Lecture 6: More on Coordinate-Independent CNNs: Convolutions and Isometry

Geometry and Topology in Machine Learning Seminar

June 30th, 2025

Outline

Recall: Why “Feature Spaces” on Manifolds?

- Classical CNNs store a feature map $f : \mathbb{R}^d \to \mathbb{R}^c$.
- A manifold M has no global coordinate, so we use sections of a vector bundle over M.
- Goal: make features independent of any chosen gauge / coordinates.

$$\boxed{G\text{-equivariant feature field}} \iff \boxed{\text{section of } \mathcal{A} := GM \times_\rho \mathbb{R}^c}$$

Key Ingredients

1. FM – frame bundle, principal $GL_n(\mathbb{R})$.
2. $GM \subset FM$ – chosen G-structure for $G \leq \mathrm{GL}_n(\mathbb{R})$.
3. $\rho : G \to GL(\mathbb{R}^c)$ – channel representation.

Recall: The Frame Bundle FM

Definition

$$FM = \bigsqcup_{p \in M} F_pM, \; F_pM = \left\{[v_1, \ldots, v_d] \mid \{v_i\} \text{ is a basis of } T_pM\right\}$$

- Action: $[v_1, \ldots, v_d] \cdot g = [gv_1, \ldots, gv_d]$ with $g \in GL_n(\mathbb{R})$ is free and transitive on each fibre.
- Projection $\pi : FM \to M$ makes FM a principal $GL_n(\mathbb{R})$-bundle.
- With the fundamental representation $\rho : \mathrm{GL}_n(\mathbb{R}) \to GL_n(\mathbb{R})$ being the identity map, $FM \times_\rho \mathbb{R}^n \cong TM$.

Examples

- $M = S^2$: each fibre $F_pM \cong GL_2(\mathbb{R})$.
- $M = T^2$: same as above but the bundle is trivial, i.e., there exists a principal-bundle isomorphism $FT^2 \cong T^2 \times GL_2(\mathbb{R})$.
- M Möbius band: FM is non-trivial; no global frame exists.

Recall: G-Structures

Definition

A G-structure on M is a principal G-sub-bundle $GM \subset FM$, where $G \leq GL_n(\mathbb{R})$.

Given a representation $\rho : G \to GL(\mathbb{R}^c)$, the feature bundle $A = GM \times_\rho \mathbb{R}^c$ carries the fields used by gauge-/manifold-equivariant CNNs.

Examples

- S^2: $G = O(2)$ — orthonormal frame bundle $O(S^2) \subset F(S^2)$.
- T^2: $G = SO(2)$ — oriented orthonormal frames; bundle is trivial $T^2 \times SO(2)$.
- Möbius band M: locally there is $G = e$ but *no* global reduction.
- Parallelizable M (e.g., $T^2, \mathbb{R}^n$): $G = \{e\}$ — a single global frame (classical CNN limit).

Recall: Feature Field

Definition

Given the principal bundle $GM \xrightarrow{\pi} M$ and a representation $\rho : G \to GL(\mathbb{R}^c)$, the associated feature bundle is

$$\mathcal{A} = GM \times_\rho \mathbb{R}^c, \quad (g, v) \sim (gh, \rho(h)^{-1} v), \;\; h \in G$$

A feature field is a smooth section $s : M \to \mathcal{A}, x \mapsto [g_x, f(x)]$.

If you switch a local frame g_α to $g_\alpha h$ by $(g_\alpha, v) \sim (g_\alpha h, \rho(h)^{-1} v)$, meaning the fibre element v is simultaneously rotated by $\rho(h)^{-1}$.

The ψ's typically refer to local trivializations.

Recall: Feature Field

The associated feature bundle $\mathcal{A}$ makes the same abstract point in $\mathcal{A}$ represented consistently in every chart. Sections of $\mathcal{A}$ can make local frames (e.g., $g_\alpha, g_\alpha h$) into a single globally defined feature field.

$$\boxed{G\text{-equivariant feature field}}^{1} \iff \boxed{\text{section of } \mathcal{A} := GM \times_\rho \mathbb{R}^c}$$

[1] called G-equivariant since we are considering the G-sub-bundle instead of the whole frame bundle

Our Goals

Recall there are still some questions we want to address:

1. What are the objects we actually want the CNN to work with and produce? In other words, what are the feature fields on M?
2. How do we define convolutions in this set-up?
3. What kind of symmetry does M have? How do we design the model to respect the symmetries?

