# Gauge Theory for Convolutional Neural Networks A Geometric Deep Learning Perspective

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#### Roadmap

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Disclaimer: Throughout the presentation the abbreviation GDL stands for Geometric deep learning as introduced in 2104.13478v (see references)

# A quick glance at Gauge theory

Gauge theory is the extension of Riemannian geometry to the study of fibre, vector and principal bundles.

**Definition.**  $(E, \pi, M; F)$  with  $\pi : E \to M$  is a *fiber bundle* with fiber F if for every  $x \in M$  there exists an open neighborhood  $U \subset M$  and a diffeomorphism

$$\phi_U: \ \pi^{-1}(U) \xrightarrow{\cong} U \times F$$

such that

$$\operatorname{pr}_{1} \circ \phi_{U} = \left. \pi \right|_{\pi^{-1}(U)},$$

where  $\operatorname{pr}_1:U\times F\to U$  is the projection.

In machine learning one usually considers a fibre of the form  $F = \mathbb{R}^r$ , or more specifically a vector bundle of rank r.

For each  $x \in M$ , a bundle chart  $(U, \phi_U)$  induces

$$\phi_{U,x} := \operatorname{pr}_2 \circ \phi_U|_{E_x} : E_x \longrightarrow F,$$

a diffeomorphism between the fibre  $E_x = \pi^{-1}(x)$  and the fibre type F.

**Transition functions.** Let  $\mathcal{U} = \{U_i\}_{i \in \Lambda}$  be an open cover of M and  $\{(U_i, \phi_i)\}_{i \in \Lambda}$  a bundle atlas. On overlaps  $U_i \cap U_k \neq \emptyset$  the change of trivialization

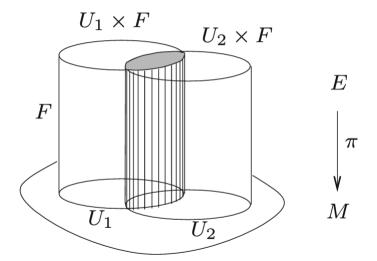
$$\phi_i \circ \phi_k^{-1} : (U_i \cap U_k) \times F \longrightarrow (U_i \cap U_k) \times F$$

defines maps into the diffeomorphism group of F,

$$\phi_{ik}: U_i \cap U_k \longrightarrow \mathrm{Diff}(F), \qquad x \longmapsto \phi_{i,x} \circ \phi_{k,x}^{-1}: F \to F,$$

where  $\phi_{i,x} := \operatorname{pr}_2 \circ \phi_i|_{E_x}$ .





**Cocycle conditions.** On triple overlaps  $U_i \cap U_j \cap U_k$ ,

$$\phi_{ik}(x) \circ \phi_{kj}(x) = \phi_{ij}(x)$$
 and  $\phi_{ii}(x) = \mathrm{Id}_F$ .

The family  $\{\phi_{ik}\}_{i,k\in\Lambda}$  is called the *cocycle* of the bundle.

It turns out that the family of cocycles is a complete description of the fibre bundle - a family of cocycles defines a unique fibre bundle.

Adding more structure to the picture one arrives at the concept of a Principal G-Bundle:

Let G be a Lie group and  $\pi: P \to M$  a smooth map. The tuple  $(P, \pi, M; G)$  is a principal G-bundle over M iff:

1. G acts smoothly on the right on P,  $(p,g) \mapsto p \cdot g$ , such that

$$\pi(p\cdot g)=\pi(p) \qquad \qquad \text{(fiber-preserving)}, \\ p\cdot g=p \iff g=e \qquad \text{(free action)}, \\ \forall x\in M, \ \forall p\in P_x: \ \{p\cdot g: g\in G\}=P_x \qquad \qquad \text{(transitive on each fiber)}.$$

Equivalently, for every  $x \in M$  and  $p \in P_x := \pi^{-1}(x)$ , the map  $G \to P_x$ ,  $g \mapsto p \cdot g$  is a diffeomorphism.

