

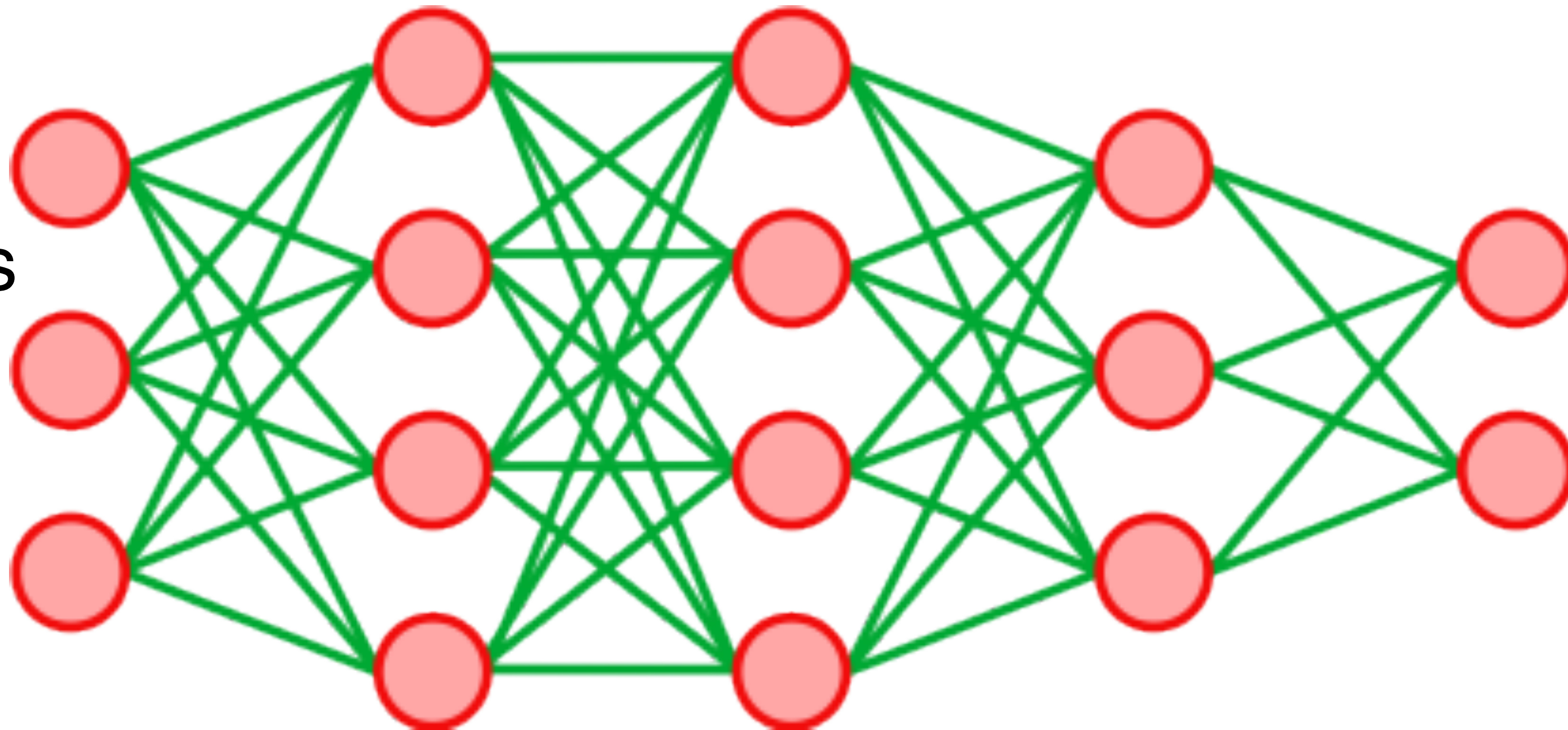
On how to incorporate spacetime symmetries into your neural networks

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Deep Neural Network (DNN)

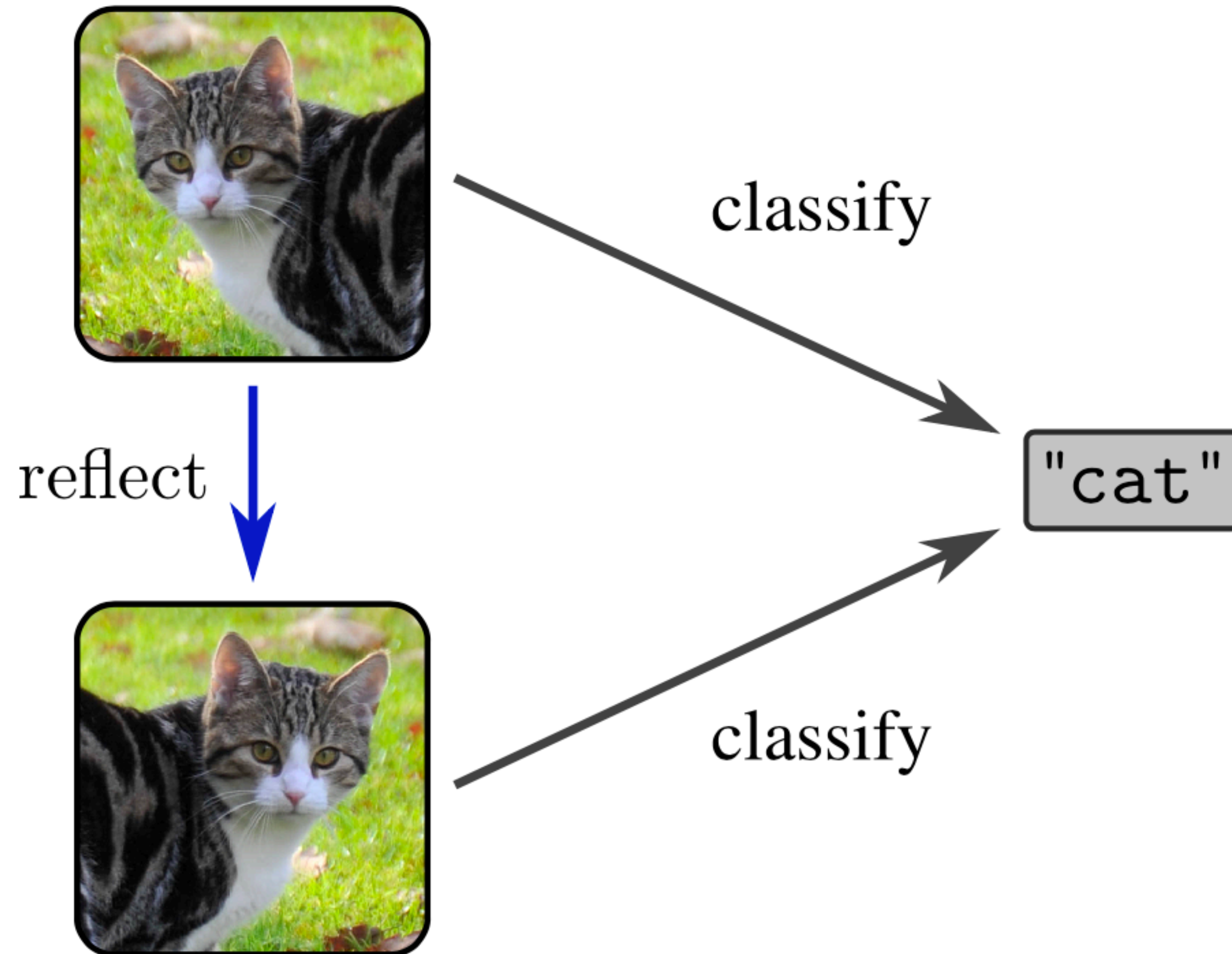
- Input: features



- Output: prediction

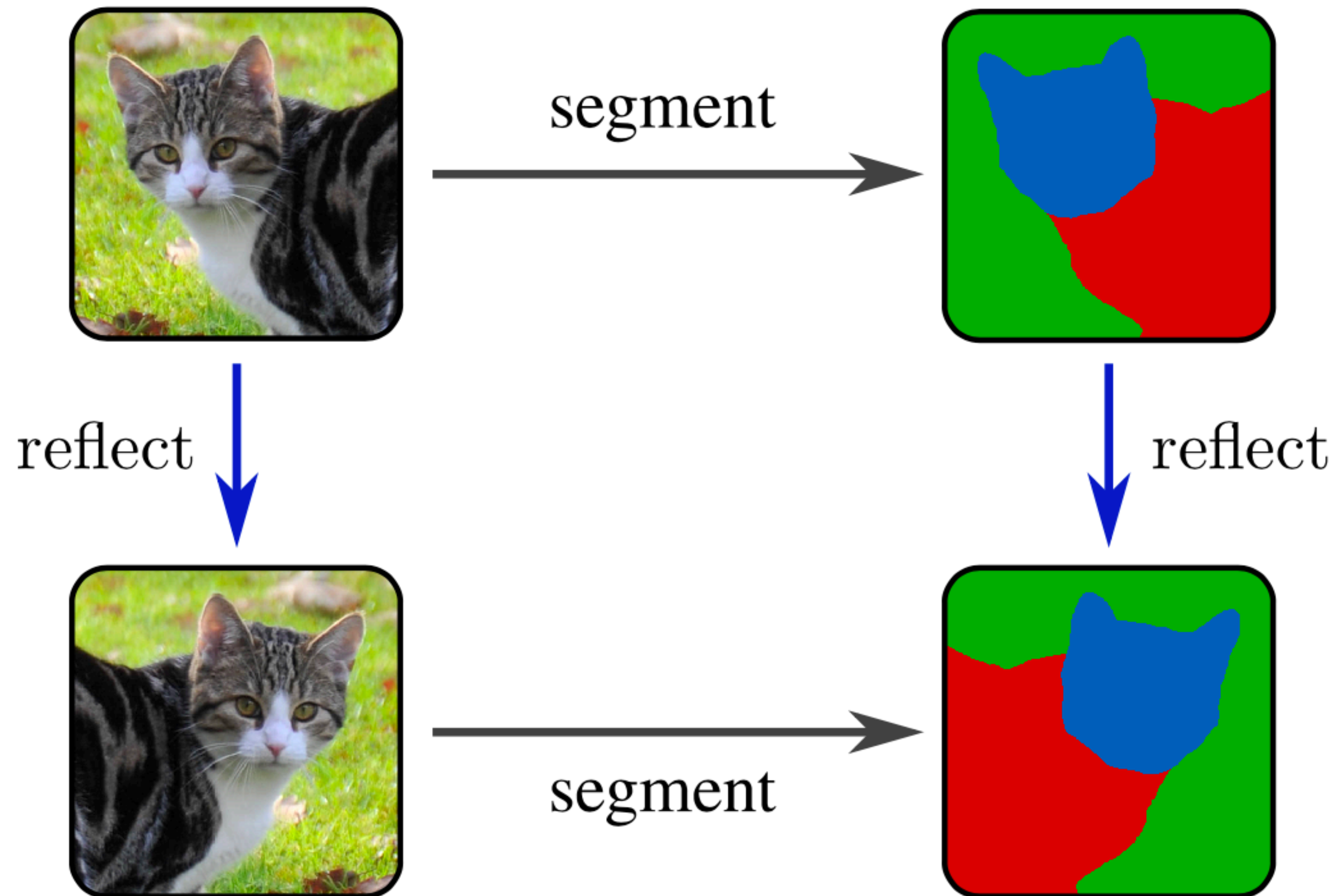
- $F : V_0 \xrightarrow{L_1} V_1 \xrightarrow{L_2} \dots \xrightarrow{L_l} V_l \xrightarrow{L_{l+1}} \dots \xrightarrow{L_\ell} V_\ell$
 - V_l finite dimensional vector spaces
 - L_l (affine) linear or simple non-linear maps