Last time, we answered the first question. Let us look at the second question now.

Neural Layers as Bundle Morphisms

Recall that a convolution layer is precisely a G-equivariant maps between two feature spaces, i.e. bundle morphism of sections $\Gamma(\mathcal{A}_{\text{in}}) \to \Gamma(\mathcal{A}_{\text{out}})$. And, neural networks are the stack of such layers.

Given a sequence of G-associated feature vector bundles

$$\mathcal{A}_0 \xrightarrow{\pi_{\mathcal{A}_0}} M, \ldots, {}_N \xrightarrow{\pi_{\mathcal{A}_N}} M \quad \text{with} \quad A_i := GM \times_{\rho_i} \mathbb{R}^{c_i}.$$

- Feature space of layer i: $\Gamma(\mathcal{A}_i)$ (global sections).
- A network is a sequence of parameterized maps

$$\Gamma(\mathcal{A}_0) \xrightarrow{L_1} \Gamma(\mathcal{A}_1) \xrightarrow{L_2} \ldots \xrightarrow{L_N} \Gamma(\mathcal{A}_N).$$

- Each L_i must be G-equivariant and coordinate independent.

Two Building Blocks

❶ **1×1 GM-convolution**[2] This is a pointwise convolution map that linearly sends each feature vector $f_{in}(p) \in \mathcal{A}_{in,p} \cong \mathbb{R}^{c_{in}}$ to an output vector $f_{out}(p) \in \mathcal{A}_{out,p} \cong \mathbb{R}^{c_{out}}$. (Mathematically, these are certain vector bundle morphisms).

❷ **Kernel-field transforms and GM-convolutions**:

- A (smooth) kernel field is a "certain" map $\mathcal{K} : TM \to \mathrm{Hom}(\mathcal{A}_{in}, \mathcal{A}_{out})$. $\mathcal{K}$ defines a kernel field transform

$$\mathcal{T}_{\mathcal{K}} : \Gamma(\mathcal{A}_{in}) \to \Gamma(\mathcal{A}_{out})$$

$$[\mathcal{T}_{\mathcal{K}}(f_{in})](x) \coloneqq \int_{T_xM} \mathcal{K}_x(v)\,\mathrm{Exp}^* f_{in}(v) dv.$$

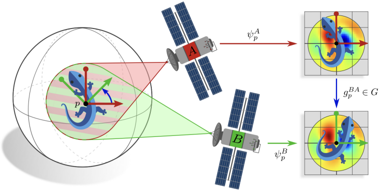
  Exp^* is related to the exponential map and to be defined.
- GM-convolutions can be viewed as specific kernel field transforms with what are so called GM-convolutional kernel fields.

[2] Gauge-Manifold-Convolution

Outline

Why point-wise (1×1) GM-convolution?

Same point, different gauges



Picture from [Weiler et al., 2021].

- Two observers A, B choose local frames ψ_p^A, ψ_p^B at one point $p \in M$.
- Coordinates of the same input vector differ by $f^B(p) = \rho_{\text{in}}\left(g_p^{BA}\right) f^A(p)$, where $g_p^{BA} \in G$ (blue arrow in figure).
- A valid layer must output exactly the same physical feature, independent of the chosen frame.

1×1 GM-Convolution

Solution: apply a 1×1 GM-convolution that operates only at the point p and multiplies by a weight matrix $K_{1\times1} \in \mathbb{R}^{c_{out} \times c_{in}}$ that is G-equivariant, i.e.

$$K_{1\times1}\rho_{\text{in}}(g) = \rho_{\text{out}}(g)K_{1\times1} \text{ for all } g \in G. \quad (\dagger)$$

We denote collection of such $K_{1\times1}$ as $\mathrm{Hom}_G(\rho_{\text{in}}, \rho_{\text{out}})$.

Intuition: A 1×1 GM-convolution is a point-wise channel mixer: at each $p \in M$ it applies the same weight matrix $K_{1\times1}$, and the equivariance condition $(\dagger)$ guarantees that "mix then change frame" equals "change frame then mix", making the output gauge-independent.

Let's figure out why this is a solution to the problem in the proceeding slides.

