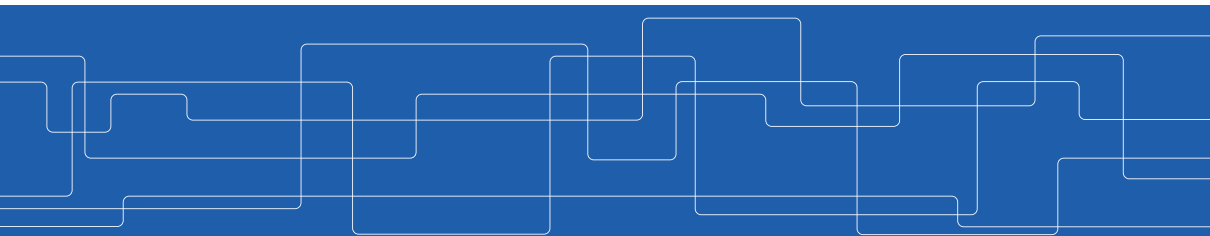




On Symmetries and Metrics in Geometric Inference

Giovanni Luca Marchetti

Supervisor: Prof. Danica Kragic
Co-Supervisor: Dr. Anastasiia Varava

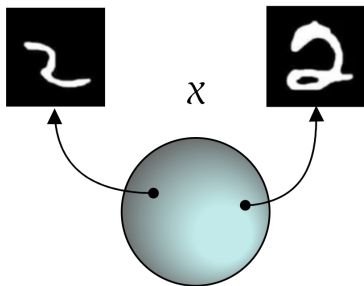




I. Overview

The Geometry of Data

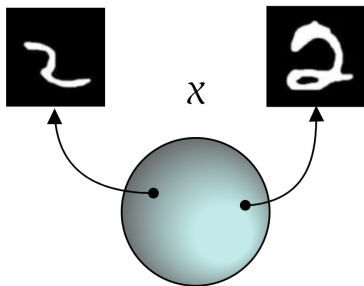
Data naturally carry **geometric structure**.



A data-set

The Geometry of Data

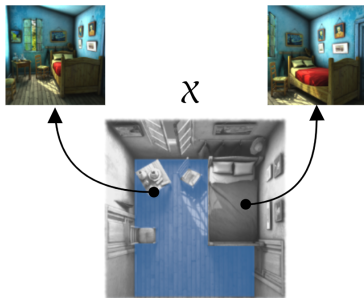
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A data ~~set~~-manifold

The Geometry of Data

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The Geometry of Data

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χ



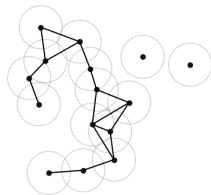
Question: How can the geometric structure be extracted statistically from data and exploited for inference?



A data set manifold

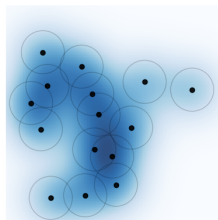
Geometric structure can be extracted in several forms.

- **Combinatorial:** graphs and simplicial complexes [4]



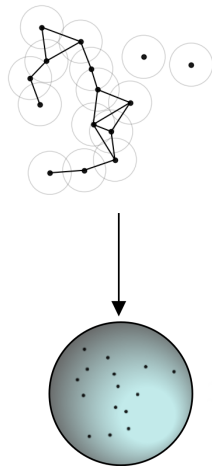
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- ▶ **Fuzzy**: density estimators [13]



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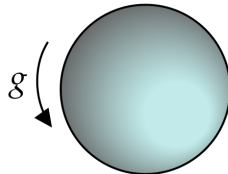
- ▶ **Combinatorial**: graphs and simplicial complexes [4]
- ▶ **Fuzzy**: density estimators [13]
- ▶ **Smooth**: representations [2]



Symmetries and Metrics



Metrics



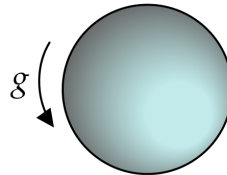
Symmetries

Symmetries and Metrics



Metrics

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



Symmetries

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



Included Papers

(A) *Active Nearest Neighbor Regression Through Delaunay Refinement*

Kravberg*, Marchetti*, Polianskii* et al., ICML 2022

(B) *Voronoi Density Estimator for High-Dimensional Data: Computation, Compactification and Convergence*