Invariant predictions tasks



- vanilla DNN could make different predictions when input is rotated or reflected
- goal: build symmetry of input space directly into the DNN

Equivariant prediction tasks



- in such tasks the output should transform correspondingly to the input
- goal: build input/output symmetry directly into your DNNs

Equivariant Deep Neural Network

- DNN: $F : V_0 \xrightarrow{L_1} V_1 \xrightarrow{L_2} \dots \xrightarrow{L_l} V_l \xrightarrow{L_{l+1}} \dots \xrightarrow{L_\ell} V_\ell$
- Let G be a group and for each $l = 0, 1, \dots, \ell$ fix:
 - $\rho_l : G \times V_l \rightarrow V_l, \quad (g, v) \mapsto \rho_l(g)(v)$ a group action
 - We call (ρ_l, V_l) a **(linear) representation for G**
- The DNN F is G -equivariant if every layer is G -equivariant.
- So focus on one **linear layer** (first): $L : V_{\text{in}} \rightarrow V_{\text{out}}$,
 - Equivariance means: $\forall g \in G. \forall v \in V_{\text{in}}.$
$$L(\rho_{\text{in}}(g)(v)) = \rho_{\text{out}}(g)(L(v)), \quad \text{or in short:} \quad L \circ \rho_{\text{in}}(g) = \rho_{\text{out}}(g) \circ L$$

Problems

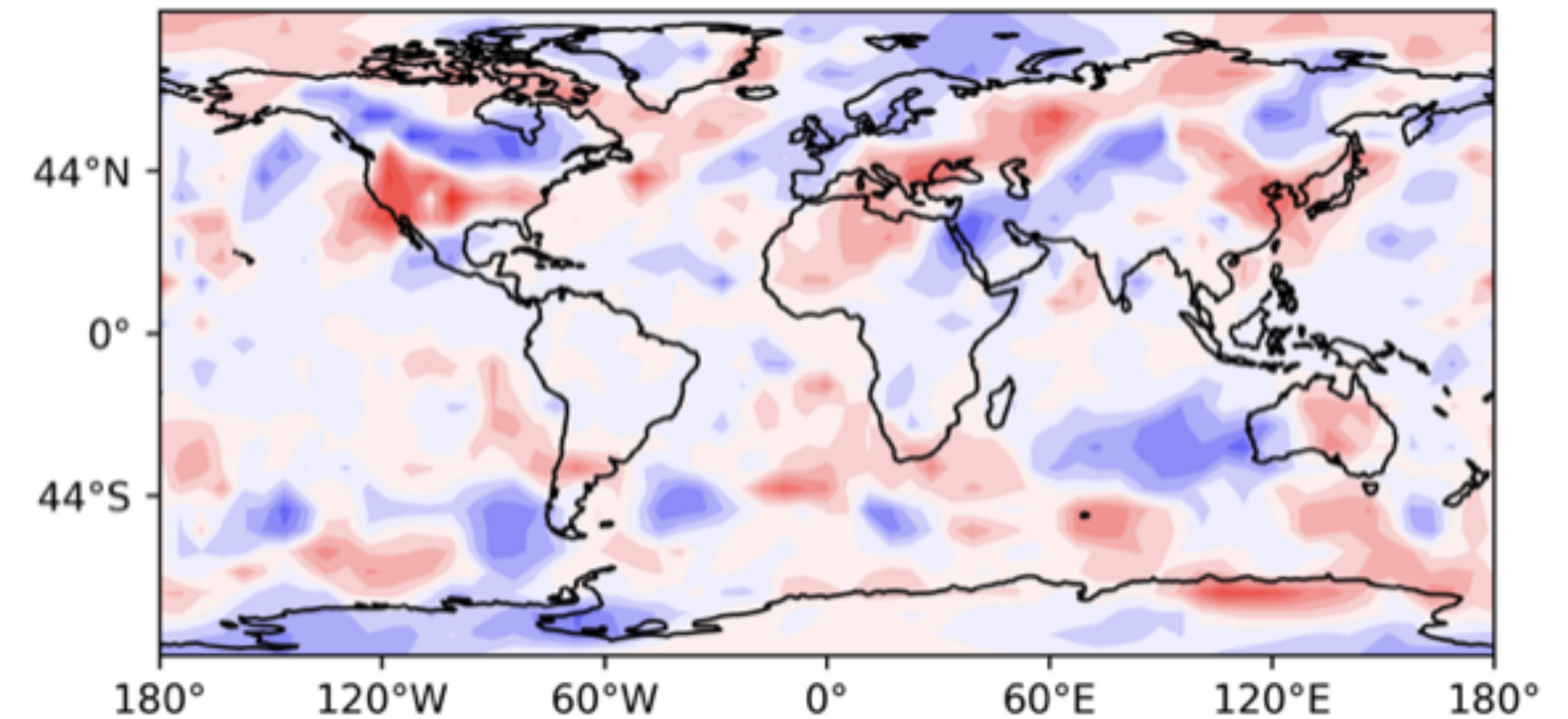
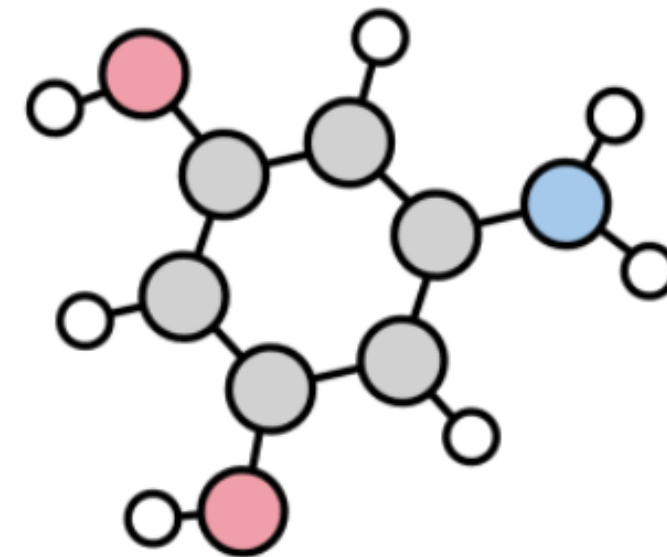
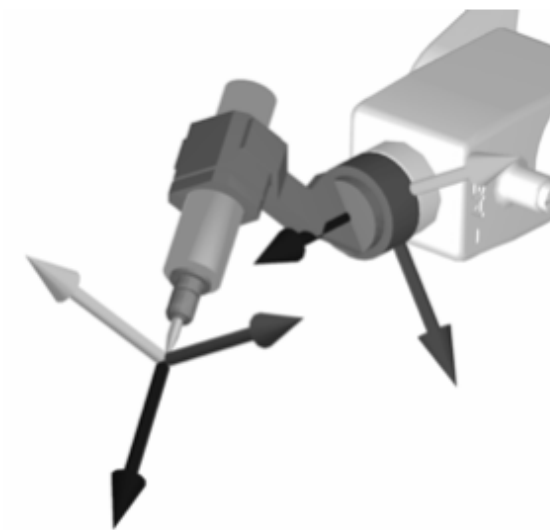
- For every different group G need to study and classify:
 - (irreducible) representations $\rho : G \times V \rightarrow V$
 - this explicitly known for finite and compact groups G
 - mainly for $SO(2)$, $O(2)$, $SO(3)$, $O(3)$ (circular and spherical harmonics)
- To increase expressivity or as partial result often needed:
 - tensor product representations: $V_i \otimes V_j$
 - need to decompose into irreducible representation again:

$$V_i \otimes V_j \cong \bigoplus_{k \in K} W_k \quad \text{and the matrices that project on such } W_k$$

Interest in Orthogonal and Pseudo-Orthogonal Transformations

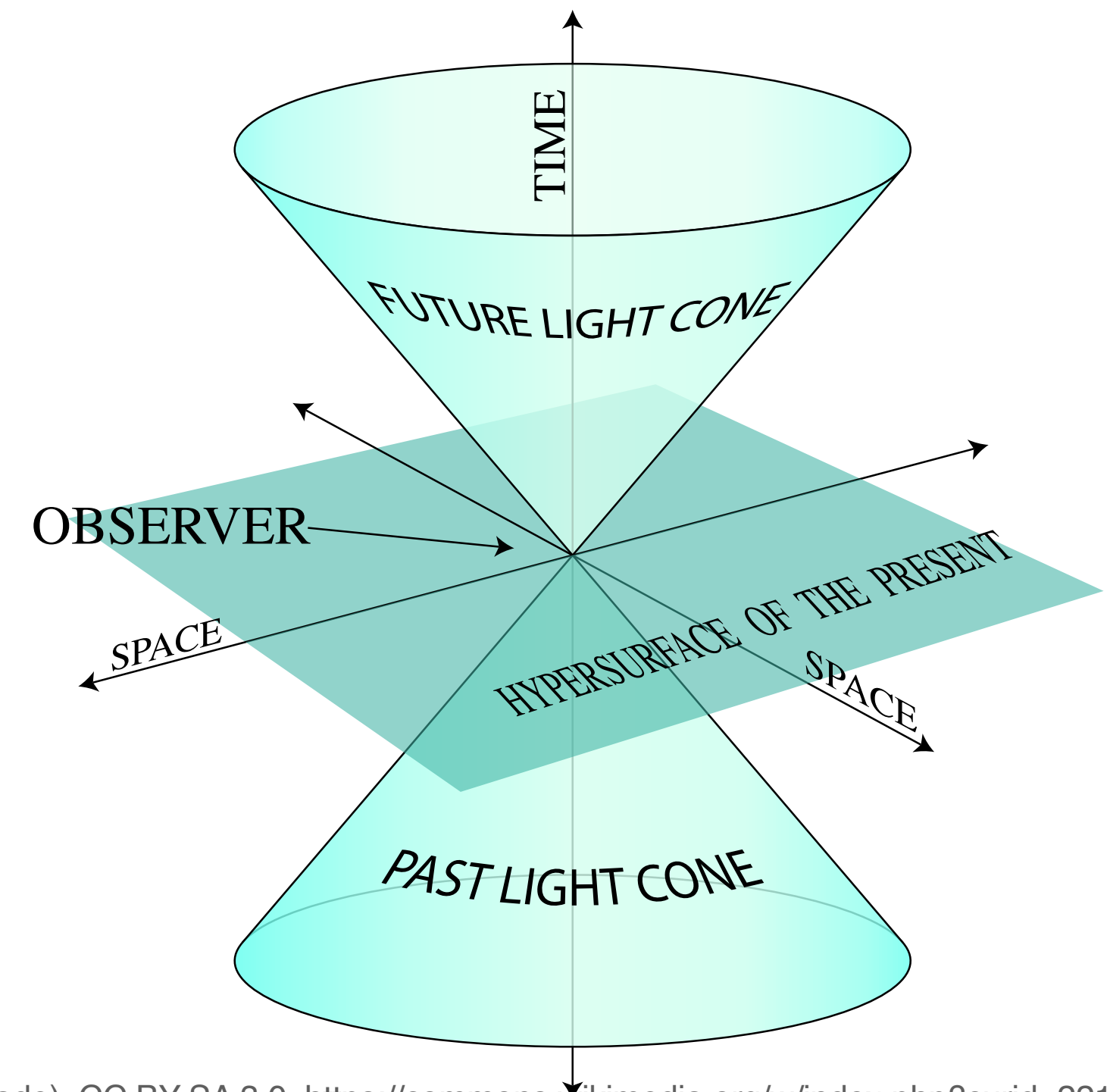
- Application area of **orthogonal transformations**:

