Geometry and Topology in Machine Learning Seminar

Summer 2025
Meeting Time: TBD
Location: Zoom

In this seminar, we will survey the application of geometric and topological machinery, including manifolds, topological invariants, and symmetry structures, to fundamental problems in machine learning across diverse applications.

Despite neural networks' remarkable successes and vast research investments over the past decade, a rigorous mathematical understanding of *why* they work so effectively remains elusive: there is no single result that simultaneously explains their expressivity, trainability, and generalization capabilities. Consequently, practical applications rely heavily on domain-specific heuristics and empirical insights, making deep learning research largely a trial-and-error endeavor.

How can we develop a unified, rigorous mathematical language to answer this question? While various research frontiers offer partial explanations, a complete picture remains out of reach. However, geometric and topological techniques provide a promising lens through which to partially address this challenge: **what shape do the learned features live on?** The most effective approaches to characterizing this shape treat the feature space either as a **manifold** (eg, spheres, projective spaces, or tori) or as a **simplicial complex**. This perspective unlocks a variety of powerful analytical tools, including **Riemannian metrics** which give a notion of distance and curvature and **topological invariants** which capture global structural properties.

Equivariance, arising from group actions and representation theory, provides another crucial geometric principle. Equivariant models are designed to respect the underlying symmetries of data, which can typically be formalized through the action of a **Lie Group** G. This mathematical framework naturally connects to **gauge theory**, traditionally a subdomain of mathematical physics, when describing how features transform consistently across different regions of the input space. These connections reveal deep relationships between geometric invariance principles and the inductive biases that make neural networks successful.

The goal of this seminar is to introduce these concepts, establish their connections to contemporary machine learning challenges, and review important works bridging the gaps between these sets of mathematics and machine learning applications. Through careful study and active discussion, we aim to develop theoretical insight and practical intuition for how geometric and topological thinking can illuminate the "black box" of neural networks.

1 Scheduled Plan for the Seminar

We plan to start at the week of **June 9th - June 13th** and end on the week of **August 18th - August 22nd**. The plan is to divide the seminar into two parts - **Foundations** and **Paper Presentations**.

Foundations: For the first 3 weeks, we will run 2 lectures per week, each roughly 1 hour long. The actual schedule is TBD based on everyone's availability. We will loosely follow the below:

- Michael M. Bronstein, Joan Bruna, Taco Cohen, and Petar Veličković. Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges, 2021

The planned contents are as follows:

Part A: Groups and Representations

1. Grids and graphs/soft introduction to ML (mainly concerning convolutional and graph neural networks)
2. Introduction to group representations, principle G-bundles, gauge theory.
3. Applications of representations and gauge theory (equivariant machine learning).

Part B: Manifolds

4. Introduction to differentiable manifolds.
5. Introduction to Riemannian manifolds.
6. Applications of manifolds in machine learning.

There's more detail on the lectures in the next section.

Paper Presentations: In the remaining weeks of the seminar, we hope to have participants electively give presentations on a research paper of their choice related to this seminar. At the end of the document, there is a list of suggested papers to choose from, but participants can certainly choose papers outside of the list. The presenter should decide the paper at least **one week** in advance, and other participants are encouraged to at least skim the paper before the presentation.

2 Geometry in Machine Learning

We will have 6 lectures, outlined roughly as **Part A** and **Part B**.
For each item in the list below, we will identify each model family with its natural geometric domain, symmetry, and representation. The explanation here is informal with the intent of providing just a "slogan/vibe" of the connections between machine learning and geometry. By no means is this exhaustive.

By a *domain*, we mean the spaces whatever particular question in machine learning lie on. By *symmetry*, we mean the possible interaction the domain can have with groups on the space our model wants to preserve. By *representation*, we mean how feature spaces with the group action.

