Preface of Geometry, Topology, and Machine Learning 2025

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The past two decades have seen unprecedented growth in the capabilities of artificial intelligence (AI), starting from foundational architectures such as deep belief networks (Hinton et al., 2006), through early efforts to scale learning algorithms (Bengio and LeCun, 2007), to the now-standard deep learning paradigm (Goodfellow et al., 2016).

The increasing utility of **AI in mathematics** is a clear example of how far these capabilities have come. Machine-learning systems now assist with the discovery of *mathematical patterns, conjectures, and constructions*, the search for programs with new mathematical content, and increasingly strong forms of *automated and neuro-symbolic theorem proving* (Davies et al., 2021; Romera-Paredes et al., 2024). Recent milestones include medal-level performance at the International Mathematical Olympiad (Trinh et al., 2024; Hubert et al., 2026), AlphaEvolve's use of evolutionary program search to improve constructions for open problems in geometry and combinatorics (Novikov et al., 2025; Georgiev et al., 2025), and the disproof of Erdős's planar unit-distance conjecture by a state-of-the-art OpenAI model (OpenAI, 2026; Alon et al., 2026).

Yet even as these tools succeed, what they actually learn and how they behave remain only partially understood—including fundamental phenomena such as *generalization in overparameterized regimes*, *optimization behavior*, *robustness*, and the role of *architectural inductive biases* (Zhang et al., 2017; Belkin et al., 2019). This *black-box character* of many high-performing AI systems has important regulatory and societal dimensions, as they increasingly affect decisions in medicine, science, finance, public administration, infrastructure, and other areas of daily life. *Transparency, traceability, auditability, robustness, and human oversight* are therefore central requirements for the deployment of AI systems (Rudin, 2019; European Parliament and Council, 2024).

A growing body of work on **mathematics in AI** addresses exactly these needs: mathematics provides the structural vocabulary through which AI models can be understood and improved. Among the branches of mathematics most directly relevant to these questions are **geometry and topology**. Modern learning systems operate on high-dimensional, structured data and are themselves high-dimensional, structured objects. Understanding these systems fundamentally requires reasoning about shape, symmetry, locality, connectivity, and multiscale organization. Geometry and topology are the mathematical disciplines that provide the formal theory to describe exactly these phenomena.

This shows up in complementary directions of research: one focused on the structure of data and representations, the other on the structure of learning architectures themselves. **Topological data analysis (TDA)** and **geometric statistics** provide tools for extracting and reasoning about the structure that data and learned representations exhibit (Edelsbrunner and Harer, 2010; Pennec et al., 2020). **Topological deep learning (TDL)** and **geometric deep learning (GDL)** build such structure directly into learning architectures: TDL incorporates information about connectivity, higher-order relations, and global shape (Bodnar et al., 2021; Hajij et al., 2022), while GDL emphasizes symmetries, invariances, curvature, and metric structure on the underlying data manifold (Bronstein et al., 2021). The value of these approaches must ultimately be tested against *practitioner-grade deep learning methods*, but they have already found application in scientific modeling, medical imaging, molecular prediction, geometry processing, and complex systems. Currently, the most promising direction appears to be not replacement but a **merging** of geometric, topological, and empirical deep learning viewpoints.

These considerations motivated the creation of a workshop on **Geometry, Topology, and Machine Learning (GTML 2025)** and shaped its scientific scope. The workshop took place at the Max Planck Institute for Mathematics in the Sciences (MPI MiS) in Leipzig, Germany, from November 10 to 14, 2025. It received institutional support from MPI MiS and the STRUCTURES Cluster of Excellence at Heidelberg University. GTML combines two earlier workshop series: *Geometry and Machine Learning (GaML)* and *Topological Methods in Data Analysis (TMDA)*. Merging them reflects our view that methods from *geometry*, *topology*, and *machine learning* have reached a stage where their interaction is methodologically productive and, in many settings, necessary. We envision GTML as the first edition of a recurring meeting that provides a space for experts in geometry, topology, and machine learning to exchange their ideas and expertise.

Workshop Scope and Topics

The workshop program was organized into several threads around a common question:

> *How can geometry and topology inform modern machine learning to understand existing systems and design better ones?*

The first thread approached this question from the side of **machine learning foundations**. Here the emphasis was on understanding the *mechanisms of deep networks themselves*: computational structure and biases, algebraic constraints on ReLU networks, the training dynamics of Riemannian stochastic gradient descent, optimal-transport perspectives on residual and shallow networks, reinforcement learning for large-scale distributed systems, and Bayesian approximations that respect the geometry of overparametrization. This provides the *diagnostic layer* of the workshop, probing what deep models can represent, how they optimize, why they generalize, and where current explanations remain incomplete.

A second thread asked how **geometric structures** can be used as an *inductive bias* and as an *analytic language* for learning. This included invariance and equivariance, covariant molecular representations, neural Fourier transforms, Platonic transformers, Gromov–Wasserstein distances, geometric statistics in computational anatomy and connectomics, score learning on shape spaces, and robust geometry processing. These contributions show how symmetries, metrics, curvature, manifolds, quotient spaces, and shape spaces can turn prior knowledge about data into *model structure*. In this sense, geometry connects the abstract analysis of learning with concrete *design principles* for models that act on molecules, point clouds, images, surfaces, signals, and scientific data.

