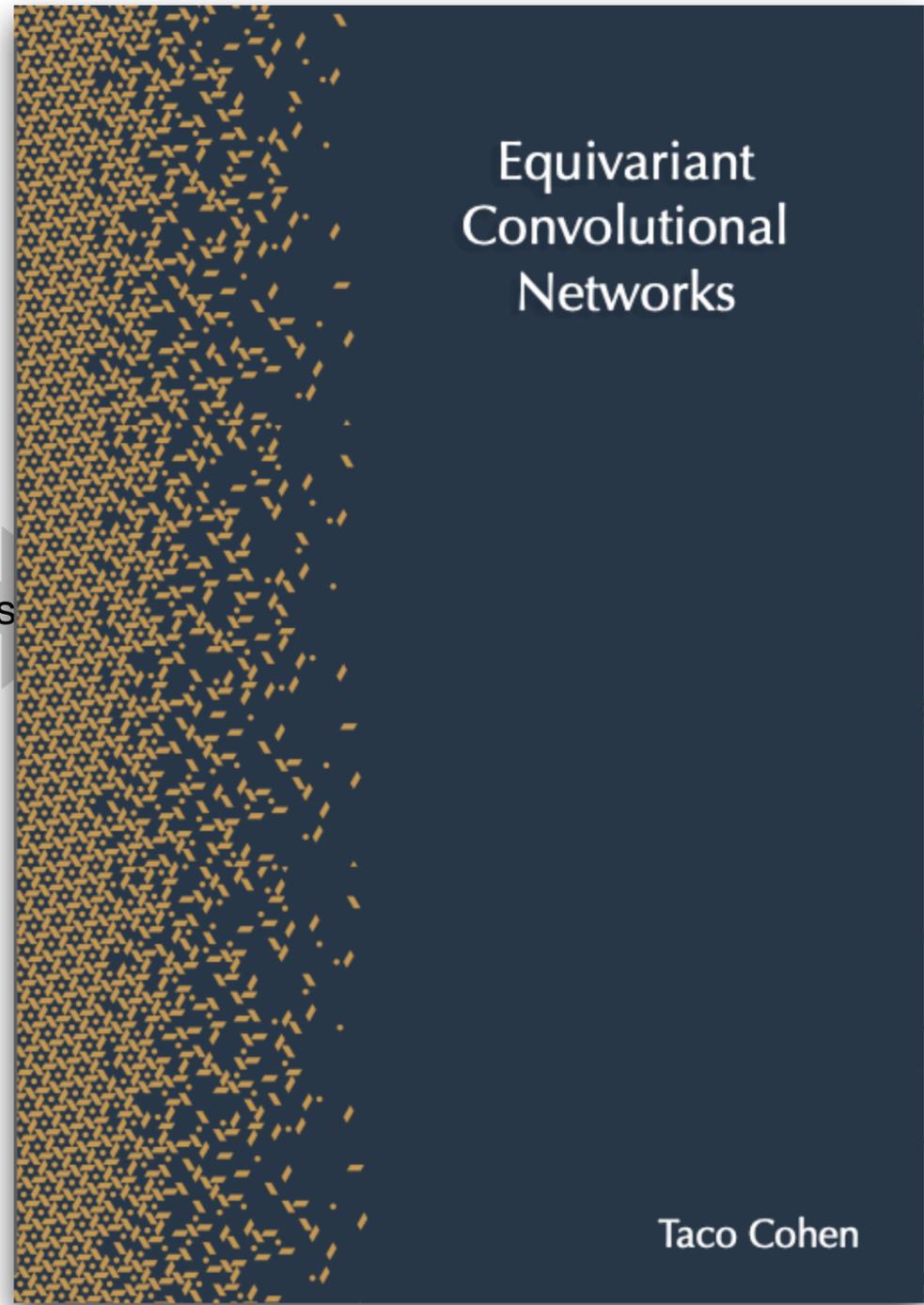


<https://github.com/e3nn/e3nn>

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

From plain NNs to Gauge-equivariant CNNs

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



Equivariant Convolutional Networks

NNs

Cohen 2018
Roto-transl.

Geboorn et al. 2018
SE(2,6)

Worrall-Brostow 2018
3D discrete roto-transl.

G-CNNs

et al. 2017
SE(2)

Esteves 2017
SO(3)

Kondor 2018
SE(3)

2017

Cohen et al. 2018
SE(3)

Kondor-Trivedi 2018
SE(3)

Weiler et al. 2018
SE(3)

Thomas et al. 2018
SE(3)

Weiler-Cesa 2019
SE(2)

Continuous rotation G-CNNs (steerable)

Bekkers 2019
Lie groups (rotation, scale)

Finzi et al. 2020
Lie groups

Chakraborty et al. 2018
Riemannian Hom. spaces

Sosnovik et al. 2020
Scale-translation

Continuous G-CNNs (Lie groups)

Gauge-equivariant CNNs (manifolds)