Domain: Ω	Where does the question live? *lattices(pixel grids), graphs, point clouds, meshes, manifolds, with possible metric structure ...*
Symmetry: $G, \alpha : G \times \Omega \to \Omega$	Which group action on Ω leaves the task invariant? $SE(2)$ *on lattices, permutation on graphs,* $SE(3)$ *on point clouds, gauge on manifolds*
Representation: $\rho : G \to \mathrm{Aut}(V) \cong GL(V)$	How the features transform under that group action *scalars, vectors, tensors, or sheaf fibres*

Chapter	**Domain** (Ω)	**Symmetry** (G, α)	**Representation** $\rho : G \to \mathrm{GL}(V)$
Pixels & CNNs	Cubical Sub-lattice of $\mathbb{Z}^{2,3}$	Translation, Rotation, Dilation, ...	e.g. if the color is RGB, then trivial on channel space ($V = \mathbb{R}^3$)
Graphs & GNNs	Graph/1-dim complex (V, E)	Permutation $S_{\lvert V \rvert}$	Trivial on node/edge features (classical MP-GNN)
SE(3)-GNNs on 3D clouds and related problems	Finite subset $P \subset \mathbb{R}^{3 \text{ or } n}$	Rigid motions	Feature vector spaces admit group action
Differentiable and Riemannian Manifolds	Smooth m-manifold M, possibly with metric or discretized	Principle G-bundles	Sections of associated bundles

Table 1: Domain–symmetry–representation triplet for each topic.

1. Pixels and CNNs (2D/3Ds with translation groups)

   (a) Convolution can be considered as an operator "$*$" combines two signals by sliding one across the other and summing pointwise products. In the discrete one-dimensional case, for zero-padded vectors x, w, it is given by

   $$(x * w)_k \;=\; \sum_{\tau=-\infty}^{\infty} x_\tau \, w_{k-\tau}$$

   while in the continuous setting one has

   $$(x * w)(t) \;=\; \int_{-\infty}^{\infty} x(\tau)\, w(t-\tau)\, \mathrm{d}\tau.$$

   (b) CNNs were first popularised for handwritten-digit recognition, where images live on a regular 2-D lattice (pixels) and translation-equivariance is enforced by weight sharing. Convolutions for 2D images in one line:

   $$(x * w)_{i,j} \;=\; \sum_{s=-\infty}^{\infty} \sum_{t=-\infty}^{\infty} x_{s,t}\, w_{i-s,\, j-t}$$

   So we see that convolutions work in the same way for two-dimensional but just take $k \times k$ matrix as the kernel w.

(c) Group-equivariant CNNs (G-CNNs) started by trying to generalize translations to larger symmetry groups. A plain CNN respects only translations. G-CNNs generalise the kernel so that the layer is equivariant to other actions such as rotations, reflections and dilations (ie. coming from the general linear group). `https://arxiv.org/abs/1602.07576`.

2. Graphs and GNNs

(a) Real-world data are rarely as tidy as image constructions, such as molecules, social networks and citation graphs. Moving to graphs forces us to replace the rigid translation group with the much larger permutation group $S_{|V|}$. The essential idea behind GNNs is the message-passing principle:

$$h_v^{(k+1)} = \mathrm{UPDATE}\Big(h_v^{(k)},\ \mathrm{AGG}\{\, h_u^{(k)} \mid u \in N(v)\}\Big),$$

where for each layer the node information are updated according to its previous state and the neighboring vertices.

(b) **GCNs, GATs, and GraphSAGE** are three of the most widely-used GNN baselines, each introducing a foundational idea—graph convolutions, attention-based aggregation, and neighbor sampling respectively, to solve the central question to GNNs: how to aggregate local information into highly expressive global representations without succumbing to oversmoothing?

i. Graph Convolutional Networks (GCN) `https://arxiv.org/abs/1609.02907`
ii. Graph Attention Networks (GAT) `https://arxiv.org/abs/1710.10903`
iii. Inductive Representation Learning on Large Graphs (GraphSAGE) `https://arxiv.org/abs/1706.02216`

(c) **Sheaves:** In GCNs, often a matrix involved in the convolution process is done by considering the graph Laplacian. A graph Laplacian, however, is a special case of what is known as a sheaf Laplacian. **Sheaf Neural Networks** does this by assigning different vector spaces to nodes/edges of the graph with learned linear restriction maps. The resulting sheaf Laplacian captures asymmetric or signed relations and yields large accuracy gains in such settings. `https://arxiv.org/abs/2012.06333`

3. Equivariant Machine Learning (e.g. point clouds & molecular geometry, SE(3)-equivariant GNNs)

(a) Point clouds in $\mathbb{R}^3$, coming from physical data such as atoms, protein residues, LiDAR returns, etc., are often invariant under continuous rigid-motion symmetry of $\mathrm{SE}(3) = \mathbb{R}^3 \rtimes \mathrm{SO}(3)$ and related groups. Often times, we would like our neural network to respect the action of these groups, leading to the idea of equivariance.