A third thread investigated how **topological structures** can be used to extract organization from data and to embed it into learning systems. The program contained contributions to topological data analysis and topological deep learning beyond persistent homology, including copresheaf neural networks, Hodge-Laplacian representations, effective resistance in simplicial complexes, Mapper and Reeb-type constructions, extended persistent homology transforms, explainable Mapper for LLM embedding spaces, and topological learning for spatial life-science data. These methods are particularly relevant when the important information is not only local or metric, but encoded in *connections, higher-order relations, flows, or changes across scale.*

Finally, the workshop featured various **applications** that served both as demonstrations of how this research can tackle real-world problems and as tests of whether the proposed structures are useful in practice. Examples included computer vision, language models, distributed data processing, medical imaging, computational anatomy, neuroscience, molecular modeling, drug design, and other data from the life sciences.

Contributions in This Volume

This PMLR volume collects contributions from invited speakers and lightning-talk presenters. The articles record current work at the **interface of geometry, topology, and machine learning**. They illustrate how geometric and topological ideas serve not only as mathematical background but as *active design principles* for models, analysis tools, and scientific applications, thus charting a sustained research program beyond the 2025 workshop.

Detailed Workshop Program

Mon 10 Nov.	**Tue** 11 Nov.	**Wed** 12 Nov.	**Thu** 13 Nov.	**Fri** 14 Nov.
Machine Learning I	Topological Deep Learning I	Topological Data Analysis I	Topological Deep Learning II	Geometric Statistics II
Geometric Deep Learning	Machine Learning II	Geometric Statistics I	Geometric Processing	Topological Data Analysis II
	Lightning Talks I		Lightning Talks II	

Machine Learning I

⋆ Keynote

Stefanie Jegelka⋆ (TUM & MIT)
Computational structure in deep networks: biases, meta networks and learning

Guido Montúfar (MPI MiS & UCLA)
Constraining the outputs of ReLU neural networks

Benjamin Gess (TU Berlin)
Effective fluctuating continuum models for Riemannian SGD

Machine Learning II

Hartmut Maennel⋆ (DeepMind)
Complete and Efficient Covariants for 3D Point Configurations with Application to Learning Molecular Quantum Properties

Robert Lilow (Deepshore)
Optimizing Distributed Data Processing with Reinforcement Learning

Jan Stühmer (HITS)
Equivariance as Design Principle for Modern Deep Learning

Geometric Deep Learning

Anna Gilbert⋆ (Yale)
Seeing the forest for the trees

François-Xavier Vialard (Université Gustave Eiffel)
Training of deep ResNets and shallow networks in the lens of optimal transport

Alice Barbora Tumpach (Wolfgang Pauli Institute)
Infinite-dimensional Geometry and Artificial Intelligence

Topological Deep Learning I

Guo-Wei Wei⋆ (Michigan State University)
Topological data analysis and topological deep learning beyond persistent homology

Bastian Grossenbacher-Rieck (University of Fribourg)
Shapes, Spaces, Simplices, and Structure: Geometry, Topology, and Machine Learning

Mustafa Hajij (University of San Francisco)
Copresheaf Topological Neural Networks: A Generalized Deep Learning Framework

Topological Deep Learning II

Kenji Fukumizu⋆ (Institute of Statistical Mathematics, Japan)
Neural Fourier Transform: a method of deep equivariant representation learning

Michael Schaub (RWTH Aachen University)
Vectorial representations of topological features: a spectral perspective

Mathilde Papillon (UC Santa Barbara)
Make Any Graph Neural Network Go Topological with TopoTune

Topological Data Analysis I

Kathryn Hess Bellwald⋆ (EPFL)
Topological perspectives on the connectome

Vanessa Robins⋆ (Australian National University)
The Extended Persistent Homology Transform for Manifolds with Boundary

Bei Wang Phillips (University of Utah)
Charting LLM Embedding Spaces with Explainable Mapper

Topological Data Analysis II

Claudia Landi⋆ (Università di Modena e Reggio Emilia)
Theoretical Insights into Effective Resistance in Simplicial Complexes

Bernadette Stolz-Pretzer (MPI of Biochemistry)
Topological learning for spatial data in the life sciences

Mathieu Carrière (Inria)
Differentiable and Measure-Based Mapper

Geometric Statistics I

Ron Kimmel⋆ (Technion)
On shape reconstruction and analysis via synthetic stereo, handling missing parts, cuts and holes

Tom Needham (Florida State University)
Variants of Gromov–Wasserstein distances

Stefan Sommer (University of Copenhagen)
Score learning and inference for diffusion processes on shape spaces

Geometric Statistics II

Xavier Pennec⋆ (Inria)
Geometric statistics in computational anatomy: old & new

Erik Bekkers (University of Amsterdam)
Platonic Transformers: A Solid Choice for Equivariance

Vincent Stimper (Isomorphic Labs)
Towards a System for Rational Drug Design with AI

Geometric Processing

Mathieu Desbrun⋆ (Inria)
Grooming with Cartan: vector field processing on triangle meshes

Søren Hauberg (Technical University of Denmark)
Reparametrization invariance in Bayesian approximations

Marco Attene (IMATI-CNR)
Robust Geometry Processing

Lightning Talks I

Hana Dal Poz Kourimska; Anupam Datta; Jan Gerken; Marco Guerra; Tom Jacobs; Maximilian Krahn; Kolya Lettl; Kelly Maggs; Nicolás Hinrichs; Matteo Pegoraro; Noémie Jaquier; Hannah Santa Cruz Baur; Yu Tian; Deniz Küçükahmetler.

Lightning Talks II

Matteo Biagetti; Yuri Gardinazzi; Eric Dolores Cuenca; Susovan Pal; David Loiseaux; Nikola Milosevic; Elias Nyholm; Shrunal Pothagoni; Sophie Rosenmeier; Celia Rubio Madrigal; Nikola Sadovek; Leonard Schmitz; Hae Jin Song; Kang-Ju Lee; Wayne Ng Kwing King; Iolo Jones; Abdul Halim.

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