2. There exists a bundle atlas  $\{(U_i, \phi_i)\}$  of *G-equivariant* bundle charts with the *G*-equivariance condition

$$\phi_i(p\cdot g) = \left(\operatorname{pr}_1(\phi_i(p)),\ \operatorname{pr}_2(\phi_i(p))\,g\right) \quad \Longleftrightarrow \quad \phi_i\circ R_g \ = \ (\operatorname{id}_{U_i}\times R_g)\circ \phi_i.$$



### A quick glance at Gauge theory, towards connections

A most central concept in Gauge theory is the extension of connections to the notion of a principal G-bundle, making concepts like curvature from Riemannian geometry available and ultimately giving rise to the Maxwell- and Yang-Mills-equations. As a prerequisite one introduces the following:

**Definition.** Let N be a smooth manifold. A (geometric) distribution of rank r on N is a smooth assignment

$$\mathcal{E}: x \longmapsto E_x \subset T_x N$$
,

where each  $E_x$  is an r-dimensional linear subspace. Smooth means: for every  $x \in N$  there exist an open neighborhood  $U \subset N$  and smooth vector fields  $X_1, \ldots, X_r \in \mathfrak{X}(U)$  such that

$$E_y = \operatorname{span}\{X_1(y), \dots, X_r(y)\}$$
 for all  $y \in U$ .

Equivalently, a rank-r distribution is a rank-r smooth subbundle  $E \subset TN$  of the tangent bundle.



# Vertical & Horizontal Spaces on a Principal Bundle

Let  $(P, \pi, M; G)$  be a principal G-bundle and  $P_x := \pi^{-1}(x)$  the fibre over  $x \in M$ .

▶ Vertical tangent space (at  $u \in P_x$ ):

$$T_u^{\mathrm{v}}P:=T_u(P_x)\subset T_uP$$
 (since  $\pi$  is a submersion,  $P_x\subset P$  is a submanifold). Equivalently,  $T_u^{\mathrm{v}}P=\ker(d\pi_u)$ .

Vertical distribution/bundle:

$$T^{\mathrm{v}}: u \mapsto T_{u}^{\mathrm{v}}P, \qquad T^{\mathrm{v}}P:=\bigcup_{u \in P}T_{u}^{\mathrm{v}}P \subset TP,$$

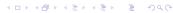
which is **right**–*G*–**invariant**:

$$dR_g(T_u^{\mathrm{v}}P) = T_{u \cdot g}^{\mathrm{v}}P$$
 for all  $u \in P, g \in G$ .

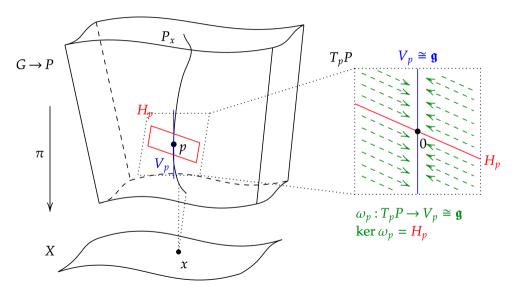
▶ Horizontal spaces: any smooth choice of complements

$$T_uP = T_u^{\mathrm{v}}P \oplus \mathrm{Th}_uP \iff d\pi_u|_{\mathrm{Th}_{P}P} : \mathrm{Th}_uP \stackrel{\cong}{\longrightarrow} T_{\pi(u)}M.$$

**Connection:** a connection on P is precisely a *right–G–invariant* smooth assignment  $u \mapsto \operatorname{Th}_u P$  of horizontal subspaces complementary to  $T_u^v P$ .



# Vertical & Horizontal Spaces on a Principal Bundle

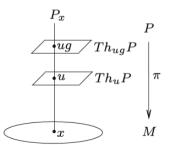


# Connection on a Principal Bundle (horizontal distribution)

**Definition.** Let  $(P, \pi, M; G)$  be a smooth principal G-bundle. A *connection* is a smooth distribution of *horizontal* subspaces

Th: 
$$u \longmapsto \operatorname{Th}_u P \subset T_u P$$

of rank dim M that is **right**–G–**invariant**:  $dR_g(\operatorname{Th}_u P) = \operatorname{Th}_{u \cdot g} P$  for all  $u \in P, g \in G$ , where  $R_g : P \to P$ ,  $u \mapsto u \cdot g$ , is the right action.