- image and video processing
- molecular dynamics
- fluid dynamics
- robotics



- Application are of **pseudo-orthogonal transformations**:

- Lorentz boosts on Minkowski space (relativistic spacetime)
- mainly in special relativistic physics applications:
 - particle physics
 - electrodynamics
 - relativistic hydrodynamics



Problems

- **Pseudo-orthogonal group** $O(p, q)$ for $p, q \geq 1$
 - not compact, not connected matrix group
 - irreps are difficult to implement and understand for ML community
- Goal: find convenient (probably not irreducible) representations such that:
 - basis easy to get (not function spaces),
 - action easy to compute,
 - are flexible and expressive,
 - their dimension can be controlled (for computational purposes),
 - work in all dimensions $d \geq 1$ and signatures (p, q) .

Proposed Solution:

The Clifford Algebra

Clifford Group Equivariant Neural Networks

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- Presented at NeurIPS 2023 (oral)
- <https://github.com/DavidRuhe/clifford-group-equivariant-neural-networks>

Inner Product Spaces

- Let V be a finite dimensional vector space over $\mathbb{R}$ with $d = \dim V$.
- Let $\eta : V \times V \rightarrow \mathbb{R}$ be a non-degenerate, symmetric, bilinear form on V .
- We then call (V, η) a **inner product space**
- We abbreviate the corresponding quadratic form:

$$\mathbf{q} : V \rightarrow \mathbb{R}, \quad \mathbf{q}(v) := \eta(v, v)$$

- Note we do **not** require η to be (positive-semi) definite !

Orthonormal Basis

- Let (V, η) be a inner product space with elements $e_1, \dots, e_d \in V$.
- $e = [e_1, \dots, e_d]$ is called an **orthonormal basis** of (V, η) if:
 - $\eta(e_i, e_j) = 0$ for all $i \neq j$ in $[d] := \{1, \dots, d\}$
 - $\eta(e_i, e_i) \in \{\pm 1\}$ for all $i \in [d]$.
- Note that such bases always exist (over $\mathbb{R}$) and the numbers (p, q) of $+1, -1$'s is an invariant of (V, η) , called the **signature of (V, η)** .

Example - Standard Pseudo-Euclidean Spaces

- Let $V = \mathbb{R}^d$ and $p, q \in \mathbb{N}_0$ with $p + q = d$.

- Consider the $d \times d$ diagonal matrix:

$$\Delta^{p,q} := \text{diag}(\underbrace{+1, \dots, +1}_{\times p}, \underbrace{-1, \dots, -1}_{\times q})$$

- and symmetric, bilinear form $\eta^{p,q}$ on (column) vectors $v_1, v_2 \in \mathbb{R}^d$ as:

$$\eta^{p,q}(v_1, v_2) := v_1^\top \Delta^{p,q} v_2$$

- We abbreviate: $\mathbb{R}^{p,q} := (\mathbb{R}^d, \eta^{p,q})$ and call it the **Standard (Pseudo-)Euclidean Space of signature (p, q)** .

The Clifford Algebra - Ad Hoc Definition

- Let (V, η) be inner product space with orthonormal basis $e = [e_1, \dots, e_d]$.
- We define the **Clifford algebra** (aka **geometric algebra**) $Cl(V, \eta)$ of (V, η) as the vector space spanned by the following formal basis elements:
 - $1_{Cl(V, \eta)}$
 - $e_1, \dots, e_d$
 - $e_{1,2}, e_{1,3}, \dots, e_{i_1, i_2}, \dots, e_{d-1, d}$ with $i_1 < i_2$
 - $e_{1,2,3}, \dots, e_{i_1, i_2, i_3}, \dots, e_{d-2, d-1, d}$ with $i_1 < i_2 < i_3$
 - etc.
 - $e_{1,2,\dots,d}$
- Note that there are no repeated indices in each element and they need to be in order.

The Clifford Algebra - Short Notations

- We can abbreviate the notation as follows.
- Define for a subset $A \subseteq [d]$ of size $k > 0$ the element:
 - $e_A := e_{i_1, \dots, i_k}$ with $A = \{i_1 < \dots < i_k\}$,
 - $e_\emptyset := 1_{\text{Cl}(V, \eta)}$
- We interpret the basis elements as products of basis vectors:
 - $e_A = e_{i_1, \dots, i_k} = e_{i_1} \bullet \dots \bullet e_{i_k}$

Clifford Algebra - The Dimension

- In particular, we have:

$$\dim \text{Cl}(V, \eta) = |\{A \subseteq [d]\}| = 2^d,$$

- and, every element $x \in \text{Cl}(V, \eta)$ can uniquely be written as:

$$x = \sum_{A \subseteq [d]} x_A \cdot e_A \quad \text{with} \quad x_A \in \mathbb{R}.$$

Geometric Product via the Fundamental Relations

- Let (V, η) be inner product space with orthonormal basis $e = [e_1, \dots, e_d]$ of signature (p, q) . We then extend the **geometric product** by the following relations:

$$e_j \bullet e_i = \begin{cases} -e_i \bullet e_j & \text{if } i < j, \\ +1 & \text{if } i = j \in [1, p], \\ -1 & \text{if } i = j \in [p + 1, p + q]. \end{cases}$$

The Fundamental Relation

- Let $v_1, v_2 \in V$ then we have the **following fundamental relation** considered as elements in $Cl(V, \eta)$:

$$v_2 \bullet v_1 = -v_1 \bullet v_2 + 2 \cdot \eta(v_1, v_2) \cdot 1_{Cl(V, \eta)}$$

The Geometric Product for General Elements

- We can now turn the **Clifford algebra** $\text{Cl}(V, \eta)$ into an algebra via extending the **geometric product**:

$$\begin{aligned} x \bullet y &= \left(\sum_{A \subseteq [d]} x_A \cdot e_A \right) \bullet \left(\sum_{B \subseteq [d]} y_B \cdot e_B \right) \\ &= \sum_{A \subseteq [d]} \sum_{B \subseteq [d]} (x_A \cdot y_B) \cdot (e_A \bullet e_B) \end{aligned}$$

- The element $e_A \bullet e_B$ can now be simplified with the above relations.

Example: The Geometric Product

- Assume $\eta(e_3, e_3) = 1$, then we have:
 - $e_2 \cdot e_3 \cdot e_1 \cdot e_3 = -e_2 \cdot e_1 \cdot e_3 \cdot e_3 = -e_2 \cdot e_1 = e_1 \cdot e_2 = e_{1,2}$.
- So we get a standard basis element back.
- The same trick can be used to simplify any element $e_A \cdot e_B$:

$$e_A \cdot e_B = \text{sgn}^{A,B} \cdot \prod_{i \in A \cap B} \eta(e_i, e_i) \cdot e_{A \Delta B}$$

Extending the Inner Product

- Let $e = [e_1, \dots, e_d]$ be an orthonormal basis of inner product space (V, η) .
- Then the system $(e_A)_{A \subseteq [d]}$ forms an **orthonormal basis** of $\text{Cl}(V, \eta)$ w.r.t. the **extended inner product** $\bar{\eta}$ defined via:

$$\bar{\eta}(e_A, e_B) := \delta_{A,B} \cdot \prod_{i \in A} \eta(e_i, e_i).$$

- This turns $\text{Cl}(V, \eta)$ into an inner product space in itself w.r.t. $\bar{\eta}$.
- Furthermore, $\bar{\eta}$ is independent of the chosen orthonormal basis.

k-Vectors

- Let $e = [e_1, \dots, e_d]$ be an orthogonal basis of the quadratic vector space (V, η) . For $k = 0, \dots, d$, we define the **grade- k -subspace** of $\text{Cl}(V, \eta)$ as follows:

$$\text{Cl}^{(k)}(V, \eta) := \text{span} \{ e_A \mid A \subseteq [d], |A| = k \}$$

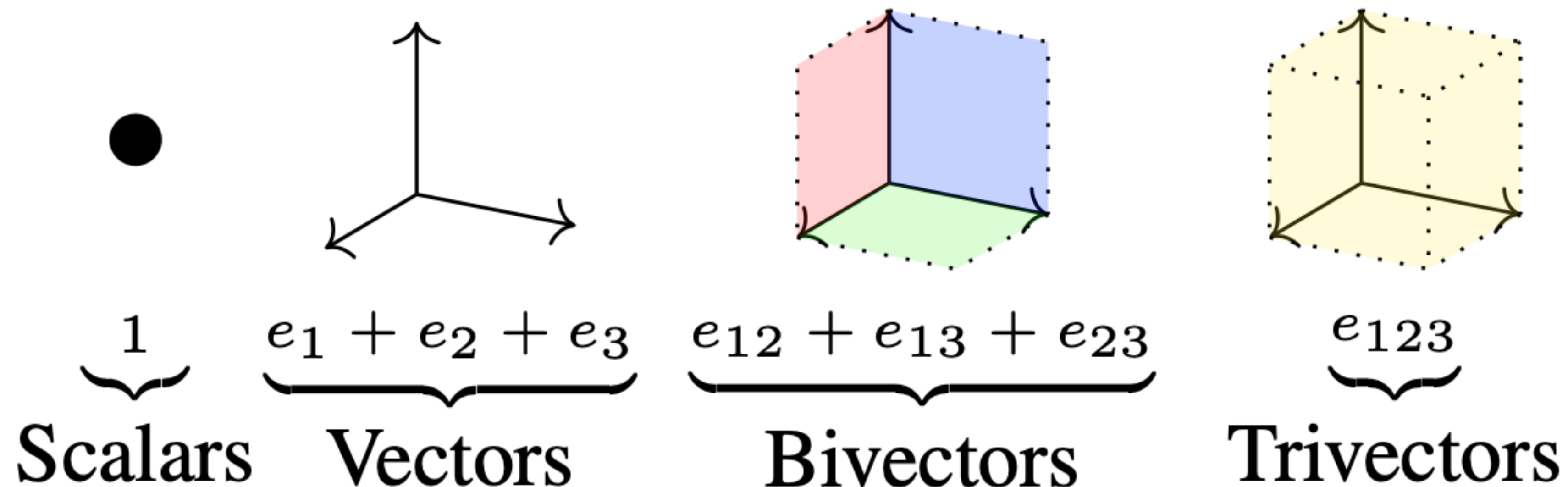
consisting of all **k -vectors** (aka **k -blade**), i.e. elements of the form:

$$x = \sum_{A \subseteq [d], |A| = k} x_A \cdot e_A.$$

- Theorem: $\text{Cl}^{(k)}(V, \eta)$ does not depend on the chosen orthogonal basis.