Step 1: What a bundle morphism looks like in gauges

We said earlier 1×1 GM-convolutions are certain bundle maps.

At the illustrated point $p \in M$, the bundle morphism

$$C_{|p} : \mathcal{A}_{\text{in},p} \longrightarrow \mathcal{A}_{\text{out},p}$$

sends the input fibre (red frame) of $\mathcal{A}_{\text{in}}$ to the corresponding output fibre (green frame) of $\mathcal{A}_{\text{out}}$, with both fibres anchored at the same base point p.

Such a vector bundle M-morphism $\mathcal{C}$ is a smooth bundle map satisfying the following commutative diagram:

$$\begin{tikzcd}
\mathcal{A}^{in} \arrow[rr, "\mathcal{C}"] \arrow[dr, "\pi_{\mathcal{A}_{in}}"'] & & \mathcal{A}^{out} \arrow[dl, "\pi_{\mathcal{A}_{out}}"] \\
& M &
\end{tikzcd}$$

Step 2: Conjugation Rule after Trivializations

- Fix a gauge[3] ψ^A on a chart U^A, at each point $p \in U^A$, the bundle map is the following matrix

$$\mathcal{C}^A_{|p} := \psi^A_{\mathcal{A}_{\text{out}},p} \circ \mathcal{C}_{|p} \circ \left(\psi^A_{\mathcal{A}_{\text{in}},p}\right)^{-1} \in \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}$$

- Change to a second gauge ψ^B with $g_p^{BA} = \psi^B {\psi^A}^{-1}$ on the overlap. Conjugation rule (Eq. 219, also gauge transformations last lecture):

$$\mathcal{C}^B_{|p} = \rho_{\text{out}}\left(g_p^{BA}\right)\mathcal{C}^A_{|p}\, \rho_{\text{in}}\left(g_p^{BA}\right)^{-1}.$$

- So any smooth bundle map C transforms like a conjugation of its local matrix when gauges change.

[3] Picking a particular gauge initializes the local trivialization

Step 3: Weight Sharing by the Intertwiner Condition

Goal: use one and the same kernel template at every point and in every gauge:

$$C^X_{K_{1\times}}|_p = K_{1\times 1} \quad \text{for all gauges } X \text{ and all } p \in U^X \quad \text{(Eq. 223).}$$

- Insert the conjugation rule from Step 2:

$$\rho_{\text{out}}(g)\, K_{1\times 1}\, \rho_{\text{in}}(g)^{-1} = K_{1\times 1} \quad \forall\, g \in G$$

- In other words, any such $K_{1\times 1}$ has to satisfy the linear constraint above, which is equivalent to being in the intertwiner space

$$\mathrm{Hom}_G(\rho_{\text{in}}, \rho_{\text{out}}) := \left\{ K \in \mathbb{R}^{c_{\text{out}}\times c_{\text{in}}} \mid \rho_{\text{out}}(g) K = K \rho_{\text{in}}(g)\ \forall g \in G \right\}$$

Formal Definition: 1×1 GM-Convolution

Definition

A 1×1 **GM-convolution** is a map

$$K_{1\times1}\circledast : \Gamma(\mathcal{A}_{in}) \to \Gamma(\mathcal{A}_{out}), f_{in} \mapsto K_{1\times1} \circledast f_{in} := C_{K_{1\times1}} \circ f_{in}.$$

where $K_{1\times1} \in \mathrm{Hom}_G(\rho_{\text{in}}, \rho_{\text{out}})$ and $C_{K_{1\times1}}|_p := \psi^{-1}_{\mathcal{A}_{out},p} \circ K_{1\times1} \circ \psi_{\mathcal{A}_{in},p}$ for arbitrary gauges $\psi_{\mathcal{A}_{out},p}$ and $\psi_{\mathcal{A}_{in},p}$.

This guarantees gauge-independent (coordinate-free) channel mixing. Here, to give some heuristics of this definition:

- ρ_{in} and ρ_{out} can be thought of as channel representations $\rho_{\text{in}}, \rho_{\text{out}} : G \longrightarrow GL(\mathbb{R}^{c_*})$ that tell us how an element $g \in G$ acts on the input and output feature vectors.
- Each feature bundle is $\mathcal{A}_* = GM \times_{\rho_*} \mathbb{R}^{c_*}$, so keeping a layer G-equivariant means its weights must respect these two representations.