#### Ehresmann vs. Levi-Civita Connection

Such a choice of a *horizontal subbundle* is also called an **Ehresmann connection** on  $\pi: TM \to M$ 

$$T(TM) = \mathcal{H} \oplus \mathcal{V}, \quad \mathcal{V} = \ker(d\pi)$$

allowing a lift of base vectors in  $T_x M$  to  $T_{(x,v)} T M$ .

▶ If  $\mathcal{H}$  is *fibrewise linear*, it corresponds to an affine connection  $\nabla$  on M:

$$u_{(x,v)}^{\mathrm{hor}} = \frac{d}{dt}\Big|_{0} (\gamma(t), V(t)),$$
 (horizontal lift at  $T_{(x,v)}TM$ )

with  $\gamma'(0) = u$  and V(t)  $\nabla$ -parallel to v. Span of these lifts gives the Ehresmann connection.

- ▶ On a Riemannian manifold (M, g), the **Levi–Civita connection**  $\nabla^{\mathrm{LC}}$  is the unique torsion-free, g-compatible affine connection.
- ▶  $\nabla^{LC}$  induces a canonical horizontal distribution  $\mathcal{H}^{LC}$  on TM: horizontal curves are exactly those whose fiber vector is parallel transported by  $\nabla^{LC}$ .



# Connection on a Principal Bundle (Connection form)

**Definition** A connection 1-form on P is a Lie-algebra-valued 1-form  $A \in M^1(P, \mathfrak{g})$  satisfying, for all  $g \in G$  and all  $X \in \mathfrak{g}$ ,

$$R_g^*A = \operatorname{Ad}(g^{-1}) \circ A$$
  $A(\widetilde{X}) = X$ 

where  $\widetilde{X}$  is the fundamental vector field generated by X,  $\widetilde{X}_u = \frac{d}{dt}\big|_{t=0}(u \cdot \exp(tX))$ .

#### Key facts.

- A connection form A determines the horizontal distribution by  $\operatorname{Th}_u P = \ker A_u$  (and conversely, any right–G-invariant horizontal distribution yields a unique A with these properties).
- ▶ On vertical vectors,  $A_u: T_u^{\vee}P \rightarrow \mathfrak{g}$  is an isomorphism sending fundamental fields to their generators.

 $\mathrm{Ad}_{\mathfrak{g}}:=(d\mathcal{C}_{\mathfrak{g}})_{\mathfrak{g}}:\mathfrak{g}\to\mathfrak{g}$  and one has  $Ad:G\to\mathrm{Aut}(\mathfrak{g}).$ 



<sup>&</sup>lt;sup>1</sup>For  $g \in G$ , consider  $C_g : G \to G$ ,  $C_g(h) = ghg^{-1}$  the differential gives a linear map:

#### Notation and basic properties.

- ▶ The horizontal tangent bundle is  $ThP := \bigcup_{u \in P} Th_u P \subset TP$ .
- ▶ The *vertical tangent bundle* is  $\operatorname{Tv} P := \ker d\pi \subset TP$ ; vectors in  $\operatorname{Tv} P$  are *vertical*, those in  $\operatorname{Th} P$  are *horizontal*.
- ▶ There are smooth projections  $\operatorname{pr}_{v}: TP \to \operatorname{Tv}P$  and  $\operatorname{pr}_{h}: TP \to \operatorname{Th}P$  (so  $TP = \operatorname{Tv}P \oplus \operatorname{Th}P$ ).
- The differential of the projection restricts to an isomorphism

$$\left. d\pi_u \right|_{\operatorname{Th}_u P} : \operatorname{Th}_u P \xrightarrow{\cong} T_{\pi(u)} M,$$

identifying horizontal vectors with base tangent vectors.

