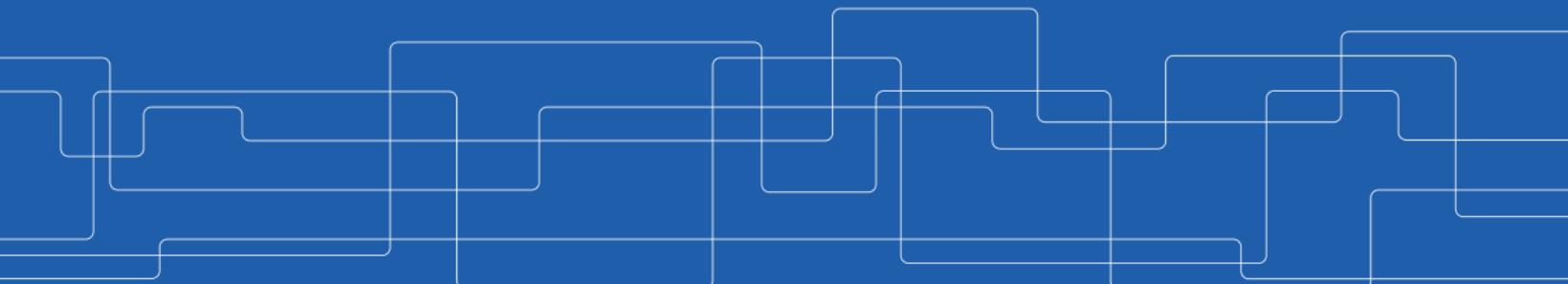


Geometric and Algebraic Aspects of Machine Learning

Giovanni Luca Marchetti

Royal Institute of Technology (KTH)



I. Overview

Bio

- ▶ **B.Sc. & M.Sc.**: pure mathematics at La Sapienza (Rome)
- ▶ **Ph.D.**: machine learning and robotics at KTH (Stockholm)
- ▶ **PostDoc**: theoretical machine learning at KTH (Stockholm)

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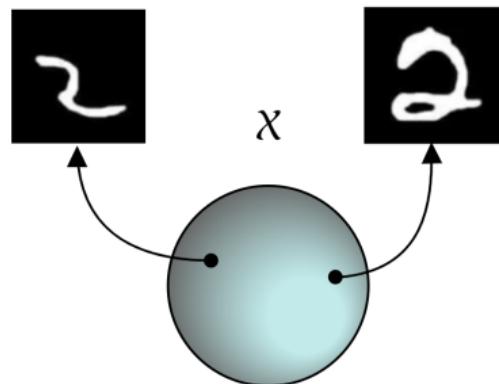
Research Interests

Geometric methods for machine learning and high-dimensional statistics:

- ▶ Geometric deep learning
- ▶ Manifold/representation learning
- ▶ Computational geometry & topology
- ▶ Statistical learning theory
- ▶ Robotics

The Geometry of Data

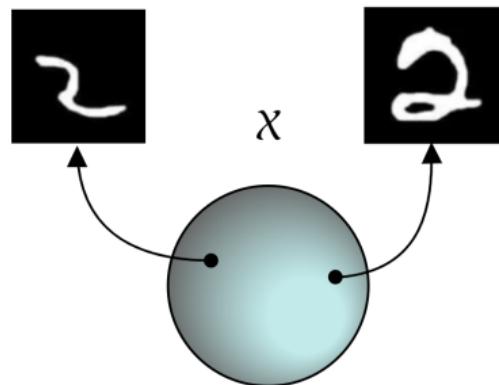
Data naturally carry **geometric structure**.



A data-set

The Geometry of Data

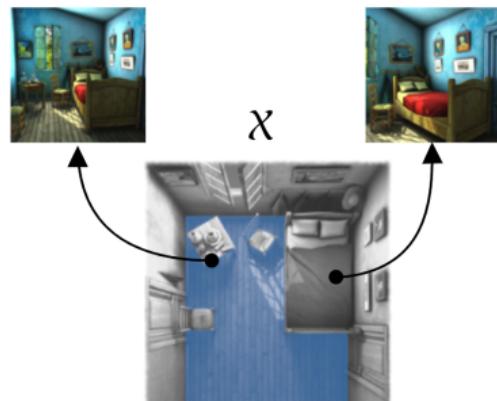
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A data**set**-manifold

The Geometry of Data

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The Geometry of Data

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Question: How can the geometric structure be extracted statistically from data and exploited for inference?

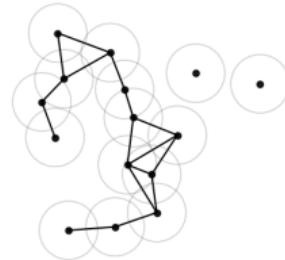


A data~~set~~-manifold

Geometric Methods

Geometric structure can be extracted in several forms.

