Séminaire Datashape - 31/01/2024

DETECTION OF REPRESENTATION ORBITS OF COMPACT LIE GROUPS FROM POINT CLOUDS

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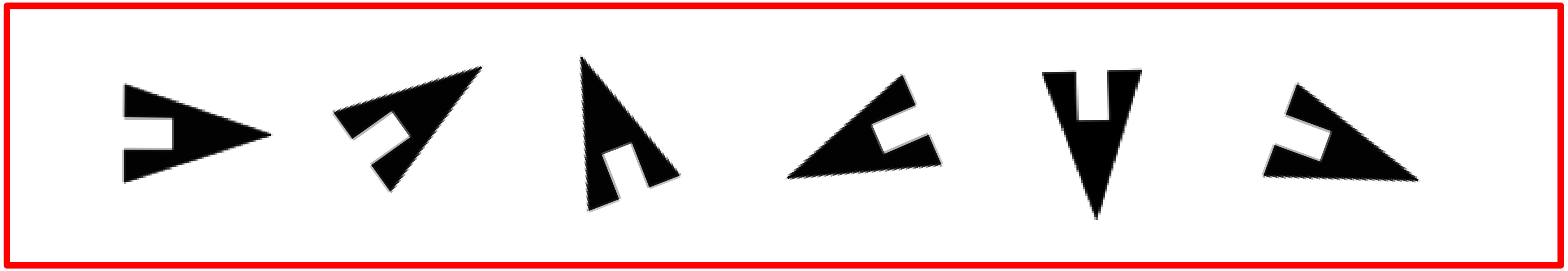
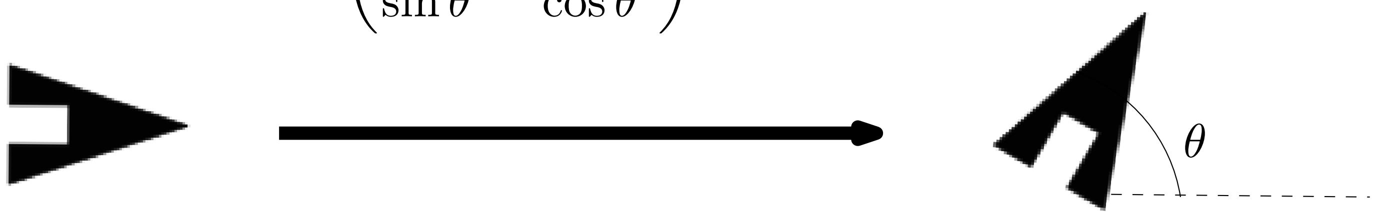
The orbit completion problem

DATA



TASK

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$



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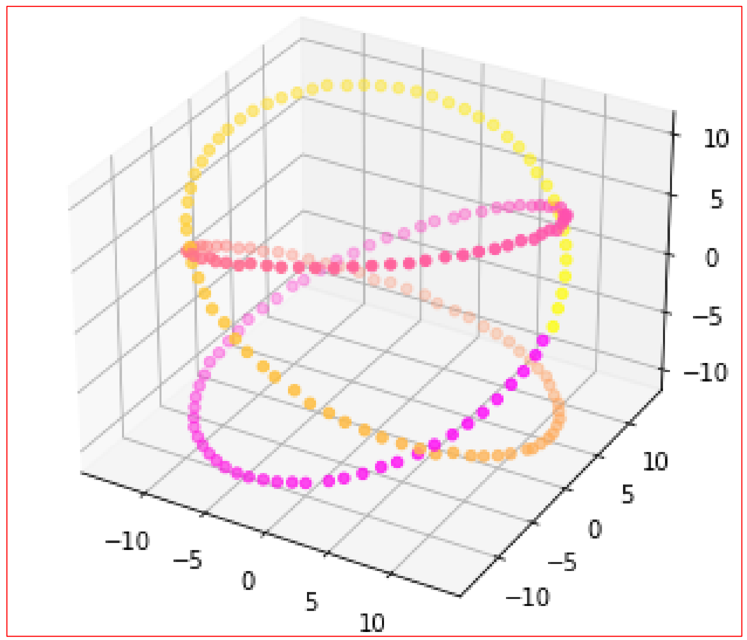
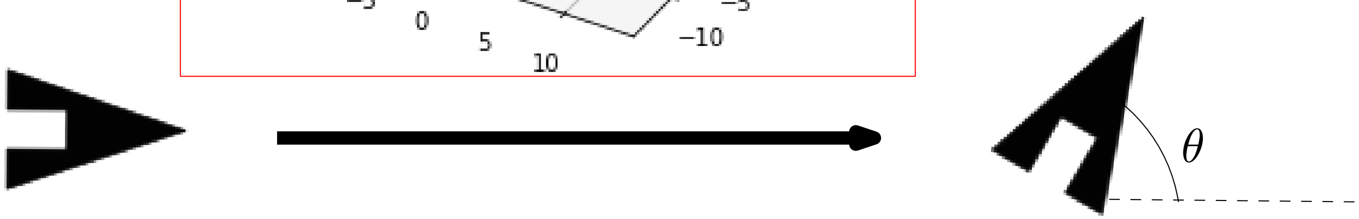
DATA