### Objects in Gauge Theory

As an important nexus of the previous constructions one may state the Maxwell equations in their most general form:

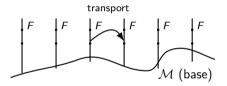
$$d_A F^A = 0$$
,  $* d_A * F^A = 4\pi i J_{
ho}$  (equiv.  $\delta_A F^A = 4\pi i J_{
ho}$ )

- ▶  $P_0 = M \times S^1$ : trivial principal  $S^1$ -bundle over spacetime M;  $(S^1) = \mathfrak{u}(1) = i\mathbb{R}$ .
- ▶  $A \in M^1(M, i\mathbb{R})$ : connection 1–form (electromagnetic potential).
- ▶  $F^A := dA \in M^2(M, i\mathbb{R})$ : curvature 2-form (in physics conventions  $F^A = iF$  for real EM field F).
- ▶  $d_A$ : covariant exterior derivative  $(d_A M = dM + [A \land M]; \text{ for } S^1 \text{ abelian, } d_A = d)$ .
- \*: Hodge star of the metric on M;  $\delta_A$  is the formal adjoint of  $d_A$ :  $\delta_A = (-1)^{n(k+1)+1} * d_A *$  on k-forms in  $n = \dim M$ .
- ▶  $J_{\rho}$ : source 1–form (electric four–current; subscript indicates charge density  $\rho$ ). The factor i appears because forms take values in  $i\mathbb{R}$ .



#### Connecting the Dots I

Gauge theory enters machine learning since fibre bundles are natural objects to model feature spaces over the base manifold M. The dimension of the fibre then equals the number of feature channels.



In GDL the term gauge is understood as follows:

**Definition** A gauge is a choice of frame for a vector bundle — originally defined as a frame for the tangent space, but more generally for any vector space (fibre) attached to each point of a base space M in a vector bundle.

#### Connecting the Dots I

A gauge transformation (as in GDL §4.5) is a change of local frame in a single chart, i.e. a smooth map

$$g_i:U_i\to G.$$

Acting on fields and parameters in that chart, it produces a new trivialization

$$\phi_i' = (\mathrm{id}_{U_i} \times g_i) \circ \phi_i$$

and hence modifies the transition functions by

$$g'_{ij}(x) = g_i(x) g_{ij}(x) g_j(x)^{-1}.$$

So gauge transformations act on the choice of frames.

# Gauge transforms on tangent bundles & the structure group

The following provides a translation from the mathematical setting into an ML-appropriate framework. The bundles under consideration reduce to vector bundles **Local frame (gauge).** At  $u \in M$ , a gauge is an isomorphism

$$\omega_u: \mathbb{R}^s \xrightarrow{\cong} T_u M.$$

Gauge transformation. A change of gauge is a map

$$g:\omega\to GL(s),\qquad u\mapsto g_u,$$

producing the new frame

$$\omega'_{u} = \omega_{u} \circ g_{u}.$$

**Components of fields.** For a vector field X, one writes  $X(u) = \omega_u(x(u))$  with  $x(u) \in \mathbb{R}^s$ . Under the gauge change,

$$X'(u) = g_u^{-1}X(u) \qquad \Rightarrow \qquad X(u) = \omega_u(\mathbf{x}'(u)) = \omega_u(g_ug_u^{-1}\mathbf{x}(u)) = \omega_u(\mathbf{x}(u)) = X(u),$$

so the *geometric* field X is unchanged—only its coordinates change.



# Gauge transforms on tangent bundles & the structure group

**General tensors via a representation.** If a field transforms by a representation  $\rho: GL(s) \to GL(V)$ , then its components obey

(e.g. matrices) 
$$A'(u) = \rho_2(g_u^{-1}) A(u) := \rho_1(g_u) A(u) \rho_1(g_u^{-1}),$$

i.e. the gauge  $g_u$  acts through  $\rho(g_u)$ .

**Takeaway.** On TM, the structure group is GL(s) (s = dim(M)); gauge transformations are GL(s)-valued maps g that change frames while leaving underlying geometric objects invariant.