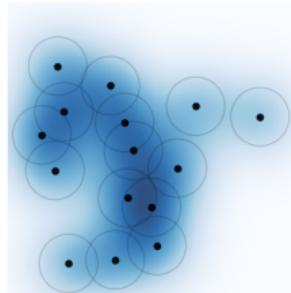
- ▶ **Combinatorial:** graphs and simplicial complexes [3]



- [3] Edelsbrunner et al., "Computational topology: an introduction", 2022
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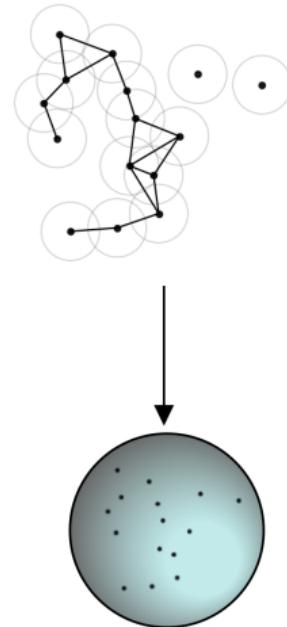
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Geometric Methods

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- ▶ **Combinatorial**: graphs and simplicial complexes [3]
- ▶ **Fuzzy**: density estimators [21]
- ▶ **Smooth**: (neural) representations [1]

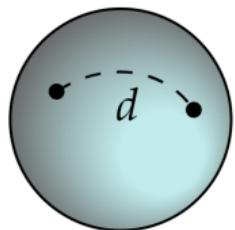


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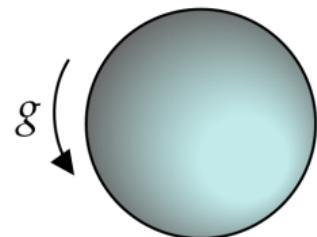
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Symmetries and Metrics

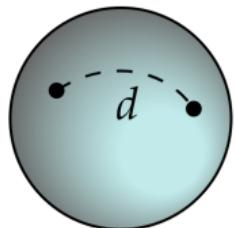


Metrics

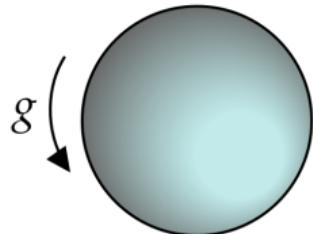


Symmetries

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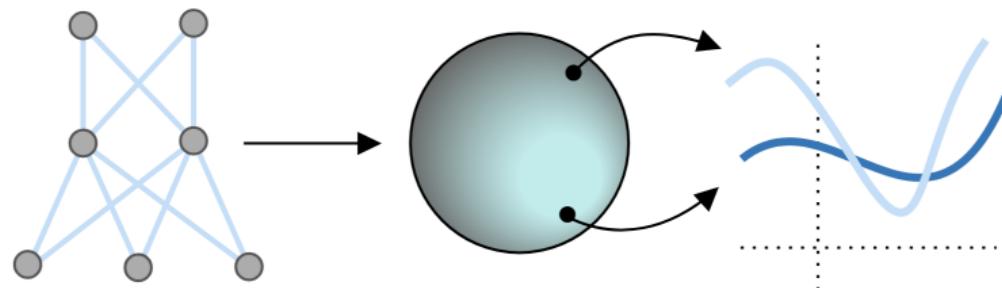
Symmetries

- ▶ Local in nature
- ▶ Can be inferred from data
- ▶ Suitable for non-parametric approaches

- ▶ Global in nature
- ▶ Unknown a priori
- ▶ Require powerful parametric approaches

The Geometry of Models

Machine learning models parametrize **spaces of functions**, whose (continuous) geometry is central in learning aspects.



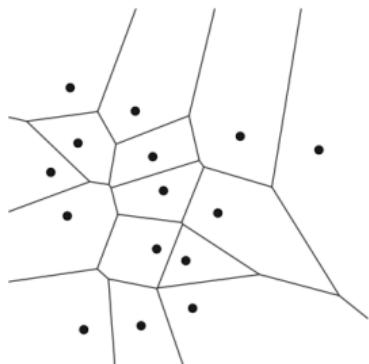
II. Geometric Density Estimation

Voronoi Tessellations

Definition

Let \mathcal{X} be a metric space and $P \subseteq \mathcal{X}$ finite. The **Voronoi cell** of $p \in P$ is defined by the nearest-neighbor relation:

$$C(p) = \{x \in \mathcal{X} \mid \forall q \in P \ d(x, q) \geq d(x, p)\}.$$



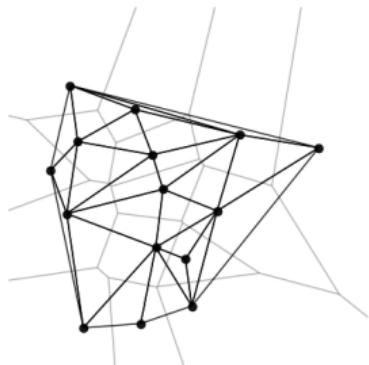
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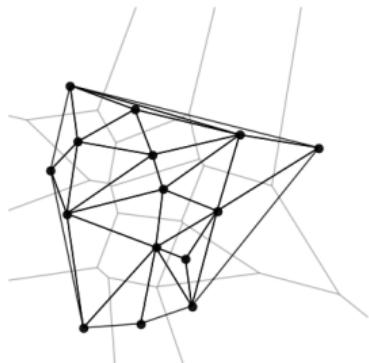
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$C(p)$ is:

- ✓ An arbitrary convex polytope
- ✓ An adaptive neighbourhood of p
- ✗ Expensive to compute

Voronoi Density Estimator (VDE)

Non-Parametric Density Estimation

Estimate a closed-form density $\hat{\rho} \in L^1(\mathcal{X})$ from finite samples $P \subseteq \mathcal{X}$, $P \sim \rho$.

[15] Ord, "How many trees in a forest", 1978

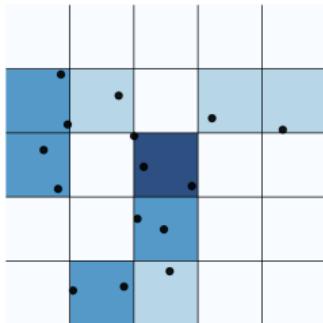
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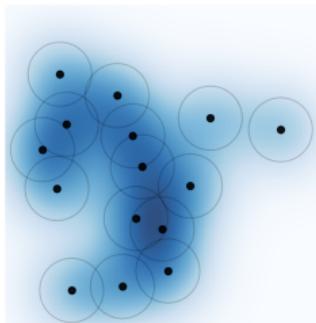
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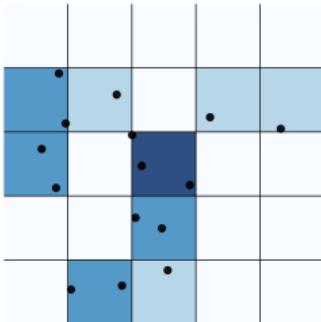
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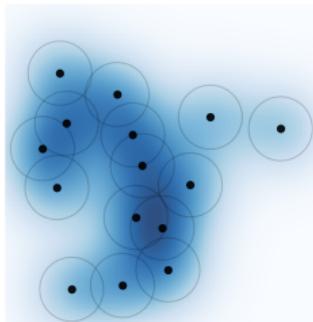
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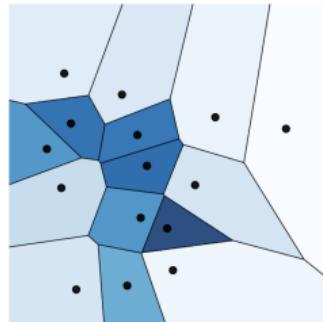
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In VDE, $\hat{\rho}(x)$ is inversely proportional to the volume of Voronoi cell $C(p) \ni x$.

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In [17], we prove **convergence** of Voronoi-based estimators to the ground-truth density ρ .

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Theorem

Consider a density estimator such that

$$\int_{C(p)} \hat{\rho} = \frac{1}{|P|}$$

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In contrast, KDE requires asymptotically-vanishing bandwidth for convergence.

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Improving the Voronoi Density Estimator

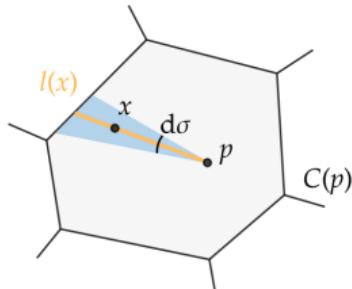
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Improving the Voronoi Density Estimator

VDE is:



- ✓ Adaptive and convergent
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In [11], we improve this by exploiting the radial geometry of Voronoi tessellations: $l(x)$ is **continuous** and **computable** in $O(|P|)$.