1. Lie theory
2. Applications of the algorithm
3. Description of the algorithm
4. Proof of robustness
5. Conclusion

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Lie groups and their representations

Lie groups are smooth finite dimensional manifolds endowed with also smooth group operation and inversions

Example: All topologically closed subgroups of $\mathrm{GL}(n, \mathbb{R})$ and $\mathrm{GL}(n, \mathbb{C})$ (i.e., the invertible $n \times n$ matrices over $\mathbb{R}$ and $\mathbb{C}$) for any integers n are Lie groups.

- $\mathrm{O}(n)$ - orthogonal $n \times n$ matrices
- $\mathrm{SO}(n)$ - orthogonal $n \times n$ matrices of determinant $+1$
- $\mathrm{Sp}(2n, \mathbb{C})$ - complex sympletic $n \times n$ matrices
- $\mathrm{U}(n)$ - complex unitary $n \times n$ matrices
- $\mathrm{SU}(n)$ - complex unitary $n \times n$ matrices of determinant $+1$

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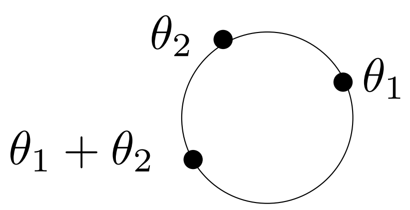
Example 2: Some Lie groups are not "naturally" groups of matrices, however

- $(S^1, +)$ - the circle group under angle addition



- $\mathrm{SE}(2) = \mathrm{SO}(2) \ltimes \mathbb{R}^2$ Euclidean group of orientation preserving isometries in the plane

$$(R_1, v_1) \cdot (R_2, v_2) = (R_1 R_2, v_1 + R_1 v_2)$$

where $R_i \in \mathrm{SO}(2)$ are rotations and $v_i \in \mathbb{R}^2$ are translations

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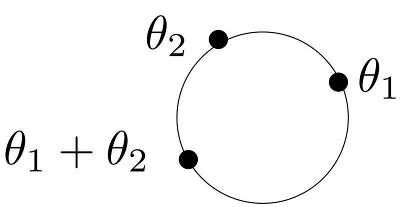
Example 2: Some Lie groups are not "naturally" groups of matrices, however

but they can be transformed into groups of matrices through **REPRESENTATIONS**

- $(S^1, +)$ - the circle group under angle addition



$$\theta_1 \mapsto \begin{pmatrix} \cos\theta_1 & -\sin\theta_1 \\ \sin\theta_1 & \cos\theta_1 \end{pmatrix}$$

$$\theta_2 \mapsto \begin{pmatrix} \cos\theta_2 & -\sin\theta_2 \\ \sin\theta_2 & \cos\theta_2 \end{pmatrix}$$

$$\theta_1 + \theta_2 \mapsto \begin{pmatrix} \cos\theta_1 & -\sin\theta_1 \\ \sin\theta_1 & \cos\theta_1 \end{pmatrix} \cdot \begin{pmatrix} \cos\theta_2 & -\sin\theta_2 \\ \sin\theta_2 & \cos\theta_2 \end{pmatrix} = \begin{pmatrix} \cos(\theta_1+\theta_2) & -\sin(\theta_1+\theta_2) \\ \sin(\theta_1+\theta_2) & \cos(\theta_1+\theta_2) \end{pmatrix}$$