Outline

From point-wise to spatial GM-convolution

- **Limitation of 1×1 GM-Conv.** Only limited to using a "point-like kernel".
- **Kernel Fields:** Instead of the point-wise(1×1) weight matrix

$$K_{1\times 1} \in \mathrm{Hom}_G(\rho_{\text{in}}, \rho_{\text{out}}),$$

we use a (unconstrained) spatial kernel field defined as a map

$$\begin{tikzcd} TM \arrow[rr, "\mathcal{K}"] \arrow[dr, "\pi_{TM}"'] & & \mathrm{Hom}(\mathcal{A}_{in}, \mathcal{A}_{out}) \arrow[dl, "\pi_{\mathrm{Hom}}"] \\ & M & \end{tikzcd}$$

Remark: $\mathcal{K}$ is not required to be a vector bundle map (ie. $\mathcal{K}_p : T_pM \to \mathrm{Hom}(\mathbb{R}^{in}, \mathbb{R}^{out})$ does not have to be linear).

Step 1: Coordinate-free Spatial Kernel

To detect local patterns around a point $p \in M$, we rewrite the coordinate-free kernel $\mathcal{K}_p$ in the numerical coordinates provided by a chosen gauge A:

Definition (Coordinate-free Kernel)

A coordinate-free kernel $\mathcal{K}_p$ at a point $p \in M$ can be expressed relative to gauges $\psi^A_{TM,p}$ (for the tangent bundle) and $\psi^A_{\mathrm{Hom},p}$ (for the homomorphism bundle) of a G-atlas via

$$\mathcal{K}^A_p : \mathbb{R}^d \longrightarrow \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}, \qquad \mathcal{K}^A_p = \psi^A_{\mathrm{Hom},p} \circ \mathcal{K}_p \circ \left(\psi^A_{TM,p}\right)^{-1}$$

For another gauge B, there is a relation

$$\mathcal{K}^B_p = \rho_{\mathrm{Hom}}(g^{BA}_p) \circ \mathcal{K}^A_p \circ (g^{BA}_p)^{-1}.$$

Step 2: From a Template Kernel to a Kernel Field

In order for kernel fields to arise from a convolution, it should come from a **template (spatial) kernel**

$$K : \mathbb{R}^d \longrightarrow \mathbb{R}^{c_{\mathsf{out}} \times c_{\mathsf{in}}}$$

be the single weight tensor learnt by the network $(K \in C^\infty(\mathbb{R}^d, \mathbb{R}^{c_{\mathsf{out}} \times c_{\mathsf{in}}}))$.

Definition

From here we define a kernel field $\mathcal{K}_K$ locally by

$$\mathcal{K}_{K,p}^X := \frac{K}{\sqrt{|\eta_p^X|}},$$

where X is any gauge, $p \in U^X$, and $\sqrt{|\eta_p^X|}$ is the reference frame volume (think of this as normalization).

Step 3: Template sharing & volume normalization

Question: How do $\mathcal{K}_K$ differ across different gauges?

Note that for gauges A, B and $p \in U^A \cap U^B$, the change of coordinates gives a essentially "Jacobian-like" relationship with

$$\sqrt{|\eta_p^A|} = |\det(g_p^{BA})|\sqrt{|\eta_p^B|}.$$

The global version of this constraint and the (aforementioned) transformation law $\mathcal{K}_p^B = \rho_{\mathrm{Hom}}(g_p^{BA}) \circ \mathcal{K}_p^A \circ (g_p^{BA})^{-1}$ implies that for every $g \in G$ and offset $\nu \in \mathbb{R}^d$, the shared template kernel $K : \mathbb{R}^d \to \mathbb{R}^{c_{\mathsf{out}} \times c_{\mathsf{in}}}$ must satisfy the following G-steerability kernel constraint:

$$\rho_{\mathsf{out}}(g)\, K(\nu)\, \rho_{\mathsf{in}}(g)^{-1} = |\det g| \cdot K(g \cdot \nu)$$

Heuristics for G-steerability

Observation: Volume normalization still only handles frame changes at a fixed point p. However, convolutions involve integrating the kernel over the entire space, which includes transformations between different points via actions g. We need the kernel to remain equivariant under global symmetry transformations. So instead of normalizing w.r.t. frame volume, we do normalization w.r.t. the group volume. To do so, we require the kernel K to satisfy a specific constraint under actions of G.