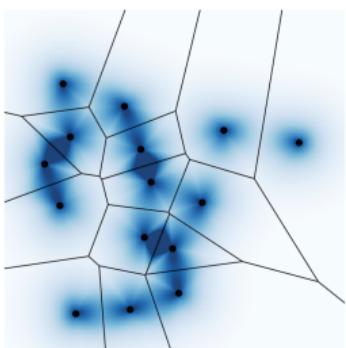
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Radial Voronoi Density Estimator

Given a kernel K , the estimated density is $K(\beta d(x, p))$, where $x \in C(p)$ and the **radial bandwidth** $\beta = \beta(I(x))$ is defined implicitly via an integral equation:

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RVDE

$$\underbrace{\int_0^{I(x)} t^{n-1} K(\beta t) dt}_{\text{Conical integral}} = \text{const}$$

In particular, $\int_{C(p)} \hat{\rho}$ is constant, implying convergence.

Modes and Performance

The map $I \mapsto \beta(I)$ generalizes Lambert's function. In particular:

Theorem

*The **modes** of RVDE are located among nodes and edges of the Delaunay triangulation.*

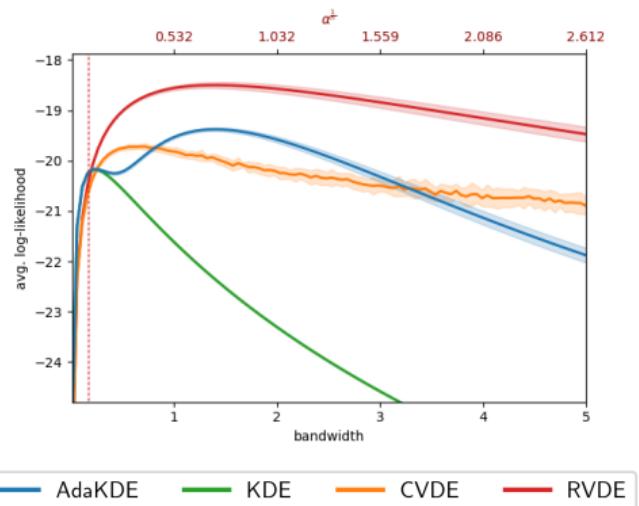
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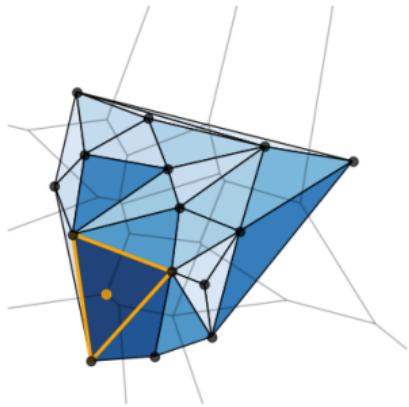
RVDE performs well:



Related Works

We have explored similar ideas for:

Non-parametric **active learning** via Delaunay triangulations [9].



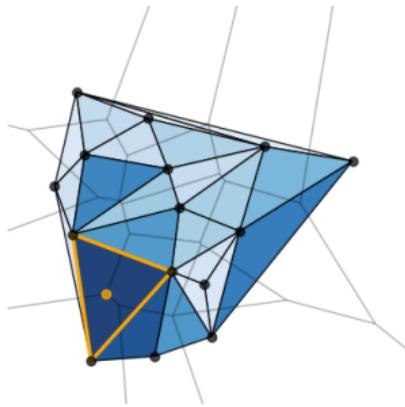
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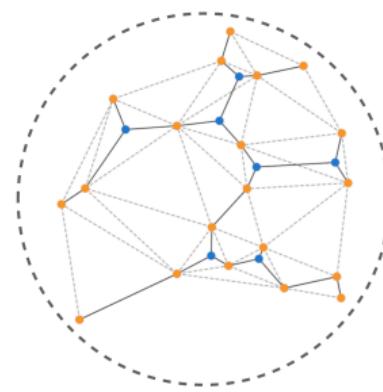
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Statistics in non-Euclidean geometries, in particular **hyperbolic spaces** [4].



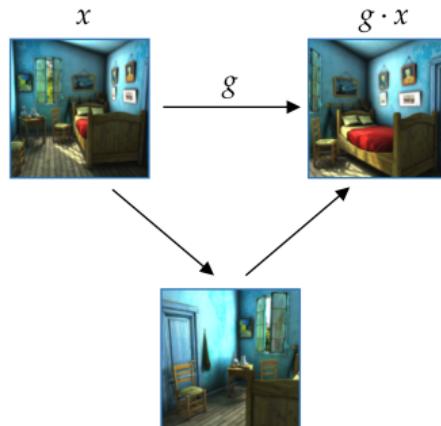
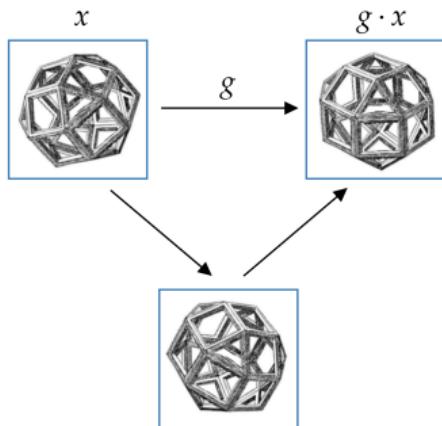
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III. Symmetry-Based Representation Learning