Cohen et al. 2019
Icosahedron

Weiler et al. 2021
Coordinate Independent CNNs

de Haan et al. 2020
Meshes

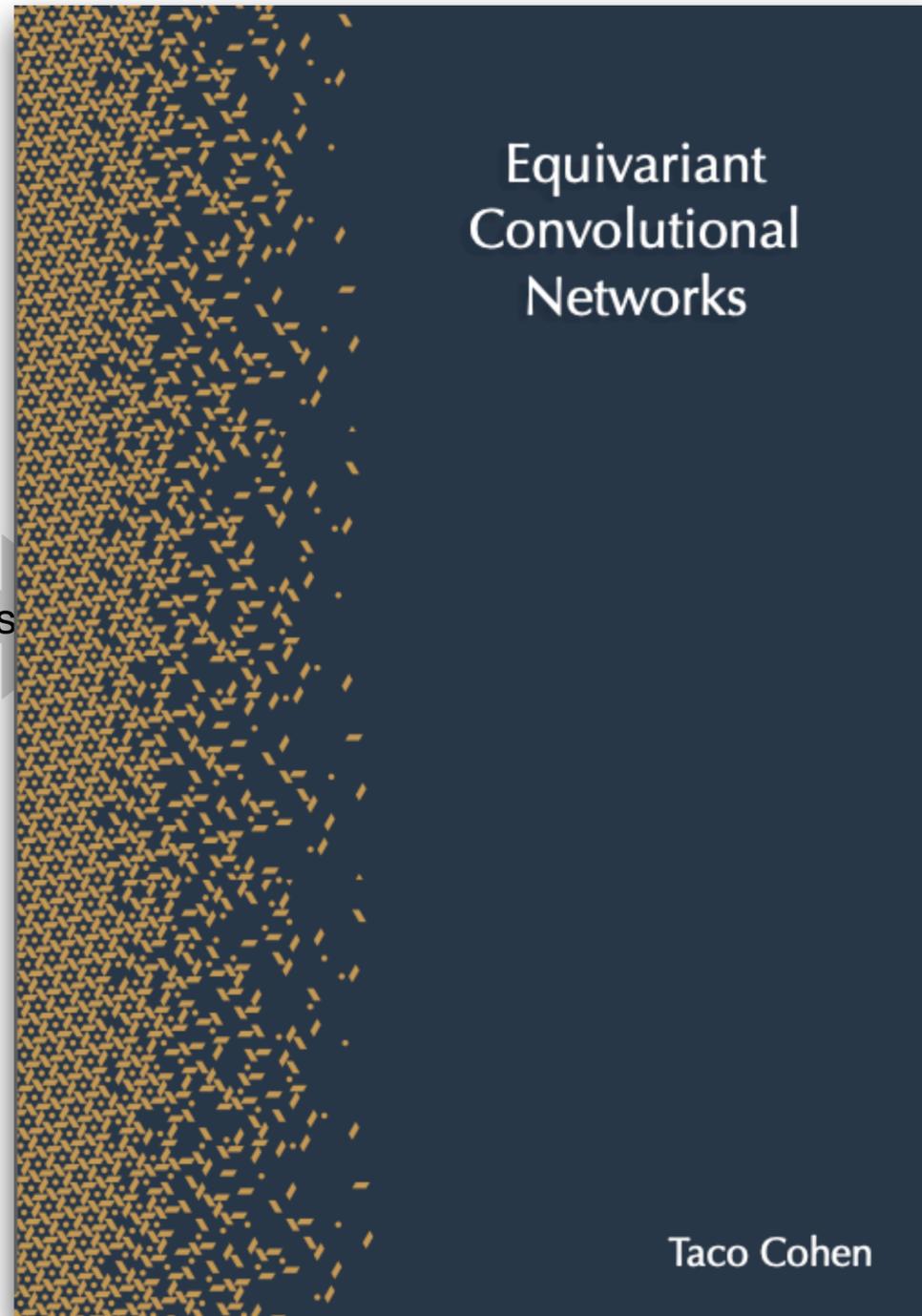
Cesa-Lang-Weiler 2022
 $G = \mathbb{R}^d \rtimes H$ with H compact

<https://pure.uva.nl/ws/files/60770359/Thesis.pdf>

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

From plain NNs to Gauge-equivariant CNNs

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Equivariant Convolutional Networks

Taco Cohen

Cohen 2018
roto-transl.

Worrall et al. 2018
SE(2,6)

Worrall-Brostow 2018
3D discrete roto-transl.

G-CNNs

Worrall et al. 2017
SE(2)

Cohen et al. 2017
SE(3)

Esteves 2017
SO(3)

Kondor 2018
SE(3)

Thomas et al. 2017
SE(3)

Continuous roto-transl. (steerable)

[e3nn/e3nn](https://github.com/Chen-Cai-OSU/e3nn/e3nn)

Gauge-equivariant

COORDINATE INDEPENDENT CONVOLUTIONAL NETWORKS
ISOMETRY AND GAUGE EQUIVARIANT CONVOLUTIONS ON RIEMANNIAN MANIFOLDS

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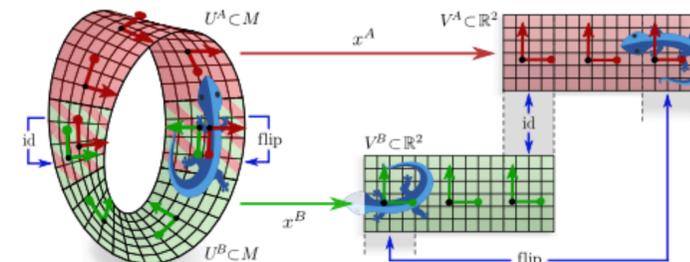
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ABSTRACT

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



NNs

<https://pure.uva.nl/ws/files/60770359/Thesis.pdf>

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