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$$(R_1, v_1) \cdot (R_2, v_2) = (R_1 R_2, v_1 + R_1 v_2)$$

$$(R_1, v_1) \mapsto \begin{pmatrix} R_1 & v_1 \\ \mathbf{0}_{1\times 2} & \mathbf{1} \end{pmatrix}$$

$$(R_2, v_2) \mapsto \begin{pmatrix} R_2 & v_2 \\ \mathbf{0}_{1\times 2} & \mathbf{1} \end{pmatrix}$$

$$(R_1, v_1) \cdot (R_2, v_2) \mapsto \begin{pmatrix} R_1 & v_1 \\ \mathbf{0}_{1\times 2} & \mathbf{1} \end{pmatrix} \cdot \begin{pmatrix} R_2 & v_2 \\ \mathbf{0}_{1\times 2} & \mathbf{1} \end{pmatrix}$$

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Lie groups and their representations

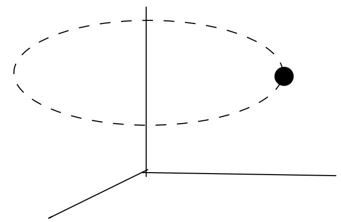
A **representation** of a Lie group G is a smooth group homomorphism $\rho : G \to GL(V)$, where $GL(V)$ is the set of invertible matrices over a vector space V

(equivalently, a representation is an action of G on V that is linear)

A same Lie group G may have several represenations

Ex.: $SO(2) = \left\{ \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \middle| \theta \in \mathbb{R} \right\} \xrightarrow{\rho_1} \{\exp(2\pi i\theta)\} \subseteq SU(1)$

$\xrightarrow{\rho_2} \left\{ \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\} \subseteq SO(3)$



- A representation (π, V) of G is **irreducible** if $W = \{0\}$ is the only proper subspace of V for which $\pi(G) \cdot W \subseteq W$, otherwise it is **reducible**

- A representation (ϕ, V) of G is **completely reducible** if it is the direct sum of irreducible representations $\pi_1, \ldots, \pi_n$ of G

$$\phi(g) = \pi_1(g) \oplus \cdots \oplus \pi_n(g), \forall g \in G$$

(there is a basis such that $\phi(g) = \text{diag}(\pi_1(g), \ldots, \pi_n(g))$)

Lie algebras

Let $L_g : G \to G$ be the left translation action of G onto itself, i.e., $L_g(h) = g \cdot h$, and X a vector field on G. Then X is called left-invariant if

$$L_g^* X = X, \forall g \in G$$

The set of left-invariant vector fields on G, $\mathfrak{g}$ is

- a vector space
- isomorphic to $T_e G$
- closed under Lie derivatives, i.e., if $X, Y \in \mathfrak{g}$, then $\mathcal{L}_X(Y) = [X, Y] \in \mathfrak{g}$
- there is a local diffeomorphism $\exp : \mathfrak{g} \to G$

The structure $(\mathfrak{g}, [\cdot, \cdot])$ is called the **Lie algebra** of G

For $\mathrm{GL}(n, F)$, we have that

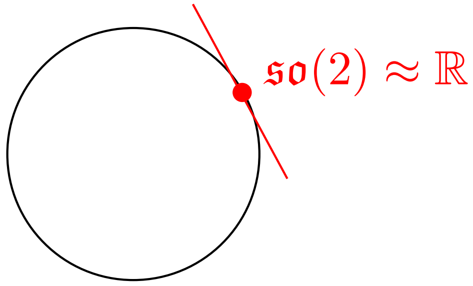
- $\mathfrak{gl}(n, F) = \mathrm{M}_{n \times n}(F)$ endowed with usual matrix commutation (i.e., $[X, Y] = XY - YX$)
- $\exp$ is just matrix exponentiation
  $\to \exp(tX)$ is a $n \times n$ invertible matrix for $X \in \mathfrak{gl}(n, F) = T_e G$
- $\exp(\mathfrak{gl}(n, \mathbb{C})) = \mathrm{GL}(n, \mathbb{C})$

Lie algebras

Example: $\mathfrak{so}(2) = t \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \approx \mathbb{R}$

$$\exp\left[t \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\right] = \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix}$$

$$\exp(\mathfrak{so}(2)) = SO(2)$$



$\mathrm{SO}(2) \approx S^1$

Example: $\mathfrak{so}(3) \approx (\mathbb{R}^3, \times)$

$$X = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \qquad Y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \qquad Z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\exp(t_X X + t_Y Y + t_Z Z) \in \mathrm{SO}(3)$$

!!! $\exp(t_X X + t_Y Y + t_Z Z) \neq \exp(t_X X) \cdot \exp(t_Y Y) \cdot \exp(t_Z Z)$!!!