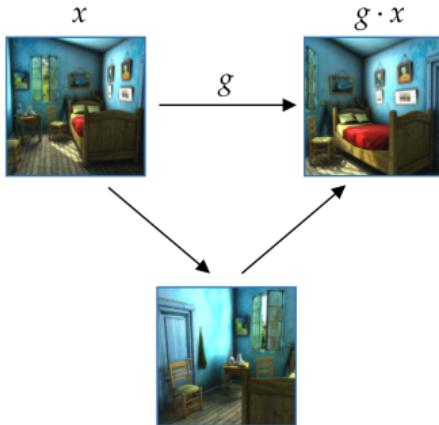
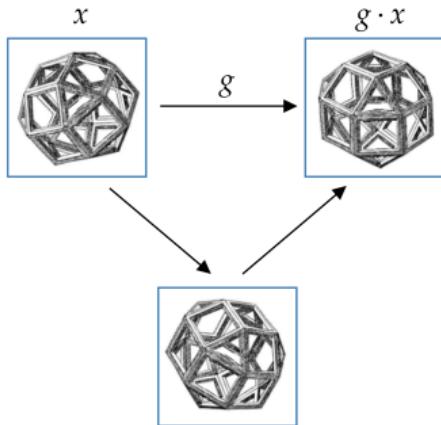
Symmetries of Data

Data naturally exhibit symmetries.



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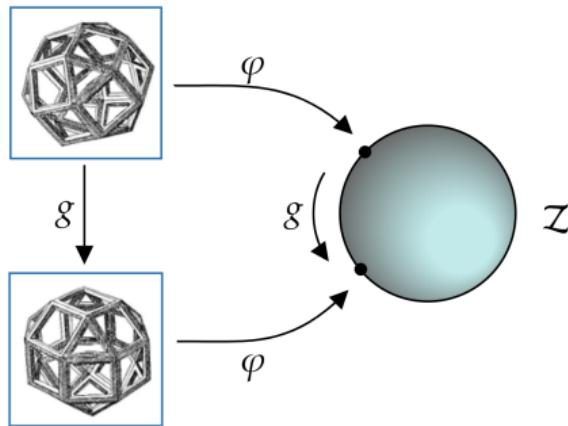
Data naturally exhibit symmetries.



Symmetries are modelled as an unknown **action** $G \times \mathcal{X} \rightarrow \mathcal{X}$ by a **group** G on \mathcal{X} .

Equivariant Representations

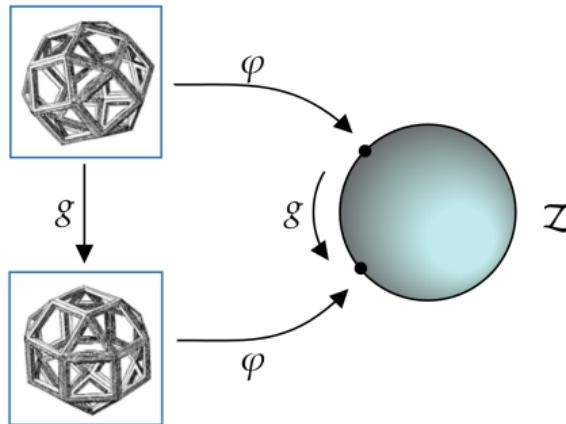
A representation respecting symmetries is deemed **equivariant**.



- [2] Bronstein et al., "Geometric deep learning: Grids, groups, graphs, geodesics, and gauges", 2021
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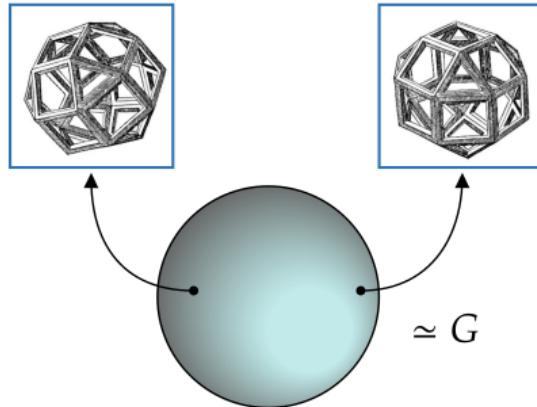
They arise in:

- ▶ **Convolutional** and graph neural networks [2]
- ▶ **World models**, incorporating interactions into representations [8]

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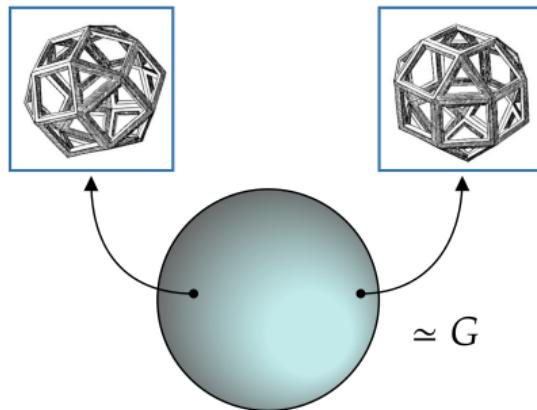
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Geometry from Symmetries



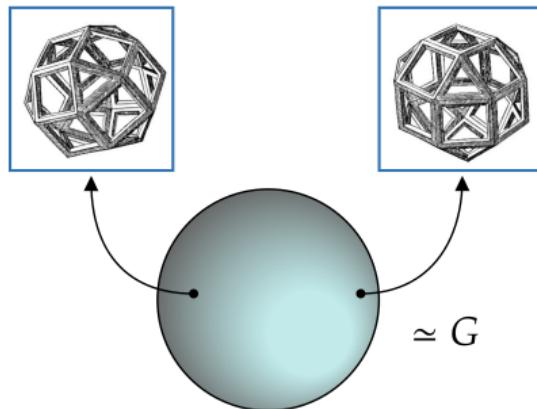
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Geometry from Symmetries



- ▶ Group actions determine classes deemed **orbits** $\mathcal{E} = \mathcal{X}/G$
- ▶ For **free** group actions, each orbit is isomorphic to G and thus $\mathcal{X} \simeq \mathcal{E} \times G$
- ▶ Every orbit-preserving equivariant map $\varphi: \mathcal{X} \rightarrow \mathcal{E} \times G$ is an isomorphism

Equivariant Isomorphic Networks (EquIN)

In [13], we propose to learn a representation $\varphi: \mathcal{X} \rightarrow \mathcal{E} \times G$. Given triplet data $(x, g, y = g \cdot x)$, EquIN optimizes:

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An ideal learner φ will infer an **isomorphism**. In particular, the representation is:

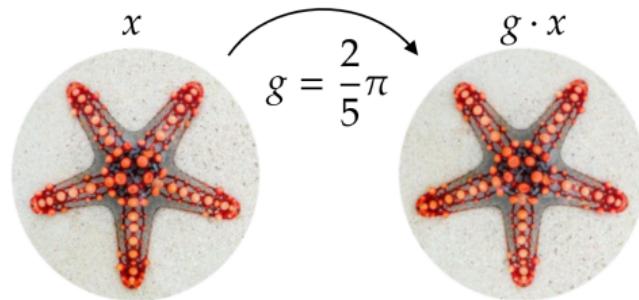
- ✓ Lossless
- ✓ Disentangled [6]
- ✗ Based on the assumption that G known a priori

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Non-Free Group Actions

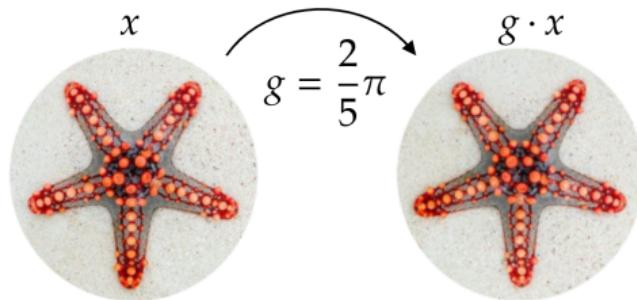
When data is **stabilized**, the action is not free.