Polianskii*, Marchetti* et al., UAI 2022

(C) *An Efficient and Continuous Voronoi Density Estimator*

Marchetti et al., AISTATS 2023, **Notable Paper Award**

(D) *Equivariant Representation Learning via Class-Pose Decomposition*

Marchetti*, Tegnér* et al., AISTATS 2023

(E) *Equivariant Representation Learning in the Presence of Stabilizers*

Rey*, Marchetti* et al., ECML 2023

(F) *Back to the Manifold: Recovering from Out-of-Distribution States*

Reichlin, Marchetti et al., IROS 2022

(G) *Harmonics of Learning: Universal Fourier Features Emerge in Invariant Networks*

Marchetti et al., preprint 2024

*Equal contribution



II. Metric-Based Methods

Papers **A**, **B** and **C**

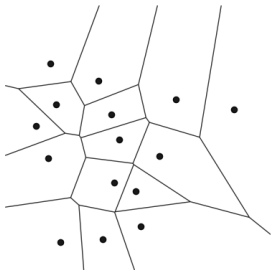
Voronoi Tessellations

Definition

Let \mathcal{X} be a metric space and $P \subseteq \mathcal{X}$ finite. The *Voronoi cell* of $p \in P$ is

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

The *Delaunay triangulation* is dual to the Voronoi tessellation.



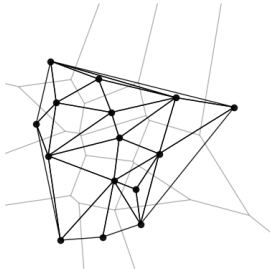
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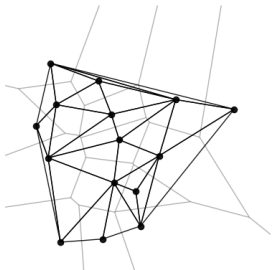
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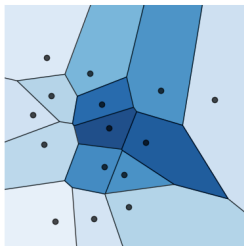
The *Delaunay triangulation* is dual to the Voronoi tessellation.



- ✓ Arbitrary convex polytopes
- ✓ Locally adaptive
- ✗ Expensive to compute

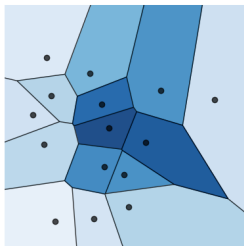
Nearest Neighbor Regressor (NNR)

NNR [5] approximates an unknown function f by the value at the closest datapoint. It is **locally constant** on Voronoi cells.



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We upgrade NNR to an **active** regressor by querying a novel datapoint p_{t+1} at step t based on the current dataset P_t .



Active Nearest Neighbor Regressor (ANNR)

Work **A**

Our querying strategy exploits the geometry of the **graph of f** discretized via the Delaunay triangulation:

[**A**] Kravberg*, Marchetti*, Polianskiĭ* et al., "Active Nearest Neighbour Regression Through Delaunay Refinement", 2022.

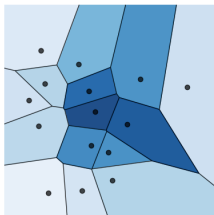
Active Nearest Neighbor Regressor (ANNR)

Work A

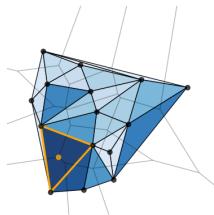
Our querying strategy exploits the geometry of the **graph of f** discretized via the Delaunay triangulation:

$$p_{t+1} = \text{Circ}(\bar{\sigma}), \quad \bar{\sigma} = \operatorname{argmax}_{\sigma \in \text{Del}P_t} \text{Vol}(\hat{\sigma}).$$

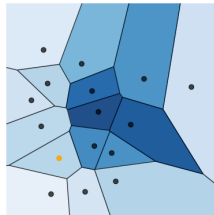
Here $\hat{\sigma}$ is the lifting of σ to the graph of λf , where λ controls **exploration-exploitation**.



P_t

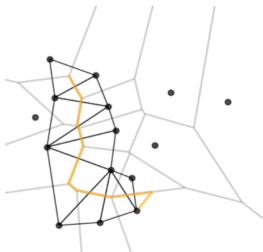


Query



P_{t+1}

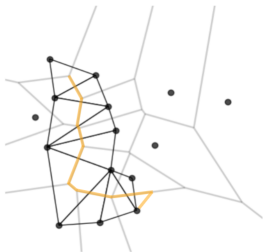
We compute the Delaunay triangulation approximately via a **random walk** over the Voronoi boundaries [11].