Lie algebras

Representations of Lie groups define representations of their Lie algebras, called **derived representation**, where the images are matrices and the Lie brackets become commutators

$$\begin{array}{ccc} G & \xrightarrow{\rho} & \mathrm{GL}(V) \\ \exp\uparrow & & \exp\uparrow \\ \mathfrak{g} & \xrightarrow{\mathrm{d}\rho} & \mathfrak{gl}(V) = \mathrm{M}(V) \end{array}$$

Ex.:

$$\begin{array}{ccc} (S^1, +) & \xrightarrow{\rho} & \mathrm{SO}(2) \\ \exp\uparrow & & \exp\uparrow \\ \mathbb{R} & \xrightarrow{\mathrm{d}\rho} & \mathfrak{so}(2) \end{array}$$

$$\begin{array}{ccc} \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} & \xrightarrow{\rho} & \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \\ \exp\uparrow & & \exp\uparrow \\ \theta & \xrightarrow{\mathrm{d}\rho} & \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \end{array}$$

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$\mathrm{d}\rho(\mathfrak{g}) \subset \mathrm{M}(V)$ is the **pushforward Lie algebra**.

Two representations $\rho_1 : G \to \mathrm{GL}(n, V)$ and $\rho_2 : G \to \mathrm{GL}(n, V)$ of are **equal (up to a change of coordinates)** if there is an invertible linear transformation $L : \mathrm{M}_{n\times n} \to \mathrm{M}_{n\times n}$ which preserves commutators (i.e., $L([X, Y]) = [L(X), L(Y)]$)

Ex.: $\rho : \mathrm{SO}(2) \to \mathrm{GL}(3, \mathbb{R})$

$$\begin{array}{ccc} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} & \stackrel{\rho}{\rightarrowtail} & \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ {\scriptstyle \exp}\uparrow & & {\scriptstyle \exp}\uparrow \\ \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} & \stackrel{d\rho}{\rightarrowtail} & \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{array}$$

Ex'.: $\rho' : \mathrm{SO}(2) \to \mathrm{GL}(3, \mathbb{R})$

$$\begin{array}{ccc} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} & \stackrel{\rho'}{\rightarrowtail} & \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} \\ {\scriptstyle \exp}\uparrow & & {\scriptstyle \exp}\uparrow \\ \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} & \stackrel{d\rho'}{\rightarrowtail} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \end{array}$$

The derived representations allow to determine if two representations are the same.

Lemma: Equal representations iff conjugated pushforward Lie algebra.

Lie algebras

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we may consider $\mathcal{G}^{Lie}(V, \mathfrak{g})$ (resp. $\mathcal{V}^{Lie}(V, \mathfrak{g})$) as the Grasmmannian (resp. Stiefel) varieties of representations of $\mathfrak{g}$ in V up to this equivalence

The derived representations allow to determine if two representations are the same.

Lemma: Equal representations iff conjugated pushforward Lie algebra.

Facts about compact Lie groups

1. Compact Lie groups are fully classified

Group	Definition	Lie algebra definition	Dimension
$\mathrm{O}(n)$	$O^T = O^{-1}$	$O^T = -O$	$\frac{n(n-1)}{2}$
$\mathrm{SO}(n)$	$O^T = O^{-1}$ $\det O = 1$	$O^T = -O$	$\frac{n(n-1)}{2}$
$\mathrm{U}(n)$	$U^\dagger = U^{-1}$	$U^\dagger = -U$	n^2
$\mathrm{SU}(n)$	$U^\dagger = U^{-1}$ $\det U = 1$	$U^\dagger = -U$ $\mathrm{tr}\, U = 0$	$n^2 - 1$

+ products
+ finite extensions

2. All representations of compact Lie groups are orthogonal under some inner product

(ϕ, V) is a rep of G $\iff$ there is an inner product $\langle \cdot, \cdot \rangle$ such that, for all $x, y \in V$ and $g \in G$, $\langle x, y \rangle = \langle \rho(g)x, \rho(g)y \rangle$

$\iff$ there is a representation (ϕ', V) with $\langle x, y \rangle_{\ell^2} = \langle \phi'(g)x, \phi'(g)y \rangle_{\ell^2}$ and a $A \in \mathrm{GL}(V)$ such that $\phi(g) = A\phi'(g)A^{-1}, \forall g \in G$