[19] Rey*, Marchetti* et al., "Equivariant Representation Learning in the Presence of Stabilizers", ECML 2023

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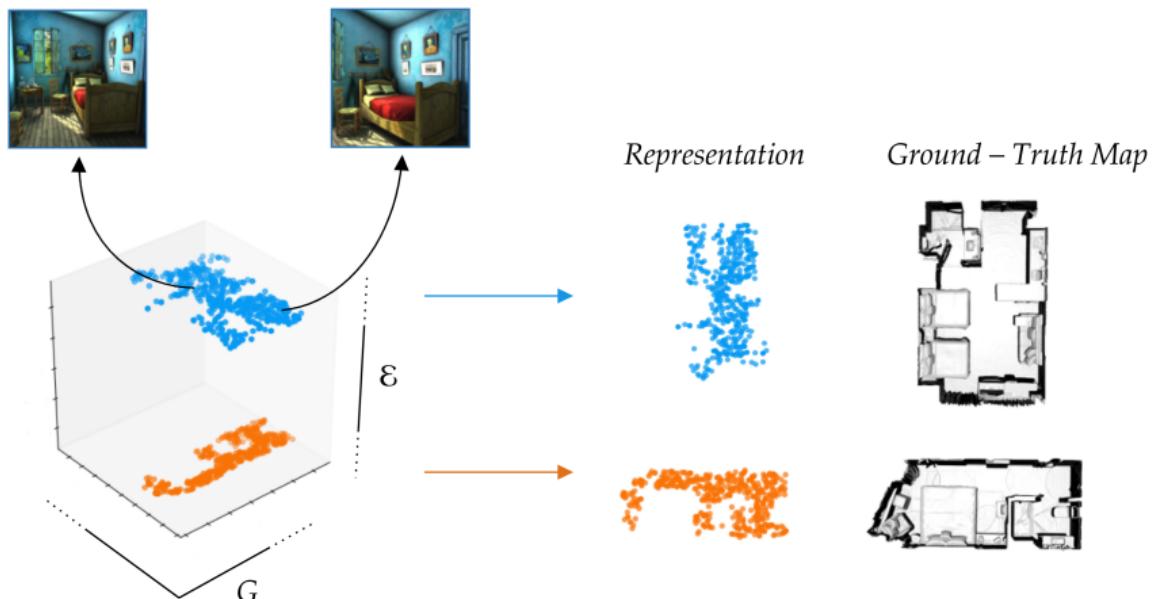


EquIN extends to this generality, but the theory is more subtle [19].

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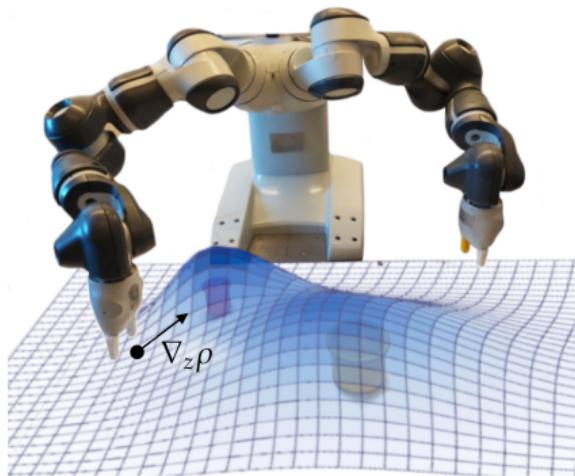
Extracting Geometry

EquIN extracts isometric maps of the world, which is crucial in **robotic perception**.



Applications to Robotics

We apply EquIN to vision-based manipulation in [18].



[18] Reichlin, Marchetti et al., "Back to the Manifold: Recovery from Out-of-Distribution States", IROS 2022

Abstract Harmonic Analysis

Suppose that G is **unknown**. Is it possible to discover symmetries from data?

Abstract Harmonic Analysis

Symmetries are intimately related to [harmonic analysis](#):

Abstract Harmonic Analysis

Symmetries are intimately related to **harmonic analysis**: the **Fourier transform** can be defined over arbitrary groups G .

The Fourier transform decomposes functions $G \rightarrow \mathbb{C}$ into harmonics, i.e. (irreducible) unitary representations $G \rightarrow \mathrm{U}(\mathbb{C}^n)$.

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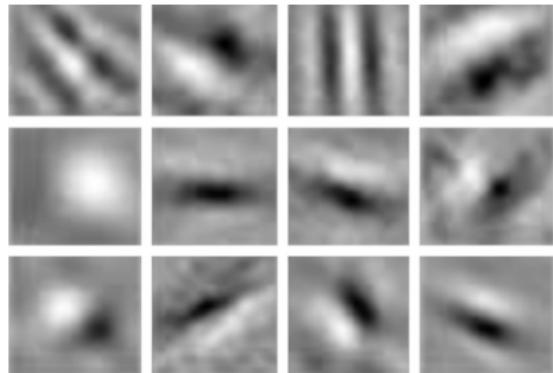
For **commutative** groups, $n = 1$, and $\mathrm{U}(\mathbb{C})$ is a circle.

Emergence of Harmonics

Harmonics are ubiquitous in both **biological** and **artificial** networks.