[A] Kravberg*, Marchetti*, Polianskii* et al., "Active Nearest Neighbour Regression Through Delaunay Refinement", 2022.

[11] Polianskii et al., "Voronoi Graph Traversal in High Dimensions", 2020

We compute the Delaunay triangulation approximately via a **random walk** over the Voronoi boundaries [11].



We prove **halting** guarantees:

Theorem

If f is Lipschitz then

$$\lim_{t \rightarrow \infty} \max_{\sigma \in \text{Del} P_t} \text{Vol}(\hat{\sigma}) = 0.$$

and provide a Riemannian interpretation:

Theorem

If $f \in C^1(\Omega)$ then

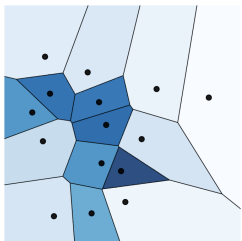
$$\log \text{Vol}(\Gamma_{\lambda f}) \gtrsim C \lambda^2 \|f - f_{\Omega} f\|_2^2 + \log \text{Vol}(\Omega).$$

[A] Kravberg*, Marchetti*, Polianskii* et al., "Active Nearest Neighbour Regression Through Delaunay Refinement", 2022.

[11] Polianskii et al., "Voronoi Graph Traversal in High Dimensions", 2020

Voronoi Density Estimator (VDE)

VDE [9] is inversely proportional to the volume of Voronoi cells.



VDE

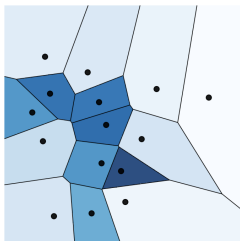
[9] Ord, "How many trees in a forest", 1978

[10] Pearson, "Contributions to the mathematical theory of evolution", 1894

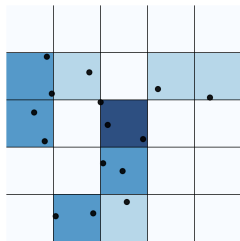
[12] Rosenblatt, "Remarks on Some Nonparametric Estimates of a Density Function", 1956

Voronoi Density Estimator (VDE)

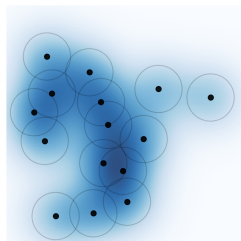
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VDE



Histograms [10]



KDE [12]

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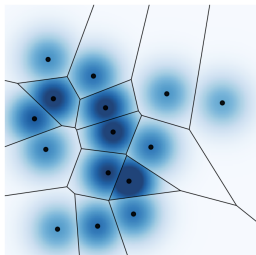
[10] Pearson, "Contributions to the mathematical theory of evolution", 1894

[12] Rosenblatt, "Remarks on Some Nonparametric Estimates of a Density Function", 1956

Compactified Voronoi Density Estimator (CVDE)

Work B

We **compactify** (unbounded) cells via a kernel K :

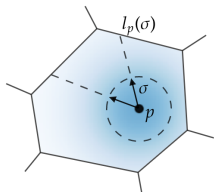


CVDE

$$\hat{\rho}(x) = \frac{K(x - p)}{|P| \int_{C(p)} K(y - p) dy}, \quad x \in C(p).$$

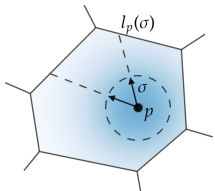
We **compute** the volumes via Monte-Carlo spherical integration:

$$\int_{\mathbb{S}^{n-1}} \int_0^{l_p(\sigma)} K(t\sigma) t^{n-1} dt d\sigma$$



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$$\int_{\mathbb{S}^{n-1}} \int_0^{l_p(\sigma)} K(t\sigma) t^{n-1} dt d\sigma$$



We prove **convergence** of CVDE to the ground-truth density ρ .

Theorem

Suppose that ρ has support in the whole \mathbb{R}^n . For any $K \in L^1(\mathbb{R}^n \times \mathbb{R}^n)$, CVDE, seen as a random measure, converges to ρ in distribution w.r.t x and in probability w.r.t. P as $|P| \rightarrow \infty$.