Example: k-Vectors

- We can identify:
 - $C1^{(0)}(V, \eta) = \mathbb{R}$ i.e. 0-vectors = scalars
 - $C1^{(1)}(V, \eta) = V$ i.e. 1-vectors = vectors



Grade Decomposition and Grade Projection

- We thus have an **orthogonal direct sum decomposition**:

$$\bullet \text{Cl}(V, \eta) = \bigoplus_{k=0}^d \text{Cl}^{(k)}(V, \eta), \quad \dim \text{Cl}^{(k)}(V, \eta) = \binom{d}{k}$$

- an **orthogonal projection map** onto the grade- k -component:

$$(_)^{(k)} : \text{Cl}(V, \eta) \rightarrow \text{Cl}^{(k)}(V, \eta),$$

$$x = \sum_{A \subseteq [d]} x_A \cdot e_A \mapsto \sum_{A \subseteq [d], |A| = k} x_A \cdot e_A =: x^{(k)}.$$

The (Pseudo-)Orthogonal Group

- Let (V, η) be a quadratic vector space / inner product space.

- The **(pseudo-)orthogonal group** of (V, η) is defined as:

$$O(V, \eta) := \{ g \in GL(V) \mid \forall v \in V. \eta(gv, gv) = \eta(v, v) \}.$$

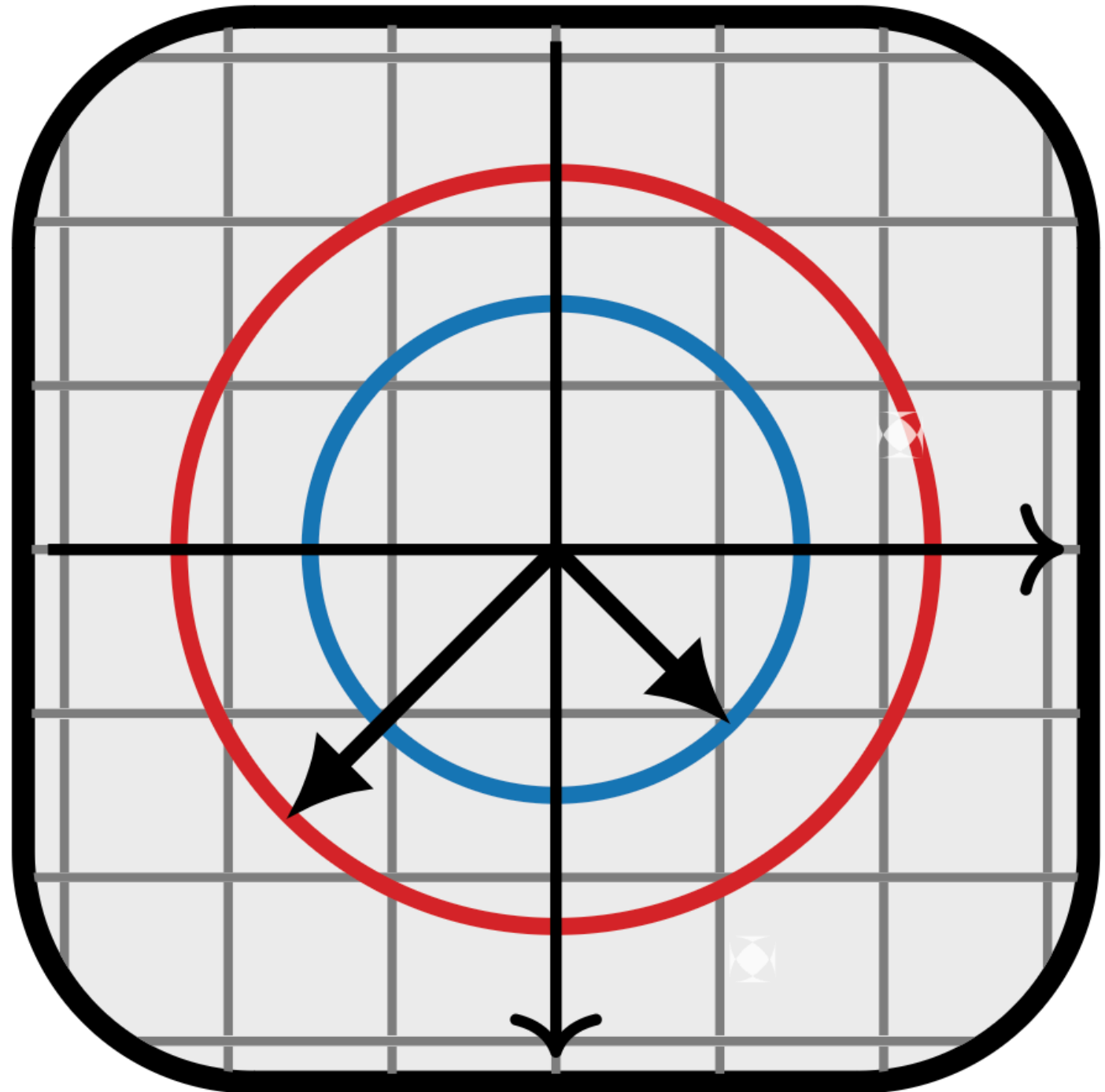
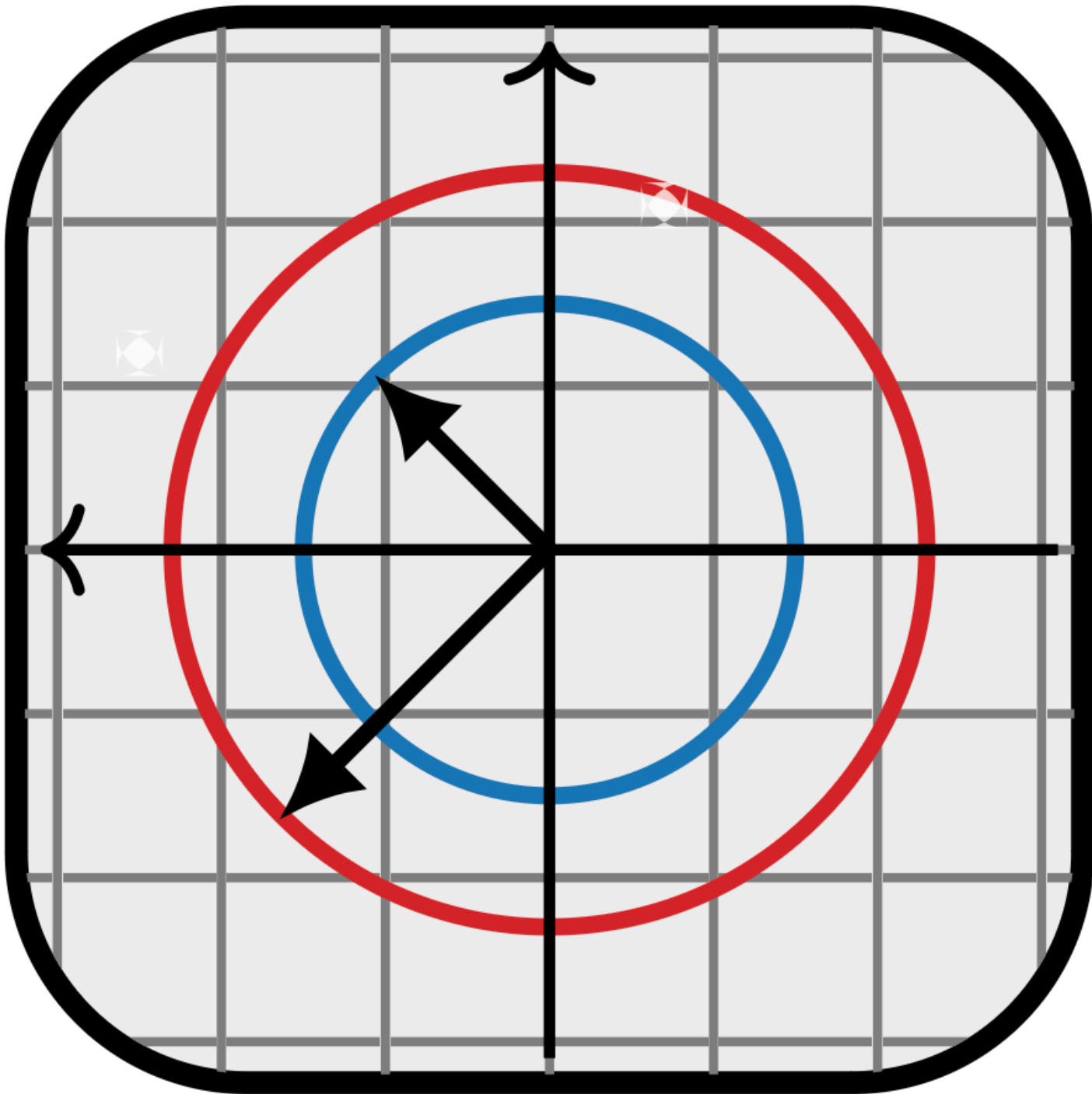
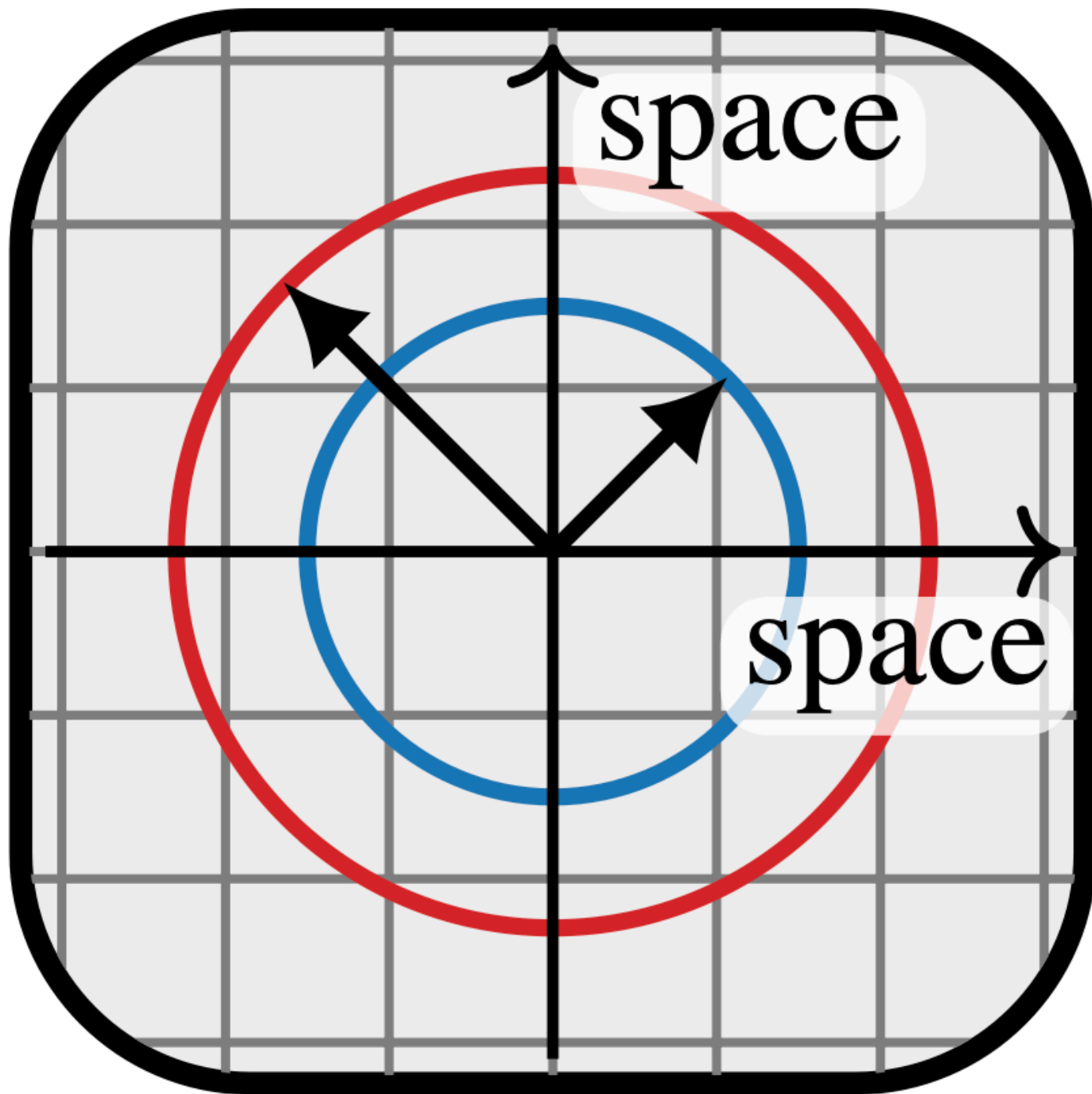
- The **special (pseudo-)orthogonal group** of (V, η) is:

$$SO(V, \eta) := \{ g \in O(V, \eta) \mid \det g = 1 \}.$$

Example: Orthogonal Transformation in Euclidean Space

rotation

reflection

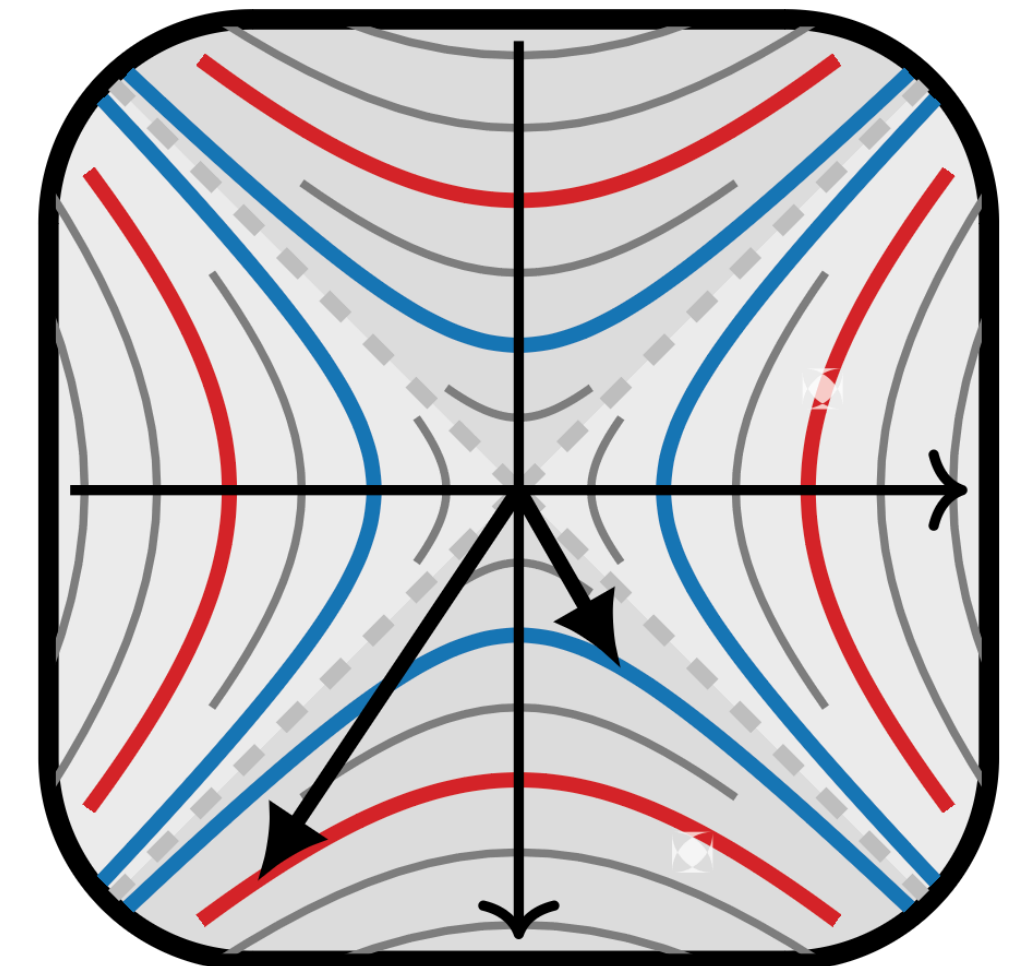
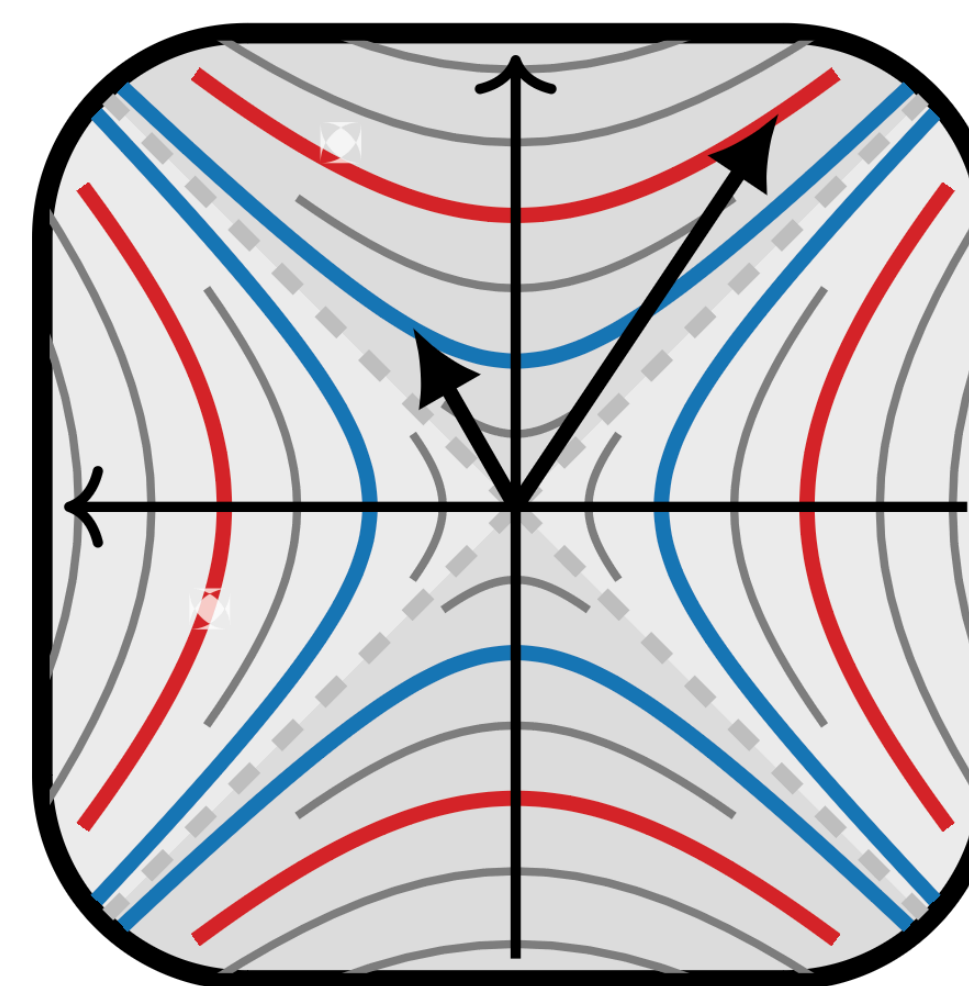
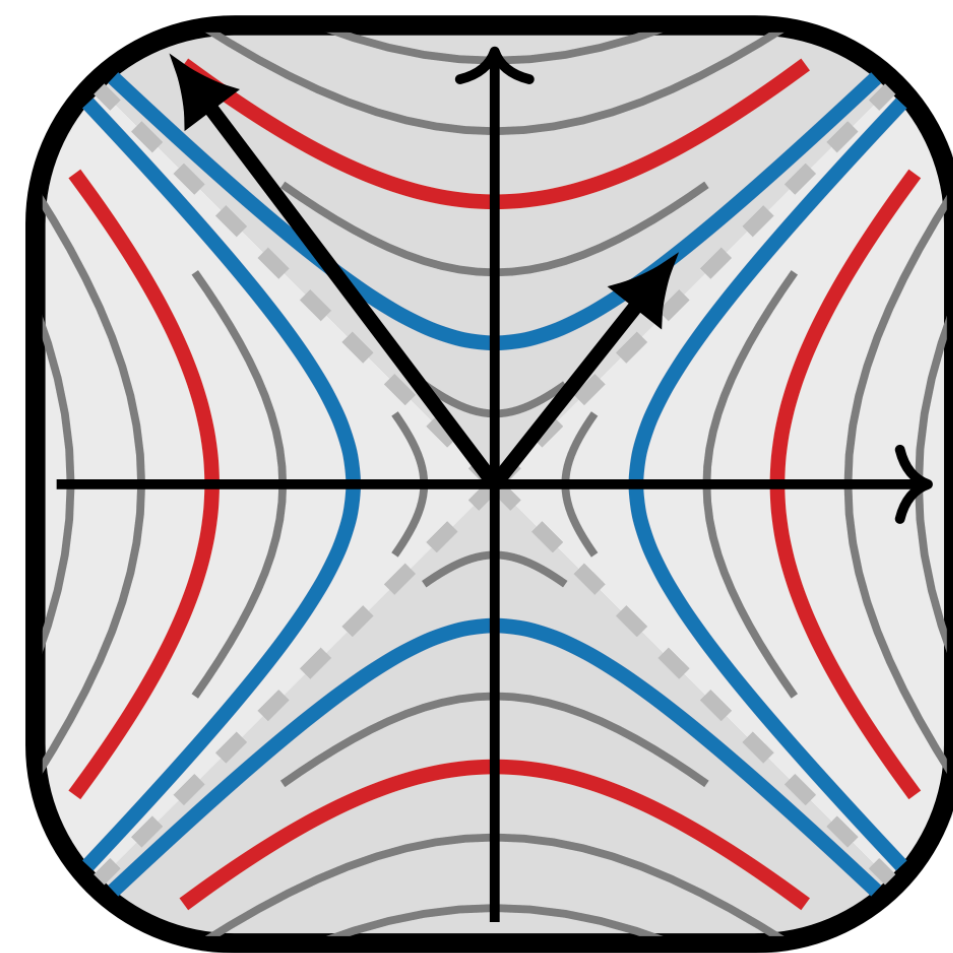
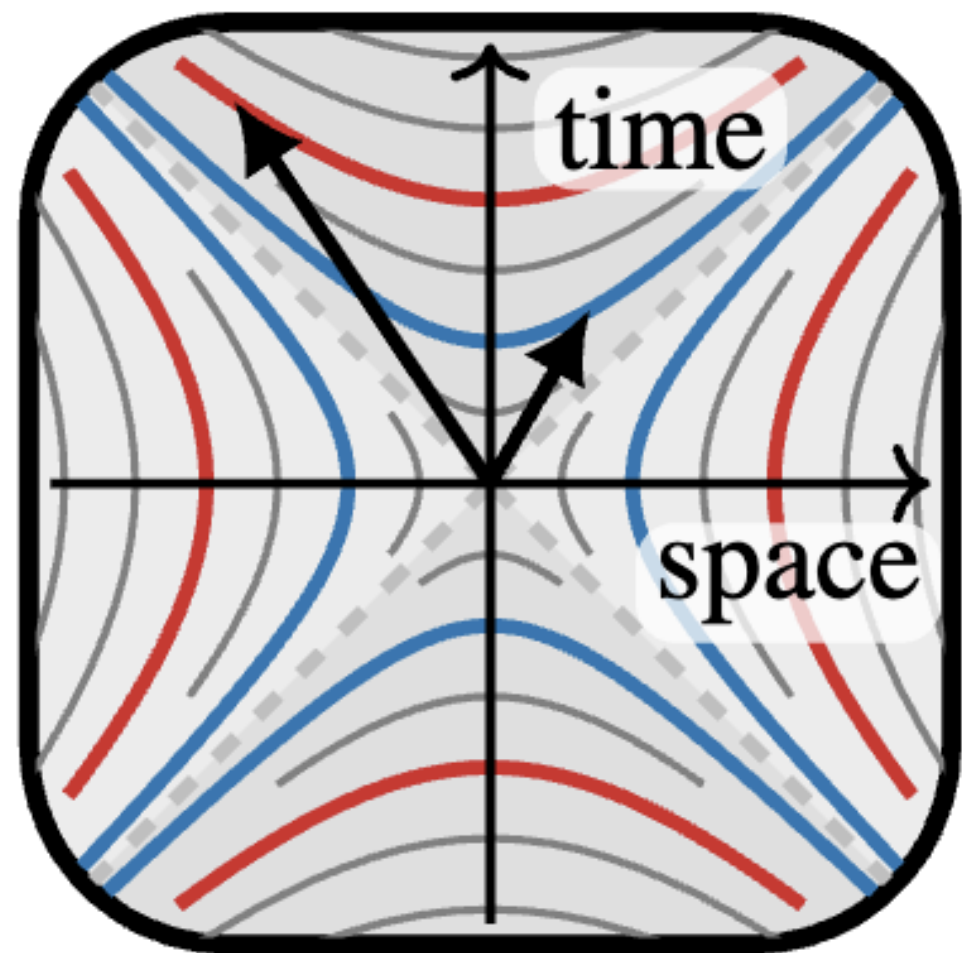