AlexNet [10]



Macaque [23]

[10] Krizhevsky et al., "Imagenet classification with deep convolutional neural networks", 2012

[23] Zylberberg et al., "A sparse coding model with synaptically local plasticity and spiking neurons can account for the diverse shapes of V1 simple cell receptive fields", 2011

Harmonics of Learning

In [14], we show that for a neural network $\varphi(W, x)$:

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Theorem

If φ is **invariant** in x w.r.t. G , then each neuron learns a harmonic of G . In particular, if W is orthonormal, it coincides with the **Fourier transform**.

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If φ is ‘almost invariant’ and the W is ‘almost orthonormal’, then G can be *recovered* from W up to isomorphism.

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This explains the emergence of harmonics in learning systems via invariance, and can be exploited for symmetry discovery via contrastive learning.

[14] Marchetti et al., "Harmonics of Learning: Universal Fourier Features Emerge in Invariant Networks", COLT 2024

IV. Algebraic Geometry of Neural Networks

Neuromanifolds

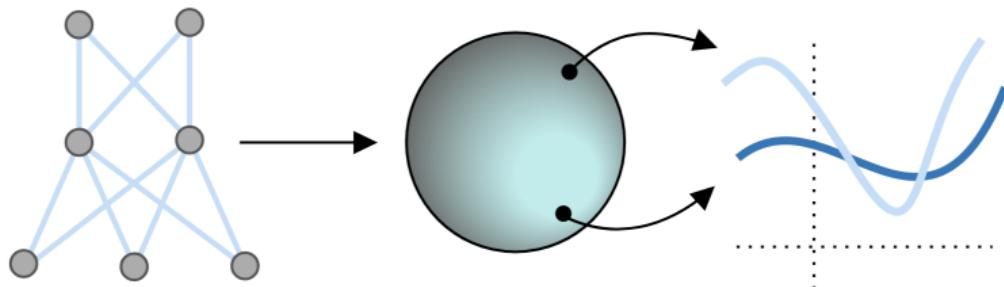
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Neuromanifolds

Machine learning models parametrize spaces of functions, referred to as:

Neuromanifolds
Information geometry

Hypothesis Spaces
Statistical learning theory



Algebraic Neuromanifolds

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By Weierstrass, any continuous activation function can be approximated by polynomial ones.

Neuroalgebraic Geometry

We refer to the study of neuromanifolds via algebraic geometry as [neuroalgebraic geometry](#) [12].

[12] Marchetti et al., "An Invitation to Neuroalgebraic Geometry", preprint 2025

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Deep Learning	Algebraic Geometry
sample complexity, expressivity	dimension, degree
subnetworks	singularities
identifiability	fibers of the parametrization
learning dynamics	gradient flow, Morse theory

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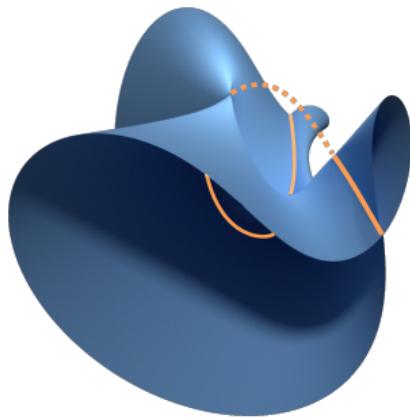
Advances in Neuroalgebraic Geometry

We have recently studied the neuroalgebraic geometry of:

- [22] Shahverdi* Marchetti* and Kohn*, "On the Geometry and Optimization of Polynomial Convolutional Networks", AISTATS 2025
- [5] Henry* Marchetti* and Kohn*, "Geometry of Lightning Self-Attention: Identifiability and Dimension", ICLR 2025
- [7] Kileel et al., "On the expressive power of deep polynomial neural networks", 2019

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Figure: Neuromanifold of self-attention

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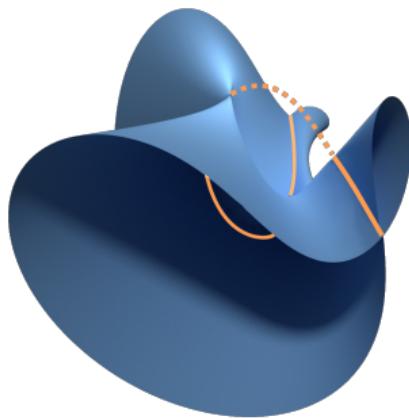


Figure: Neuromanifold of self-attention

- ▶ Deep polynomial **convolutional** networks [22]
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For **fully-connected** networks, most problems are still open [7]!

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Directions for future work:

- ▶ Voronoi cells for social networks/graphs.
- ▶ Emergence of features, especially in large vision/language models.
- ▶ A prescriptive theory of neural architectures; what's next after Transformers?

Grazie!

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