#### Why the need for a Connection?

It is of general interest to have a rigorous notion of convolution in ML. The difficulty in doing so comes from the need to match a filter  $\theta: M \times M \to \mathbb{R}$  at different points on M. One possible way is to simply take position dependent filters  $\theta_u$ ,  $u \in M$  and define for  $Y \in \Gamma(TM)$ 

$$(x \star \theta)(u) = \int_{T_u M} x(\exp_u Y) \, \theta_u(Y) \, dY$$

Various chart dependent obstacles complicate this approach. For one, the vector field Y needs to be expressed relative to a local frame  $\omega_u : \mathbb{R}^s \to T_u M$ .

Another point is the question of gauge invariance i.e. independence of the choice of frames. For scalar functions this comes for free, but it's much more subtle for a general  $f:\Gamma(TM)\to\Gamma(TM)$ . Given a chosen gauge, the input and output of such functions f are vector-valued functions  $x,y\in\mathcal{X}(M,\mathbb{R}^s)$ .

#### Why the need for a Connection?

A general linear map between such functions may be written through convolution with a kernel  $\Theta: M \times M \to \mathbb{R}^{s \times s}$  as before, having to transform non-trivially according to a gauge transformation as

$$\Theta(u,v) = \rho^{-1}(g(u))\,\Theta(u,v)\,\rho(g(v))$$

There is, however, a better implementation through the use of parallel transport: One first parallel transports all the vectors to a common tangent space and then imposes gauge equivariance w.r.t a single gauge transformation:

$$(\mathbf{x} \star \Theta)(u) = \int_M \Theta(u, v) \, \rho(\mathfrak{g}_{v \to u}) \mathbf{x}(v) \, \mathrm{d}v.$$

Here  $\mathfrak{g}_{v\to u}$  denotes the parallel transport from v to u as dictated by the Ehresmann connection on TM. Given that  $\rho\circ\theta=\theta\circ\rho$ , the above transforms gauge invariantly as

$$(\mathbf{x}' \star \mathbf{\Theta})(u) = \rho^{-1}(\mathbf{g}_u)(\mathbf{x} \star \mathbf{\Theta})(u).$$



### Example of an RGB Image, Base & Fibre

The following is an illustrative example showcasing gauge transformations in a concrete setting.

#### Base space & fibre.

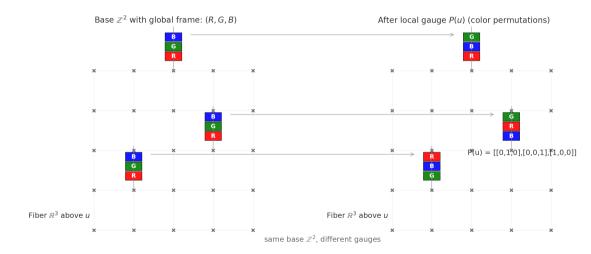
- ▶ Domain  $M = \mathbb{Z}^2 = 2D$  pixel grid.
- ▶ Each pixel  $u \in M$  has an RGB value  $x(u) \in \mathbb{R}^3$ .
- Interpret as a vector bundle:
  - ► Base space: *M*
  - Fibre:  $\mathbb{R}^3$  (color space)

#### Gauge choice (frame).

- ▶ Choose an ordering of color channels (R, G, B) as a *local frame*.
- ightharpoonup A gauge transformation g(u) permutes channels independently at each pixel.
- ▶ Structure group:  $G = S_3$  (all RGB channel permutations).
- ▶ The gauge specifies how the vector components (r, g, b) are arranged in each fibre.



### RGB Images as a Fibre Bundle



# RGB Images as a Fibre Bundle — Equivariance

#### Equivariance requirement.

- ▶ Let  $f: \mathbb{R}^3 \to \mathbb{R}^C$  represent a  $1 \times 1$  convolution <sup>2</sup>
- ▶ Input representation:  $\rho_{in}: S_3 \to GL(3)$  (permutation matrices).
- ▶ Output representation:  $\rho_{\text{out}}: S_3 \to GL(C)$ .
- Gauge-equivariance means:

$$f(\rho_{\sf in}(g)x) = \rho_{\sf out}(g)f(x)$$

for all  $g \in S_3$ ,  $x \in \mathbb{R}^3$ .