Example: Orthogonal Transformation in Pseudo-Euclidean Space

Lorentz boost

space reflection

time reflection



(+ rotations)

The Orthogonal Group Action

- Let (V, η) be a quadratic vector space / inner product space and

$$x = \sum_{i \in I} c_i \cdot v_{i,1} \cdot \cdots \cdot v_{i,l_i} \in \text{Cl}(V, \eta) \quad \text{and} \quad g \in \text{O}(V, \eta).$$

- Then we define the action of g on x as follows:

$$\rho_{\text{Cl}}(g)(x) := \sum_{i \in I} c_i \cdot (gv_{i,1}) \cdot \cdots \cdot (gv_{i,l_i}) \in \text{Cl}(V, \eta)$$

- By the universal property this is well-defined and gives action:

$$\rho_{\text{Cl}} : \text{O}(V, \eta) \times \text{Cl}(V, \eta) \rightarrow \text{Cl}(V, \eta), \quad (g, x) \mapsto \rho_{\text{Cl}}(g)(x).$$

Orthogonal Group Action - Properties

- We have the following properties for ρ_{C1} :
- linear: $\rho_{C1}(g)(c_1 \cdot x_1 + c_2 \cdot x_2) = c_1 \cdot \rho_{C1}(g)(x_1) + c_2 \cdot \rho_{C1}(g)(x_2)$
- composing: $\rho_{C1}(g_2)(\rho_{C1}(g_1)(x)) = \rho_{C1}(g_2 g_1)(x)$
- invertible: $\rho_{C1}(g)^{-1}(x) = \rho_{C1}(g^{-1})(x)$
- orthogonal: $\bar{\eta}(\rho_{C1}(g)(x_1), \rho_{C1}(g)(x_2)) = \bar{\eta}(x_1, x_2)$
- multiplicative: $\rho_{C1}(g)(x_1 \cdot x_2) = \rho_{C1}(g)(x_1) \cdot \rho_{C1}(g)(x_2)$
- grade preserving: $(\rho_{C1}(g)(x))^{(k)} = \rho_{C1}(g)(x^{(k)})$

Corollary

- So the following maps are $O(V, \eta)$ -equivariant:

$$\begin{array}{ccc} \mathrm{Cl}(V, \eta) \times \mathrm{Cl}(V, \eta) & \xrightarrow{\quad \bullet \quad} & \mathrm{Cl}(V, \eta) \\ \rho_{\mathrm{Cl}}(g) \times \rho_{\mathrm{Cl}}(g) \downarrow & & \downarrow \rho_{\mathrm{Cl}}(g) \\ \mathrm{Cl}(V, \eta) \times \mathrm{Cl}(V, \eta) & \xrightarrow{\quad \bullet \quad} & \mathrm{Cl}(V, \eta) \end{array}$$

- Geometric product.

$$\begin{array}{ccc} \mathrm{Cl}(V, \eta) & \xrightarrow{(\cdot)^{(k)}} & \mathrm{Cl}^{(k)}(V, \eta) \\ \rho_{\mathrm{Cl}}(g) \downarrow & & \downarrow \rho_{\mathrm{Cl}}(g) \\ \mathrm{Cl}(V, \eta) & \xrightarrow{(\cdot)^{(k)}} & \mathrm{Cl}^{(k)}(V, \eta) \end{array}$$

- Grade projections.

- $\mathrm{Cl}^{(k)}(V, \eta)$ are thus sub-representations!

Clifford Group Equivariant Neural Networks

- A **Clifford Group Equivariant Neural Network (CGENN)** is a composition:

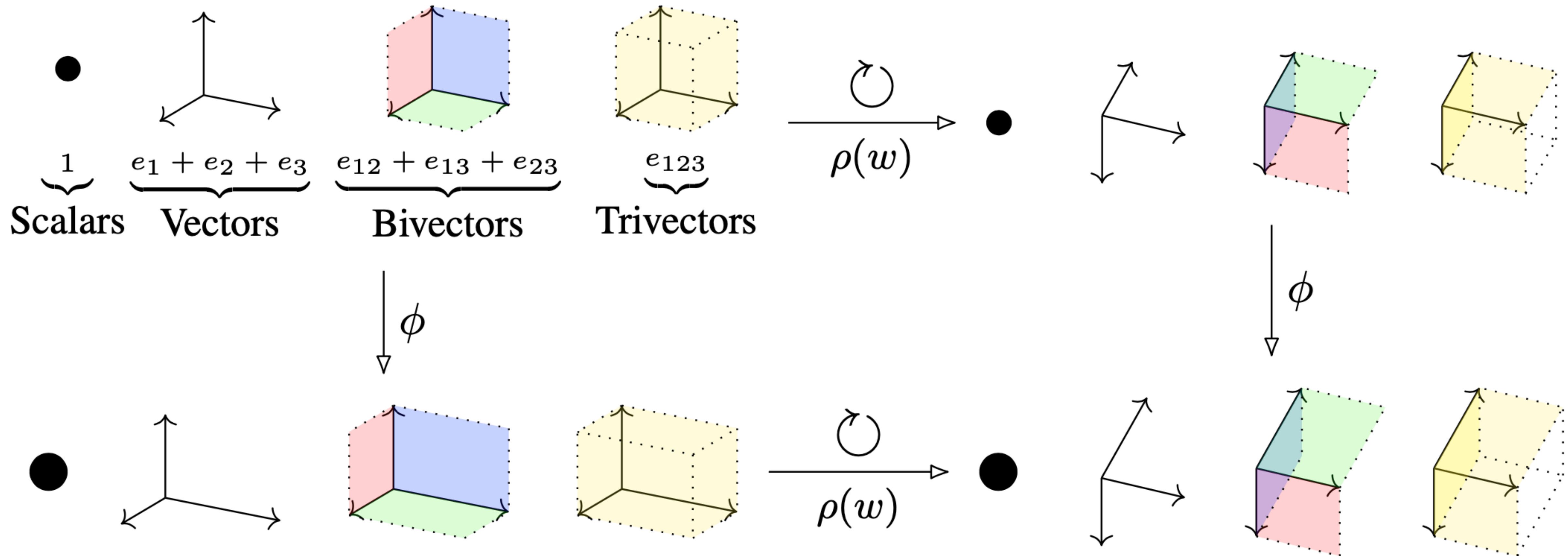
$$F : V_0 \xrightarrow{L_1} V_1 \xrightarrow{L_2} \dots \xrightarrow{L_l} V_l \xrightarrow{L_{l+1}} \dots \xrightarrow{L_\ell} V_\ell$$

where $V_l = \text{Cl}(V, \eta)^{c_l}$ and $L_l = L : V_{\text{in}} \rightarrow V_{\text{out}}$ is either:

- **Linear layer:** $\forall m \in [c_{\text{out}}]: \quad L_m^{(k)}(x_1, \dots, x_{c_{\text{in}}}) := \sum_{n=1}^{c_{\text{in}}} w_{m,n}^k \cdot x_n^{(k)},$
- **Geometric Product layer:** $P^{(k)}(x_1, x_2) := \sum_{m=0}^d \sum_{n=0}^d w_{m,n}^k \cdot (x_1^{(m)} \bullet x_2^{(n)})^{(k)}$
- **Nonlinearity:** $A(x) := \sigma(x^{(0)}) \cdot x, \quad \text{or} \quad A^{(k)}(x^{(k)}) = \sigma(\bar{q}(x^{(k)})) \cdot x^{(k)}.$

Theorem - CGENN are $O(V, \eta)$ -equivariant

- Theorem: All CGENN are automatically $O(V, \eta)$ -equivariant.