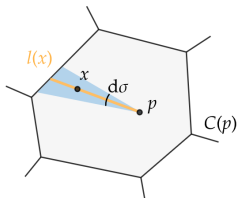


An Improved Voronoi Density Estimator

CVDE is:

- ✓ Adaptive and convergent
- ✓ More efficient than VDE but less than KDE
- ✗ Discontinuous

An Improved Voronoi Density Estimator



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We improve this by exploiting the radial geometry of Voronoi tessellations: $l(x)$ is **continuous** and **computable** in $O(|P|)$.



Radial Voronoi Density Estimator (RVDE)

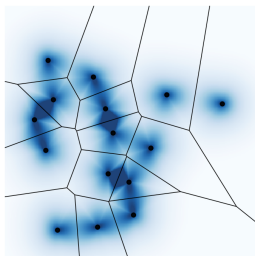
Work C

For a kernel K , we define a **radial bandwidth** $\beta = \beta(I(x))$ implicitly via an integral equation:

Radial Voronoi Density Estimator (RVDE)

Work C

For a kernel K , we define a **radial bandwidth** $\beta = \beta(l(x))$ implicitly via an integral equation:



RVDE

$$\hat{\rho}(x) \propto \frac{K(\beta d(x, p))}{|P|}, \quad x \in C(p),$$

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

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



Modes and Performance

Work C

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

Theorem

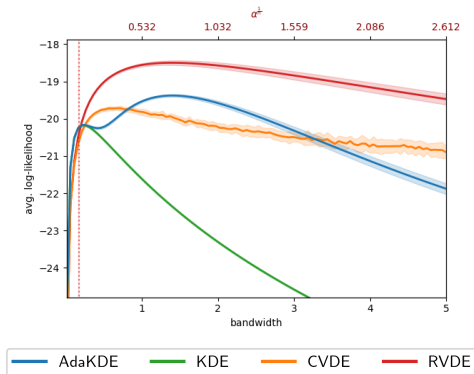
*The **modes** of RVDE are located among nodes and edges of the Gabriel graph.*

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 Gabriel graph.

RVDE performs well:



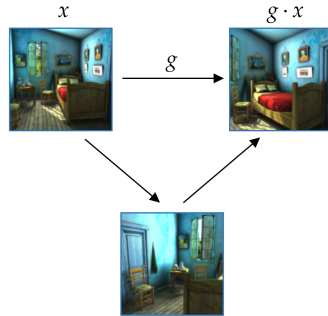
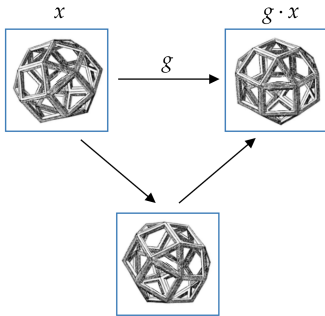


III. Symmetry-Based Methods

Papers **D**, **E**, **F** and **G**

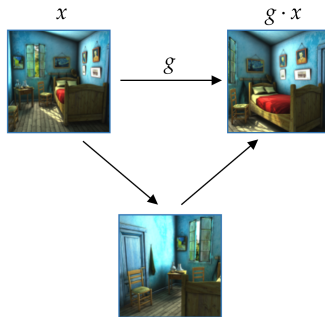
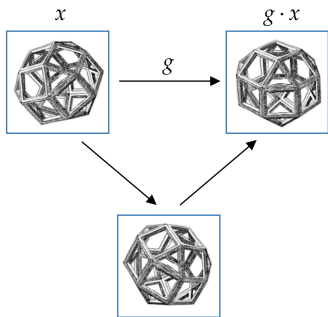
Symmetries of Data

Data naturally exhibit symmetries.



Symmetries of Data

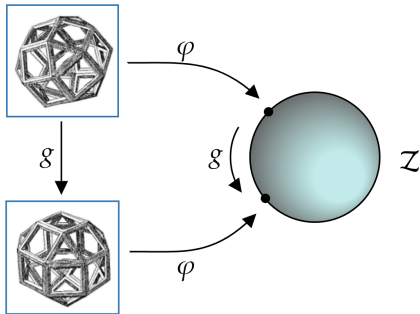
Data naturally exhibit symmetries.



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**.