#### **Takeaway**

- ► The RGB gauge model enforces that network layers treat all color channels *equivalently* under local permutations.
- ► This ensures that the learned functions respect gauge symmetry in the colour space.
- ► Conceptually: a change of colour channel order at each pixel should not affect the semantic meaning of the output.

<sup>&</sup>lt;sup>2</sup>Given an image  $x: M \to \mathbb{R}^3$ , a  $1 \times 1$  conv with C output channels applies the same matrix to each pixel:  $y(u) = f(x(u)) = W \ x(u) + b \in \mathbb{R}^C$ ,  $W \in \mathbb{R}^{C \times 3}$ ,  $b \in \mathbb{R}^C$ ,  $u \in M$ 

#### Connecting the Dots II

The previous framework applies to GDL in a concrete sense. In ML terms (GDL): a gauge transformation is "re-expressing features in a different local frame" (no physical change), while transition functions are the relative frame changes one must respect on chart overlaps. The following four points serve to unravel the picture.

- 1) Data as a vector bundle; gauges as local frames.
  - ▶ Domain M with a fibre  $F_u \cong \mathbb{R}^C$  at each  $u \in M$  (e.g., RGB features per pixel).
  - ▶ Choosing a channel basis at each u is a gauge  $\omega_u : \mathbb{R}^s \xrightarrow{\cong} F$  (local frame).
  - ▶ Gauge transformatoin acts by a representation  $\rho: G \to \operatorname{GL}(F)$ :  $x'(u) = \rho(g(u))^{-1}x(u)$ .

### Connecting the Dots II, gauge transformations & per-point layers

- 2) Equivariance of  $1 \times 1$  convolutions (fibrewise linear maps).
  - ▶ A  $1 \times 1$  convolution is a linear map  $f : F \to F'$  applied at each u.
  - ► Gauge consistency / equivariance:

$$f \circ \rho_{\mathrm{in}}(g) = \rho_{\mathrm{out}}(g) \circ f \quad \Leftrightarrow \quad f' = \rho_{\mathrm{out}}(g)^{-1} \circ f \circ \rho_{\mathrm{in}}(g).$$

▶ Then outputs transform predictably:  $y'(u) = \rho_{\text{out}}(g(u)) y(u)$  with y(u) = f(x(u)).

#### 3) Comparing different fibres requires transport.

- $\triangleright$  For spatial ops (true convolutions/message passing), features at v must be transported to the frame at u before aggregation.
- ▶ With parallel transport  $g_{v \to u}$  and representation  $\rho$ :

$$h_u = \Theta_{\mathrm{self}} x_u + \sum_{v \in N_u} \Theta_{\mathrm{neigh}}(\alpha_{uv}) \rho(g_{v \to u}) x_v.$$

▶ This construction is gauge-equivariant by design.



### Connecting the Dots II, why this matters in ML

#### 4) Benefits of the gauge view.

- ightharpoonup Encodes local symmetries via a structure group G on fibres.
- Layers yield predictable transformations:  $y'(u) = \rho_{\text{out}}(g(u)) y(u)$ ; global invariants via pooling.
- ▶ Improves data efficiency & robustness; generalises CNN equivariance beyond translations.

In machine learning applications, one is interested in constructing functions  $f \in \mathcal{F}(\mathcal{X}(M))^3$  on such images (e.g. to perform image classification or segmentation), implemented as layers of a neural network. It follows that if, for whatever reason, we were to apply a gauge transformation to our image, one would need to also change the function f (network layers) so as to preserve their meaning.

$$\mathcal{X}(M) = \{x : M \to V\}.$$

 $<sup>^{3}\</sup>mathcal{X}(M)$  is the space of signals/fields on  $\Omega$ . Formally,

# References (core source)

- M. M. Bronstein, J. Bruna, T. S. Cohen, P. Veličković, Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges, arXiv:2104.13478.
- ► Helga Baum, Eichfeldtheorie: Eine Einführung in die Differentialgeometrie auf Faserbündeln (Masterclass), Springer, 2014

#### Fiber bundle schematic