3. Representations of compact Lie groups are completely reducible (there is a basis for V such that $\rho(g) = \mathrm{diag}(\pi_1(g), \ldots, \pi_n(g))$)

4. If G is connected, then $\exp : \mathfrak{g} \to G$ is surjective

Our algorithm

The goal: Given a point cloud $\{x_i\}_{i=1}^N$ in $\mathbb{R}^n$ which we believe to within the orbit of a representation $\rho : G \to \mathrm{GL}(n, \mathbb{R})$ of G. We want to decompose ρ as a direct sum of irreducible representations, i.e., there is an orthogonal change of basis $A : \mathbb{R}^n \to \mathbb{R}^n$ such that $\rho = A(\pi_1 \oplus \pi_2 \oplus \cdots \oplus \pi_k)A^{-1}$.

Ex.: The non-trivial real irreducible representations of $\mathrm{SO}(2)$ are all of $\pi_n : \mathrm{SO}(2) \to \mathrm{GL}(2, \mathbb{R})$ and given by

$$\pi_n(\theta) = \begin{pmatrix} \cos(n\theta) & -\sin(n\theta) \\ \sin(n\theta) & \cos(n\theta) \end{pmatrix}$$

Any $\rho : \mathrm{SO}(2) \to \mathbb{R}^{2n}$ has form $\rho(\theta) = \begin{pmatrix} \pi_{i_1}(\theta) & & & \\ & \pi_{i_2}(\theta) & & \\ & & & \\ & & & \pi_{i_{n/2}}(\theta) \end{pmatrix}$ up to a change of basis, where the non-negative integers $i_1, \ldots, i_{n/2}$ are called the representation **types**.

Ex. 2: The non-trivial real irreducible representations of $\mathrm{SO}(3)$ are more complicated, but there are, up to change of basis, one irreducible representation of $\mathrm{SO}(3)$ for all odd positive integers

Our algorithm

The challenge: Find this decomposition, together with the change of basis A.

The solution: Work at the Lie algebra level to find a basis $\{T_j\}_{j=1}^{\dim G}$ for $\mathrm{d}\rho(\mathfrak{g})$ and decompose each T_j into representation types.

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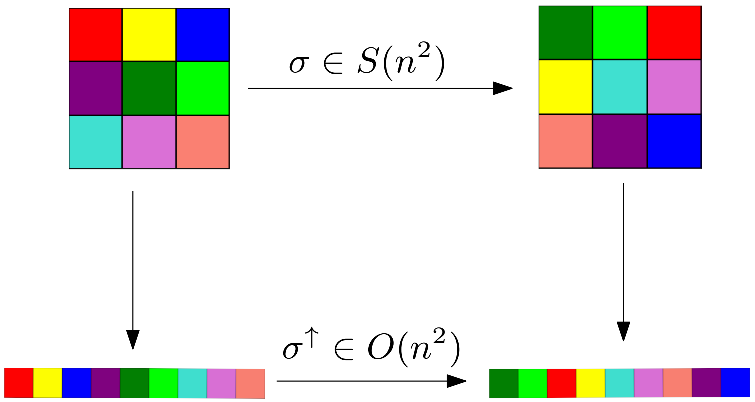
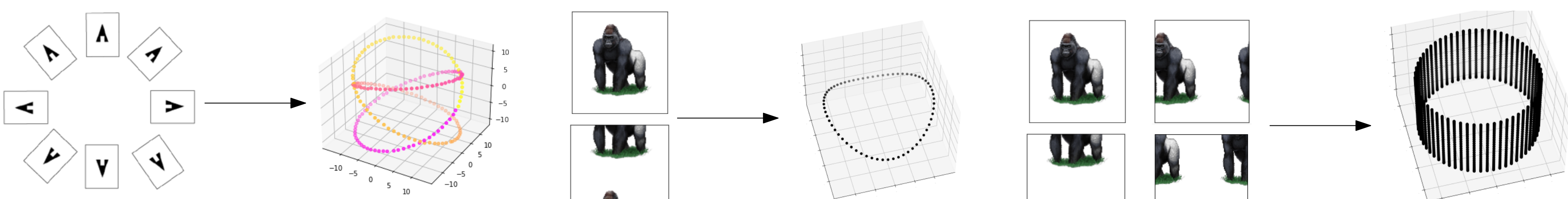
Pixel Permutation Transformations