(b) Here are some examples of groups-equivariant architectures with respect to SE(3) and/or related groups.

i. *Tensor Field Networks* achieves local equivariance to 3D rotations, translations, and permutations, and they use spherical-harmonic convolutions to build the filters `https://arxiv.org/abs/1802.08219`.
ii. SE(3)-*Transformers* use tensor fields with attention for long-range interactions `https://arxiv.org/abs/2006.10503`.
iii. E(n) *GNN / EGNN* generalizes the equivariant architecture to the general Euclidean group in $\mathbb{R}^n$ `https://arxiv.org/abs/2102.09844`.

Analogously, there are also many interests in studying equivariant convolutional neural networks.

(c) Gauge theory arises when trying to describe features of the domain that varies over space. In the study of CNNs, the perspective of gauge theory gave a unified framework for classifying much of the equivariant CNN archittectures `https://arxiv.org/abs/1811.02017`.

4. Differentiable and Riemannian Manifolds

   (a) The consideration of a **(Riemannian) metric** (similar to the dot product on $\mathbb{R}^n$) on such manifolds is relevant in questions such as optimization. This is because optimization problems often involve a gradient descent of sorts, which has to be defined with respect to a Riemannian metric. Geodesics regression has also become the analog of linear regression for statistical methods.

   (b) In the world of machine learning, they have notable applications such as:

      i. The theory of stochastic gradient descents have been developed on Riemannian manifolds to tackle problems in machine learning `https://arxiv.org/abs/1111.5280`.

      ii. *Geodesic CNN* establishes CNNs on non-Euclidean manifolds by using geodesics to extract the analog of “patches" for images `https://arxiv.org/abs/1501.06297`.

      iii. Methods involving the Poincaré ball and hyperbolic geometry have shown gains in the area `https://arxiv.org/abs/1705.08039`.

3 Suggested Papers

Here are some suggested papers to present in this seminar.

Papers concerning **metric and geometry**:

1. Iasonas Kokkinos, Michael M. Bronstein, Roee Litman, and Alex M. Bronstein. Intrinsic shape context descriptors for deformable shapes. In *2012 IEEE Conference on Computer Vision and Pattern Recognition*, pages 159–166, 2012

2. Silvère Bonnabel. Stochastic gradient descent on riemannian manifolds. *IEEE Transactions on Automatic Control*, 58(9):2217–2229, 2013

3. Jonathan Masci, Davide Boscaini, Michael M. Bronstein, and Pierre Vandergheynst. Geodesic convolutional neural networks on riemannian manifolds. In *2015 IEEE International Conference on Computer Vision Workshop (ICCVW)*, pages 832–840, 2015

4. Zhiwu Huang, Ruiping Wang, Shiguang Shan, Xianqiu Li, and Xilin Chen. Log-euclidean metric learning on symmetric positive definite manifold with application to image set classification. In *Proceedings of the 32nd International Conference on International Conference on Machine Learning - Volume 37*, ICML’15, page 720–729. JMLR.org, 2015

5. Maximilian Nickel and Douwe Kiela. Poincaré embeddings for learning hierarchical representations, 2017

6. Federico Monti, Davide Boscaini, Jonathan Masci, Emanuele Rodolà, Jan Svoboda, and Michael M. Bronstein. Geometric deep learning on graphs and manifolds using mixture model cnns. In *2017 IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pages 5425–5434, 2017

7. Zhiwu Huang, Jiqing Wu, and Luc Van Gool. Building deep networks on grassmann manifolds. In *Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence and Thirtieth Innovative Applications of Artificial Intelligence Conference and Eighth AAAI Symposium on Educational Advances in Artificial Intelligence*, AAAI'18/IAAI'18/EAAI'18. AAAI Press, 2018

8. Brandon Hansen, Zhiwei Wu, Michael M. Bronstein, and David Vázquez. Geomgcn: Geometric graph convolutional networks. In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2020

Papers concerning **groups and equivariance**.