Step 4: Formal Definition of a G-steerable kernel

Definition (vector space of G-steerable kernels)

The vector space of smooth G-steerable kernels that map between field types ρ_{in} and ρ_{out} is defined by

$$\mathscr{K}^{G}_{\rho_{\text{in}},\rho_{\text{out}}} := \Big\{ K : \mathbb{R}^d \to \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}} \text{ smooth} \;\Big|\; \rho_{\text{out}}(g) K(\nu) \rho_{\text{in}}(g)^{-1} = |\det g| K(g \cdot \nu) \,\forall g \in G, \nu \in \mathbb{R}^d \Big\}$$

Here $\det(g)$ refers to taking the determinant of the linear map given by the representation.

- The LHS rotates the channels, while the RHS rotates the spatial offset and rescales by $|\det g|^{-1}$ to keep the integral measure invariant.
- Check: At $\nu = 0$, we have $\rho_{\text{out}}(g) K(0) = K(0) \rho_{\text{in}}(g)$, i.e. $K(0)$ is exactly the intertwiner $K_{1 \times 1}$.

Step 5: Kernel Field Transform

Recall given a kernel field $\mathcal{K}$, we define its corresponding kernel field transform to be:

$$\mathcal{T}_{\mathcal{K}} : \Gamma(\mathcal{A}_{in}) \to \Gamma(\mathcal{A}_{out})$$

$$[\mathcal{T}_{\mathcal{K}}(f_{in})](x) \coloneqq \int_{T_x M} \mathcal{K}_x(v) \operatorname{Exp}^* f_{in}(v) dv,$$

where Exp^* is to be defined.

Definition

Let $f \in \Gamma(\mathcal{A})$, its transporter pullback is a map $\operatorname{Exp}^* f : TM \to \mathcal{A}$ such that

$$v \mapsto P_{A,\pi_{TM}(v) \leftarrow \exp(v)} \circ f \circ \exp(v).$$

where $\mathcal{P}_{A,\pi_{TM}(v) \exp(v)}$ is some parallel transport with respect to a "G-compatible connection".[4]

[4] More details in the reference [Weiler et al., 2021].

Step 6: GM-Convolution

Definition

A GM-convolution $K\star$ is a kernel field transformation coming from a G-steerable template kernel K.

Is a GM-convolution (or more generally a kernel field well-defined?). It turns out that this is if we add a compactly-supported condition.

Theorem

Suppose $\mathcal{K}$ is a kernel field such that $\mathcal{K}_p : T_pM \to \mathbb{R}^{c_{out} \times c_{in}}$ is compactly supported in a closed ball of radius R, then $\mathcal{T}_{\mathcal{K}}$ exists and is smooth.

The Convolution Operator: Summary

Putting it together, let (M, G) be a Riemannian manifold with an associated G-structure. Let $\mathcal{A}_{in}, \mathcal{A}_{out}$ be two G-associated vector bundles over M.

Let $(W_{in}, \rho_{in}), (W_{out}, \rho_{out})$ be the two associated representations and K be a **G-steerable template convolution kernel**, the convolution operator is

$$L : \Gamma(\mathcal{A}_{in}) \to \Gamma(\mathcal{A}_{out}), f_{in} \mapsto f_{out} \coloneqq L(f_{in}),$$

where L is a GM-convolution.

Theorem (Coordinate Independence)

The output f_{out} is a well-defined global section of $\mathcal{A}_{out}$.

Remark: Why the spatial kernel field can vary over TM

- Point-wise case. The matrix $K_{1\times1} \in \mathrm{Hom}_G(\rho_{\text{in}}, \rho_{\text{out}})$ is constant: it has no dependence on position or direction, so it only mixes channels at the single point p.
- In contrast, the kernel field

$$\mathcal{K} : TM \to \mathrm{Hom}\big(\mathbb{R}^{c_{\text{in}}}, \mathbb{R}^{c_{\text{out}}}\big), \;\; \mathcal{K}(g \cdot u) = \rho_{\text{out}}(g)\mathcal{K}(u)\rho_{\text{in}}(g)^{-1},$$

depends on the offset $u \in T_pM$. For each u we

1. parallel-transport $f(x')$ from $x' = \exp_p(u)$ back to p,
2. multiply by $\mathcal{K}(u)$,
3. integrate over $\|u\| \leq r$.