Remark - CGENNs

- Note that the geometric product layers are non-linear, but still $O(V, \eta)$ -equivariant. We could also simplify them to:
$$P(x_1, x_2) = w \cdot x_1 \bullet x_2$$
- Note that we can just replace all occurring deep learning architectures with corresponding Clifford layers to make them $O(V, \eta)$ -equivariant,
 - e.g. graph or message-passing neural networks.

CGENN - Experiments

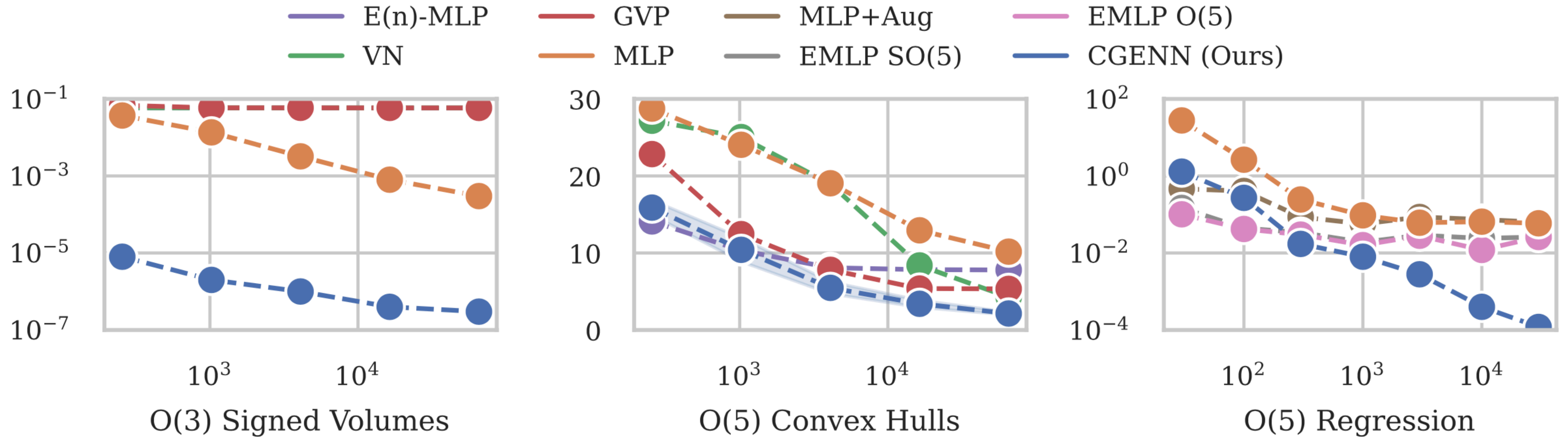


Figure 3: Left: Test mean-squared errors on the $O(3)$ signed volume task as functions of the number of training data. Note that due to identical performance, some baselines are not clearly visible. Right: same, but for the $O(5)$ convex hull task.

Figure 4: Test mean-squared-errors on the $O(5)$ regression task.

CGENN - Top Tagging: $O(1,3)$ -Experiment

- Particle collider experiment at CERN's ATLAS detector
- produces and measures particle jets
- goal: **predict** if particle jet contains **top quark**
- each jet has ~ 200 particles, each given with energy-momentum vector
- those live in relativistic spacetime = Minkowski space $V = \mathbb{R}^{1,3}$
- due to special relativity, prediction should be invariant under Lorentz boosts, i.e. under action of the Lorentz group $O(1,3)$.
- train/validation/test set: 1.2M, 0.4M, 0.4M entries
- only LGN is steerable, EGNN and LorentzNet scalarized (invariant), rest not

CGENN - Top Tagging: $O(1,3)$ -Experiment

Model	Accuracy ($\uparrow$)	AUC ($\uparrow$)	$1/\epsilon_B$ ($\uparrow$) ($\epsilon_S = 0.5$)	$1/\epsilon_B$ ($\uparrow$) ($\epsilon_S = 0.3$)
ResNeXt [XGD ⁺ 17]	0.936	0.9837	302	1147
P-CNN [CMS17]	0.930	0.9803	201	759
PFN [KMT19]	0.932	0.9819	247	888
ParticleNet [QG20]	0.940	0.9858	397	1615
EGNN [SHW21]	0.922	0.9760	148	540
LGN [BAO ⁺ 20]	0.929	0.9640	124	435
LorentzNet [GMZ ⁺ 22]	0.942	0.9868	498	2195
CGENN	0.942	0.9869	500	2172

Table 2: Performance comparison between our proposed method and alternative algorithms on the top tagging experiment. We present the accuracy, Area Under the Receiver Operating Characteristic Curve (AUC), and background rejection $1/\epsilon_B$ and at signal efficiencies of $\epsilon_S = 0.3$ and $\epsilon_S = 0.5$.

- Minkowski metric: $(1, -1, -1, -1)$, group: $G = O(1,3)$

Equivariant Simplicial Message Passing

Algorithm 1 Shared Simplicial Message Passing

Require: $K, \forall \sigma \in K : h^\sigma, \phi^m, \phi^h$

Repeat:

$$m^\sigma \leftarrow \text{Agg}_{\substack{\tau \in B(\sigma) \\ \tau \in C(\sigma) \\ \tau \in N_\uparrow(\sigma) \\ \tau \in N_\downarrow(\sigma)}} \phi^m(h^\sigma, h^\tau, \dim \sigma, \dim \tau)$$

$$h^\sigma \leftarrow \phi^h(h^\sigma, m^\sigma, \dim \sigma)$$

- where the message and update functions: ϕ^m, ϕ^h are CGENNs

Equivariant Convolution Layer for Multi-Vector Fields

- Let (V, η) be an inner product space of signature (p, q) , $d = p + q$.
- Consider linear layer $L : \Gamma(V, \text{Cl}(V, \eta)^{c_{\text{in}}}) \rightarrow \Gamma(V, \text{Cl}(V, \eta)^{c_{\text{out}}})$ given by:

$$L(f)(x) := \int_V K(v)[f(x - v)] dv, \quad \text{with kernel } K = H \circ Y,$$

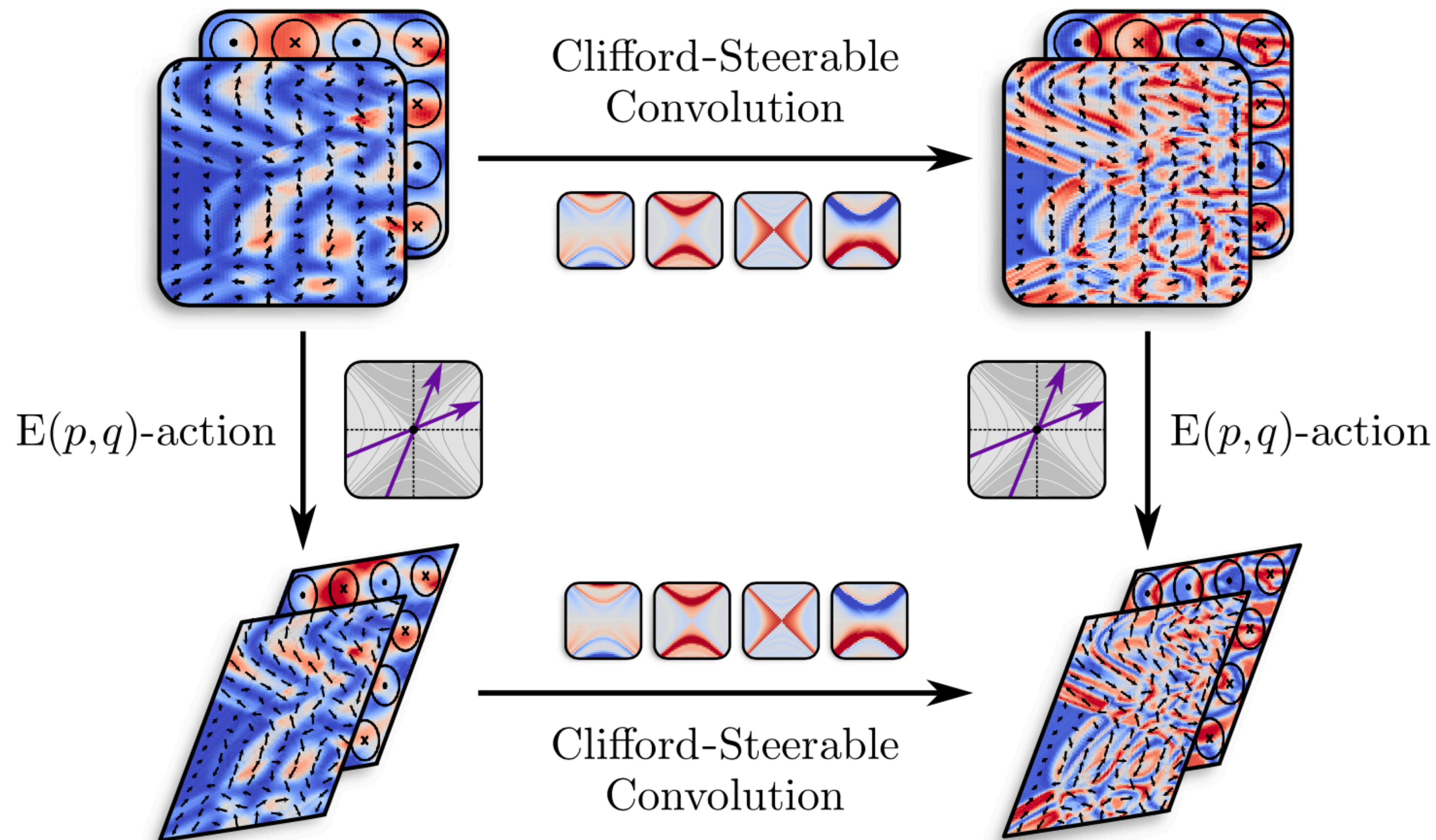
- where Y is CGENN and **kernel head** H is linear $\text{O}(V, \eta)$ -equivariant top layer:

$$K : V \xrightarrow{Y} \text{Cl}(V, \eta)^{c_{\text{out}} \times c_{\text{in}}} \xrightarrow{H} \text{hom}(\text{Cl}(V, \eta)^{c_{\text{in}}}, \text{Cl}(V, \eta)^{c_{\text{out}}}).$$

- Then K is always $\text{O}(V, \eta)$ -**steerable** and L is $\text{E}(V, \eta)$ -**equivariant**:
 - i.e. for all $(t, g) \in \text{E}(V, \eta)$ and $f \in \Gamma(V, \text{Cl}(V, \eta)^{c_{\text{in}}})$ we have:

$$L((t, g) \triangleright f) = (t, g) \triangleright L(f).$$

Clifford-Steerable Convolutional Neural Networks



Experiments:

- Forecasting task: trained on past, predict future:
 - Fluid dynamics on $\mathbb{R}^2$ (incompressible Navier-Stokes)
 - Electrodynamics on $\mathbb{R}^3$ (Maxwell equations)
 - Electrodynamics on $\mathbb{R}^{1,2}$ (Maxwell equations)

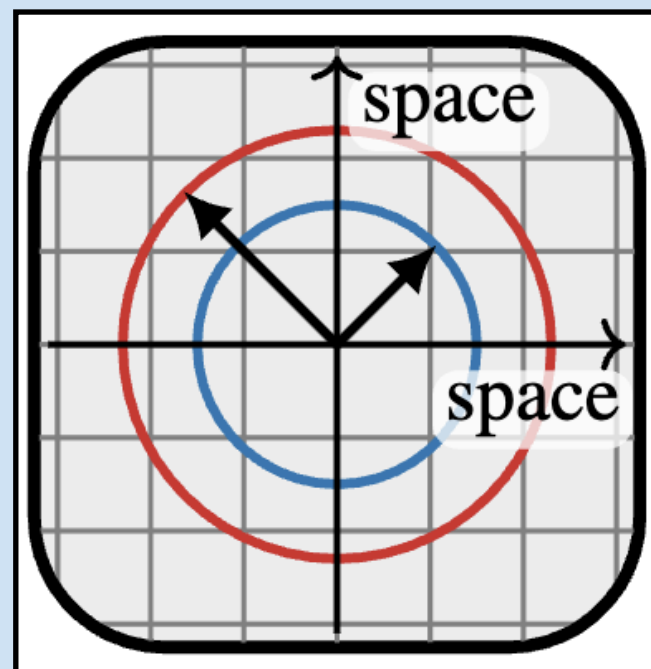
Steerable Convolutional Neural Networks

prior research

main paper

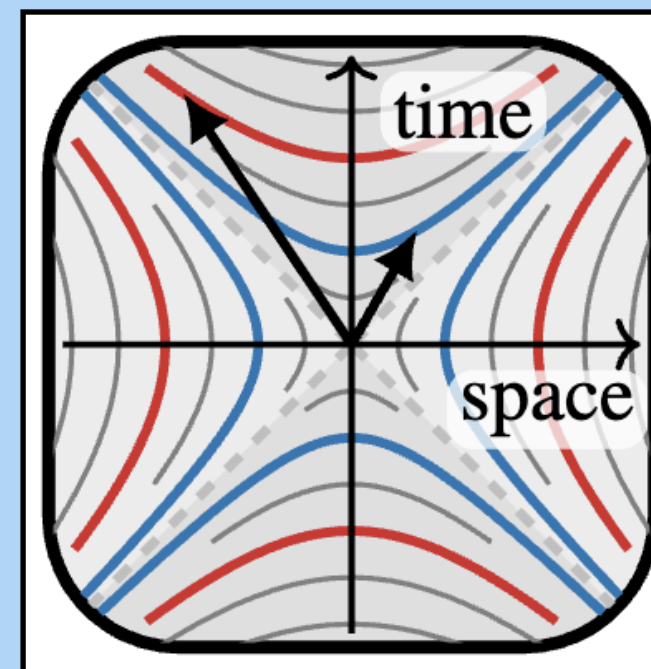
appendix

Euclidean space



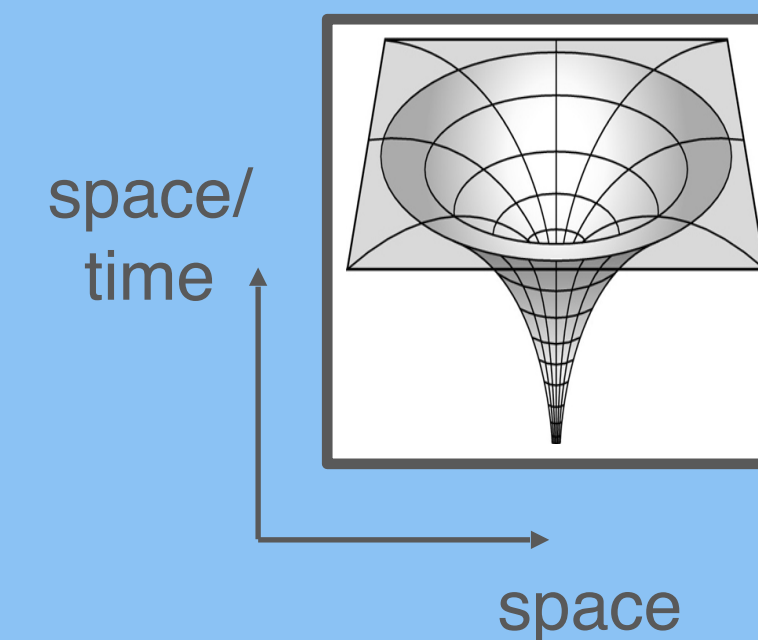
classical physics

pseudo-Euclidean space



special relativity

pseudo-Riemannian manifold



general relativity

Equivariant Attention Layer for Transformers

$$\text{Attention}(Q, K, V)_{i,c'} := \sum_{t=1}^T \text{Softmax}_t \left(\sum_c^C \frac{\bar{\eta}(Q_{i,c}, K_{t,c})}{\sqrt{16C}} \right) \cdot V_{t,c'}$$

- query multi-vectors: Q
 - key multi-vectors: K
 - value multi-vectors: V
 - number of multi-vector channels: C
-
- J. Brehmer, P. de Haan, S. Behrends, T. Cohen. **Geometric Algebra Transformers**. NeurIPS 2023.
 - J. Spinner, V. Bresó, P. de Haan, T. Plehn, J. Thaler, J. Brehmer. **Lorentz-Equivariant Geometric Algebra Transformers for High-Energy Physics**. NeurIPS 2024.

Equivariant Diffusion Model

- $p(z_t^{(m)} | z^{(m)}) := \mathcal{N} \left(z_t^{(m)} | \sqrt{\bar{\alpha}_t} \cdot z^{(m)}, (1 - \bar{\alpha}_t) \cdot I \right)$
 - $p(z_t | z) = \prod_{m=0}^d p(z_t^{(m)} | z^{(m)})$
 - $\text{Loss} := \mathbb{E}_{t \sim U, x_1 \sim q, \epsilon \sim \mathcal{N}(0, I)} [\|\phi_w(x_t(x_1)), t) - \epsilon\|^2]$
 - with CGENN ϕ_w
-
- C. Liu, S. Vagstad, D. Ruhe, E. Bekkers, P. Forré. **Clifford Group Equivariant Diffusion Models for 3D Molecular Generation**. ICLR 2025 Workshop: Frontiers in Probabilistic Inference.

Summary - CGENNs

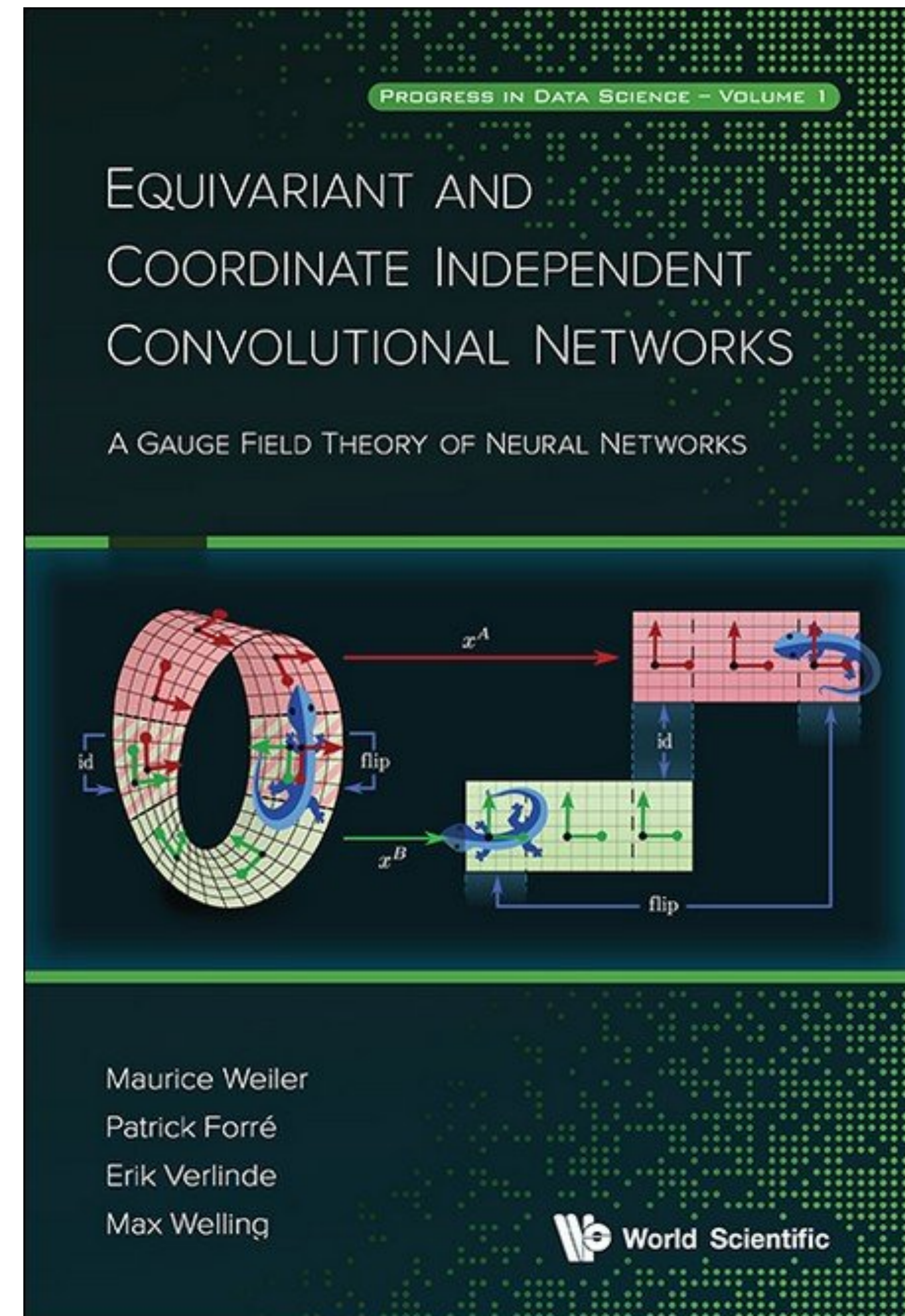
- CGENNs are based on Clifford algebra layers
- process multi-vector features
- incorporate space/spacetime symmetries, i.e. are $O(V, \eta)$ -equivariant
- work in any dimension d and signature (p, q, r) with same code base
- are flexible, expressive, practical
- can be combined with other architectures (graph NN, simplicial message passing NN, convolutional neural networks, diffusion models, transformers, etc.)
- perform well in comparison to other methods on $O(V, \eta)$ -equivariant prediction tasks
- can be improved by more efficient implementations

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 - => last 3 papers also presented at AGACSE 2024.



Thank you for your attention!