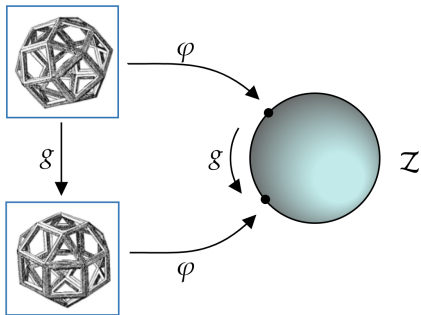


[3] Bronstein et al., "Geometric deep learning: Grids, groups, graphs, geodesics, and gauges", 2021

[7] Kipf et al., "Contrastive learning of structured world models", 2020

[1] Ahuja et al., "Properties from mechanisms: an equivariance perspective on identifiable representation learning", 2022

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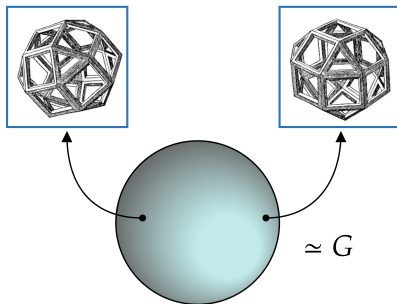
They are related to:

- ▶ **Convolutional** and graph neural networks [3]
- ▶ **World models**, incorporating interactions into representations [7, 1]

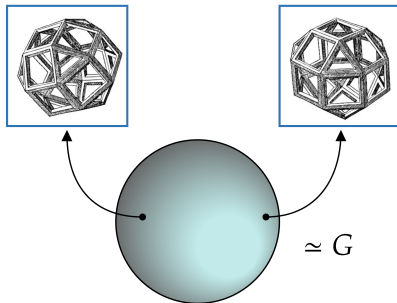
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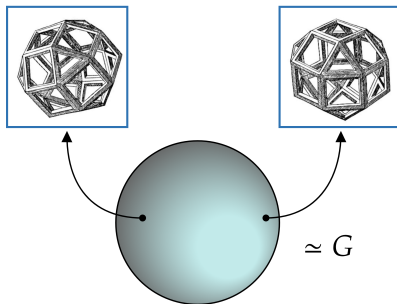
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- ▶ For **free** group actions, each orbit is isomorphic to G and thus $\mathcal{X} \simeq \mathcal{E} \times G$
- ▶ Every orbit-preserving equivariant map $\varphi : \mathcal{X} \rightarrow \mathcal{E} \times G$ is an isomorphism



Equivariant Isomorphic Networks (EquIN)

Work D

We propose to learn a representation $\varphi: \mathcal{X} \rightarrow \mathcal{E} \times G$ by optimizing:

$$\mathcal{L}(x, g, y = g \cdot x) = \underbrace{d_{\mathcal{E}}(\varphi_{\mathcal{E}}(y), \varphi_{\mathcal{E}}(x))}_{\text{Invariant/Contrastive}} + \underbrace{d_G(\varphi_G(y), g\varphi_G(x))}_{\text{Multiplication-Equivariant}}$$

[5] Marchetti*, Tegner* et al., "Equivariant Representation Learning via Class-Pose Decomposition", 2023.

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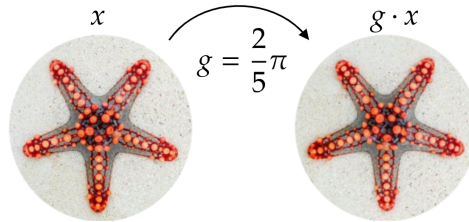
At the optimum, φ is an **isomorphism**. In particular, it is:

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

[D] Marchetti*, Tegner* et al., "Equivariant Representation Learning via Class-Pose Decomposition", 2023.

[6] Higgins et al., "Towards a definition of disentangled representations", 2018

Non-Free Group Actions



In general, it is necessary to consider **stabilizer subgroups**:

$$G_x = \{g \in G \mid g \cdot x = x\}.$$



EquIN with Stabilizers

Work E

- ▶ Each orbit $O \subseteq \mathcal{X}$ is isomorphic to the coset space G/G_{x_0} , $x_0 \in O$.



EquIN with Stabilizers

Work **E**

- ▶ Each orbit $O \subseteq \mathcal{X}$ is isomorphic to the **coset** space G/G_{x_0} , $x_0 \in O$.
- ▶ Any orbit-preserving equivariant map

$$\varphi: \mathcal{X} \rightarrow \coprod_{O \in \mathcal{X}/G} G/G_{x_0}$$

is an isomorphism.



EquIN with Stabilizers

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is an isomorphism.