Intuition: The steerability condition ensures this direction-dependent kernel still commutes with every gauge change, making the filter both spatially aware and G-equivariant.

Outline

Isometric Equivariance with GM

So far, we have been considering GM structures, with $G \leq \mathrm{GL}_n(\mathbb{R})$. This is done without much compatibility with a possible metric on M.

Thus, we would like to consider the following data.

$$\mathrm{Isom}_{GM} \coloneqq \{\phi \in \mathrm{Isom}(M) \mid [\phi_*(e_i)]_{i=1}^d \in GM, \forall [e_1, .., e_d] \in GM\}.$$

In other words, this is exactly the subgroup of isometries respecting the GM structure.

Note: When G contains $O(d)$, $\mathrm{Isom}_{GM} = \mathrm{Isom}_M$.

Action of the G-Isometry Group

There is a clear action of Isom_{GM} on GM by

$$\phi \cdot [e_1, ..., e_d] \mapsto [\phi_*(e_1), ..., \phi_*(e_d)]$$

with the pushforward induced on tangent spaces.

This leads to an induced action of Isom_{GM} on $\mathcal{A}_{in}$ and $\mathcal{A}_{out}$ given by

$$\phi_{*,\mathcal{A}_\bullet} : \mathcal{A}_\bullet \to \mathcal{A}_\bullet, [e, v] \mapsto [\phi_{*,GM}(e), v],$$

for $\bullet \in \{\mathrm{in}, \mathrm{out}\}$. This clearly gives an action on $\Gamma(\mathcal{A}_\bullet)$ as well.

We say a map

$$L : \Gamma(\mathcal{A}_{in}) \to \Gamma(\mathcal{A}_{out})$$

is **G-isometry equivariant** if for each $\phi \in \mathrm{Isom}_{GM}(M)$,

$$L(\phi \cdot f_{in}) = \phi \cdot L(f_{in}).$$

Isometry Equivariance

Theorem

A GM-convolution given earlier $K\star : \Gamma(\mathcal{A}_{in}) \to \Gamma(\mathcal{A}_{out})$ with a G-steerable kernel K is G-isometry equivariant.

Corollary: Full Isometry Equivariant

For any G that contains $O(d)$, a GM-convolution operator is fully isometry equivariant.

Proof: Recall if G contains $O(d)$, then

$$\mathrm{Isom}_{GM}(M) = \mathrm{Isom}(M)$$

Corollary: $\mathrm{Isom}_+(M)$-Equvariant

When $G = \mathrm{SO}(d)$, then the GM-convolutions are equivariant w.r.t to all orientation preserving isometries.

Outline

Icosahedral CNNs

Gauge Equivariant CNNs on the icosahedron [Cohen et al., 2019] provide a handcrafted approach to processing spherical signals.

Utilizing the regular grid of the icosahedral discretization as the approximation of the sphere that sampling from the icosahedron(illustration next slide), the convolution operation can be equivariant to both local gauge transformations and global icosahedral symmetries.

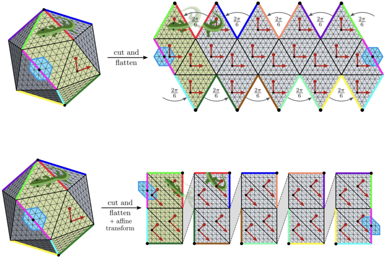
Given a manifold M (the icosahedron) and a feature field $f : M \to \mathbb{R}^n$, the gauge equivariant convolution is defined as:

$$(K \star f)(p) = \int_{\mathbb{R}^d} K(v)\rho_{\text{in}}(g_{p\leftarrow q_v})f(q_v)dv,$$

where K is a learnable kernel, $q_v = \exp_p w_p(v)$ is obtained via the exponential map, and ρ_{in} represents the transformation of features under gauge changes.

Icosahedral CNNs

- each hexagonal grid is a locally flat approximation of S^2
- each hexagonal grid admits $\mathbb{Z}_6$-structure as the G-structure since the Levi-Civita connection has holonomy group $\mathbb{Z}_6$
- flatten icosahedron by cutting it at the north and south pole but the parallel transport is non-trivial over cut edges (upper). So we also need to apply an affine transformation (lower) to align boundaries.



Pictures from [Cohen et al., 2019]

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