We can treat permutation of $n \times n$ pixeled images as orthogonal matrices in $\mathbb{R}^{n \times n}$



the embedded images $\{x\} \in \mathbb{R}^{n \times n}$ lie in a **orbit of a $\mathrm{O}(n^2)$ representation**

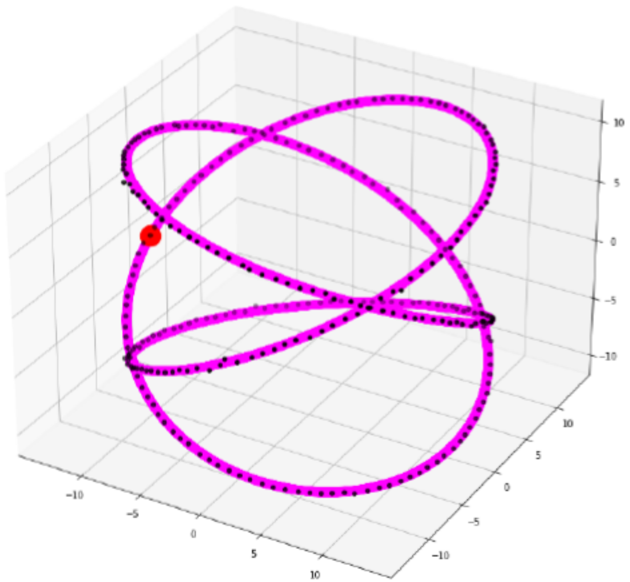
But special set of transformations may be within the **orbit of representations of "smaller" Lie groups**



$SO(2)$ $SO(2)$ $SO(2) \times SO(2) \approx T^2$

Lemma: If a set of $n \times n$ images $\{x_i\}_{i=0}^{N}$ is generated by applications of an Abelian group of rank d to x_0, then their embeddings $\{x_i^{\uparrow}\}_{i=0}^{N}$ lie in an orbit of a $\mathrm{SO}(2)^d \approx T^d$ representation in $\mathbb{R}^{n \times n}$. Moreover, they are still in orbit of a $SO(2)^d \approx T^d$ representation after (smart) applications of PCA.

Application 1: orbit completion



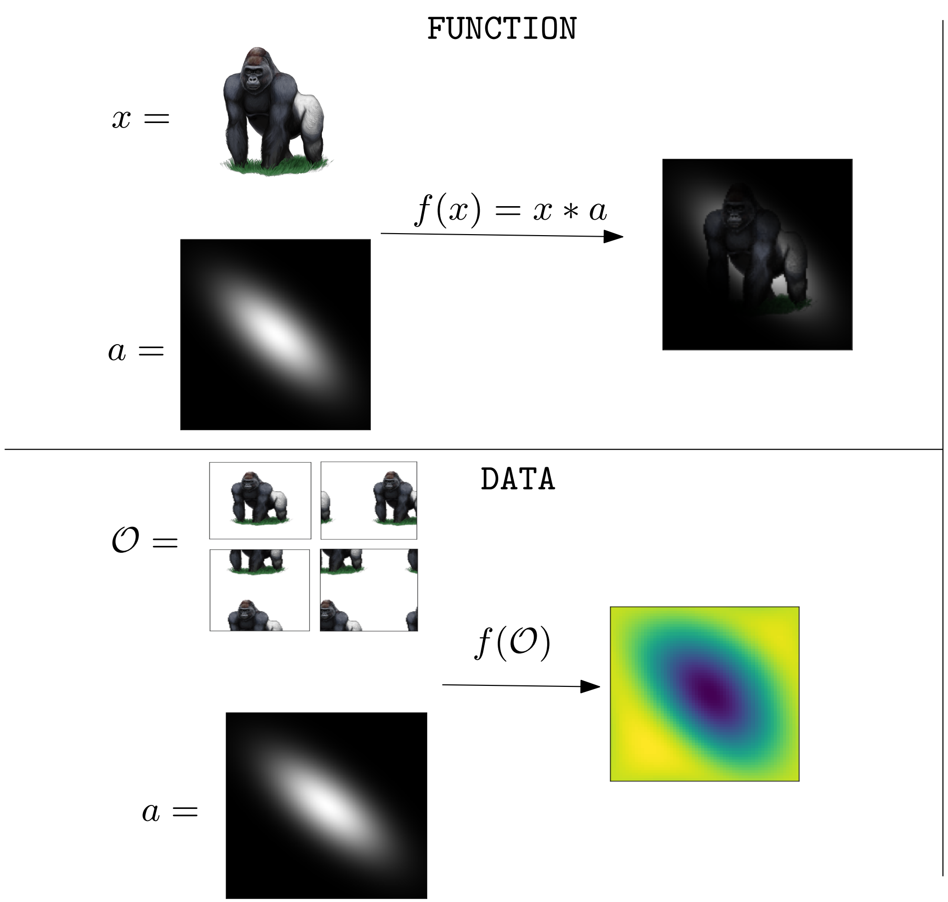
PCA dimension	Upscale of initial image	Hausdorff distance	Upscale of orbit generated
4		0.039	
6		0.029	
8		0.065	
10		0.084	