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EquIN with Stabilizers

Work E

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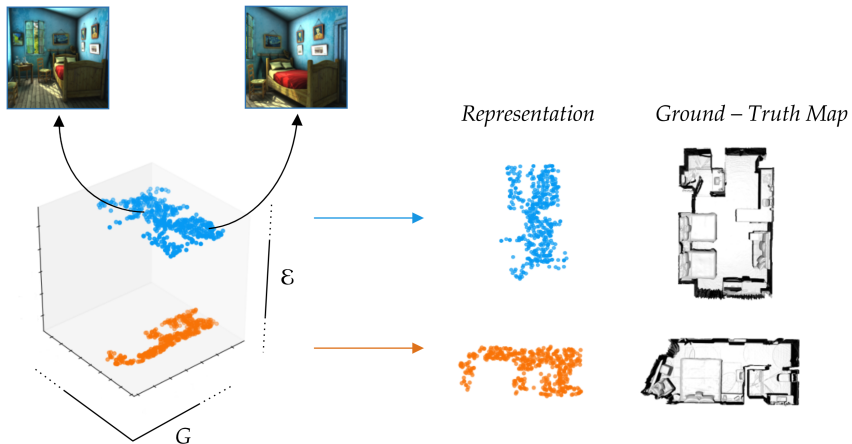
- ▶ Stabilizers are unknown a priori. However, the outputs of an equivariant map $\varphi: \mathcal{X} \rightarrow 2^G$ contain stabilizer subgroups.

We generalize EquIN to $\varphi: \mathcal{X} \rightarrow \mathcal{E} \times 2^G$, with an entropy loss term for [minimality](#).

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

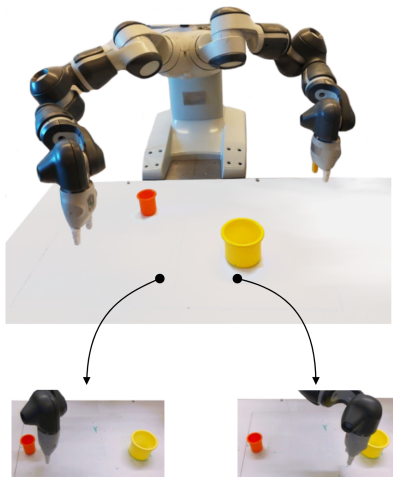
Extracting Geometry

EquiN extracts isometric maps of the world.



Back to the Manifold

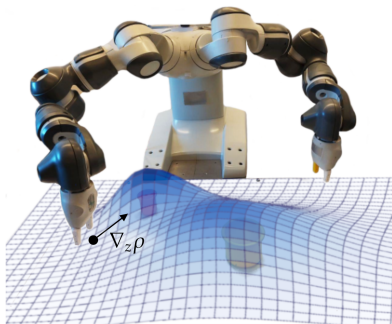
Work **F**



The extracted geometry can be exploited to address problems via classical methods.

Back to the Manifold

Work **F**



The extracted geometry can be exploited to address problems via classical methods.

We propose to **stabilize** a policy by using the estimated latent density ρ as a potential:

$$\tilde{\pi}(x) = \nabla_z \rho(\varphi(x)).$$



Abstract Harmonic Analysis

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



Abstract Harmonic Analysis

Group theory is intimately related to [harmonic analysis](#).



Abstract Harmonic Analysis

Group theory is intimately related to [harmonic analysis](#).

Definition

The *Fourier transform* is a linear isometric isomorphism of the form:

$$\mathbb{C}^G \rightarrow \bigoplus_{\rho: G \rightarrow \text{U}(V)} \text{End}(V),$$

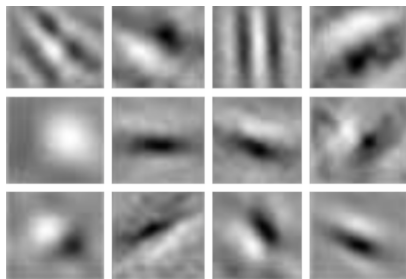
where ρ is an irreducible unitary representation (irrep) of G in a Hilbert space V .

Emergence of Harmonics

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



AlexNet



Macaque

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

[14] 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

Work G

We show that, under certain conditions, **invariance** of $\varphi(W, x)$ in x w.r.t. to a finite group G implies emergence of harmonics in W .



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Informal Theorem

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



Future Work

Extensions to other metric spaces, e.g.
Riemannian manifolds.

- ▶ Spheres for directional statistics.
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Extensions to **algebraic structures** beyond groups:

- ▶ Groupoids for local symmetries.
- ▶ C^* -algebras for more general transformations.



Tack!



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