1. Taco S. Cohen, Mario Geiger, Jonas Köhler, and Max Welling. Spherical CNNs. In *International Conference on Learning Representations*, 2018

2. Taco Cohen and Max Welling. Group equivariant convolutional networks. In Maria Florina Balcan and Kilian Q. Weinberger, editors, *Proceedings of The 33rd International Conference on Machine Learning*, volume 48 of *Proceedings of Machine Learning Research*, pages 2990–2999, New York, New York, USA, 20–22 Jun 2016. PMLR

3. Taco Cohen and Max Welling. Learning the irreducible representations of commutative lie groups. In Eric P. Xing and Tony Jebara, editors, *Proceedings of the 31st International Conference on Machine Learning*, volume 32 of *Proceedings of Machine Learning Research*, pages 1755–1763, Bejing, China, 22–24 Jun 2014. PMLR

4. Taco S. Cohen, Mario Geiger, and Maurice Weiler. *A general theory of equivariant CNNs on homogeneous spaces.* Curran Associates Inc., Red Hook, NY, USA, 2019

5. Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. In Kamalika Chaudhuri and Ruslan Salakhutdinov, editors, *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pages 1321–1330. PMLR, 09–15 Jun 2019

6. Nathan Thomas, Tess Smidt, Steven Kearnes, Li Yang, Lixuan Li, Kevin Kohlhoff, and Patrick Riley. Tensor field networks. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2018

7. Maurice Weiler and Gabriele Cesa. General E(2)-Equivariant Steerable CNNs. In *Conference on Neural Information Processing Systems (NeurIPS)*, 2019

8. Kristof Schütt, Stefan Chmiela, Hector E. Sauceda, Klaus-Robert Müller, and Alexandre Tkatchenko. E(3)-equivariant graph neural networks. In *Proceedings of the International Conference on Machine Learning (ICML)*, volume 139, pages 9329–9339. PMLR, 2021

9. Víctor Garcia Satorras, Emiel Hoogeboom, and Max Welling. E(n) Equivariant Graph Neural Networks. In Marina Meila and Tong Zhang, editors, *Proceedings of the 38th International Conference on Machine Learning*, volume 139 of *Proceedings of Machine Learning Research*, pages 9323–9332. PMLR, 18–24 Jul 2021

10. Rafal Karczewski, Amauri H Souza, and Vikas Garg. On the generalization of equivariant graph neural networks. In *Forty-first International Conference on Machine Learning*, 2024

11. Najwa Laabid, Severi Rissanen, Markus Heinonen, Arno Solin, and Vikas Garg. Equivariant denoisers cannot copy graphs: Align your graph diffusion models. In *The Thirteenth International Conference on Learning Representations*, 2025

12. Alexandru Dumitrescu, Dani Korpela, Markus Heinonen, Yogesh Verma, Valerii Iakovlev, Vikas Garg, and Harri Lähdesmäki. E(3)-equivariant models cannot learn chirality: Field-based molecular generation. In *The Thirteenth International Conference on Learning Representations*, 2025

Papers concerning **topology and shape**.

1. Christopher Hofer, Patrick Berzin, Martin Niethammer, and Caroline Uhler. Topological convolutional neural networks. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2017

2. Christopher Hofer, Roland Kwitt, Martin Niethammer, and Caroline Uhler. Deep learning with persistence images. In *Proceedings of the NeurIPS Workshop on Topological Data Analysis*, 2017

3. Raymond Ho, Thien F. Nguyen, and Gunnar Carlsson. Topolayer: A topological layer for convolutional neural networks. In *International Conference on Learning Representations (ICLR)*, 2018

4. Mathieu Carrière, Steve Oudot, and Umut Ozertem. Structure-aware machine learning with topological features. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pages 3509–3516, 2019

5. Mathieu Carrière, Filippo Chazal, and Steve Oudot. Stable topological signatures for points on 3d surfaces. *Journal of Machine Learning Research*, 21:1–43, 2020

6. Christopher Hofer, Roland Kwitt, Martin Niethammer, and Caroline Uhler. Deep learning with persistent homology—a survey. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 43(1):31–53, 2021

7. Cristian Bodnar, Francesco Di Giovanni, Benjamin Paul Chamberlain, Pietro Liò, and Michael M. Bronstein. Neural sheaf diffusion: A topological perspective on heterophily and oversmoothing in gnns, 2023