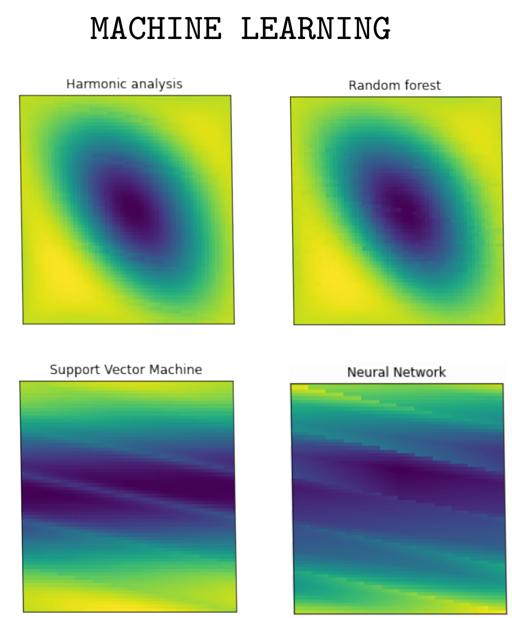
Harmonic analysis

Application 2: harmonic analysis

Theorem: Suppose $\mathcal{O}$ is an orbit of a representation of a Lie group G in $\mathbb{R}^n$. Then there is a known enumerable set of functions $\{\tilde{f}_i : \mathcal{O} \to \mathbb{C}\}_{i=0}^{\infty}$ such that, for any continuous $f : \mathcal{O} \to \mathbb{C}$, there are $\{a_i\}_{i=0}^{\infty} \in \mathbb{C}$ such that $f = \sum_{i=0}^{\infty} a_i \tilde{f}_i$.

Ex.: for $G = (S^1, +)$, this reduces to the ordinary Fourier decomposition





Model	MSE on test data
Harmonic analysis	**0.02057**
Random Forest	0.09336
Support Vector Machine	24.91
Neural Network	25.33

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Overview of the algorithm

Input: A point cloud $X = \{x_1 \dots, x_N\} \subset \mathbb{R}^n$ and a compact Lie group G.

Output: A representation $\widehat{\phi}$ of G in $\mathbb{R}^n$, and an orbit $\widehat{\mathcal{O}}$ close to X.

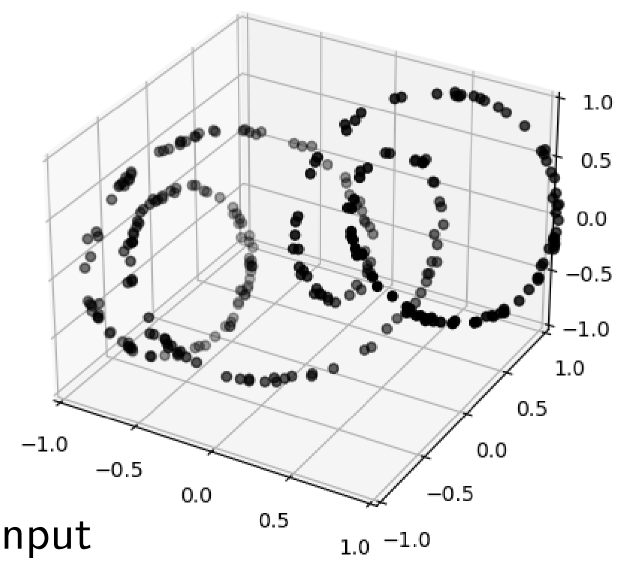
Example: Let $X \subset \mathbb{R}^4$ be a 300-sample of

$$\mathcal{O} = \left\{(\cos t, 2\sin t, \cos 4t, \sin 4t) \mid t \in [0, 2\pi)\right\}.$$

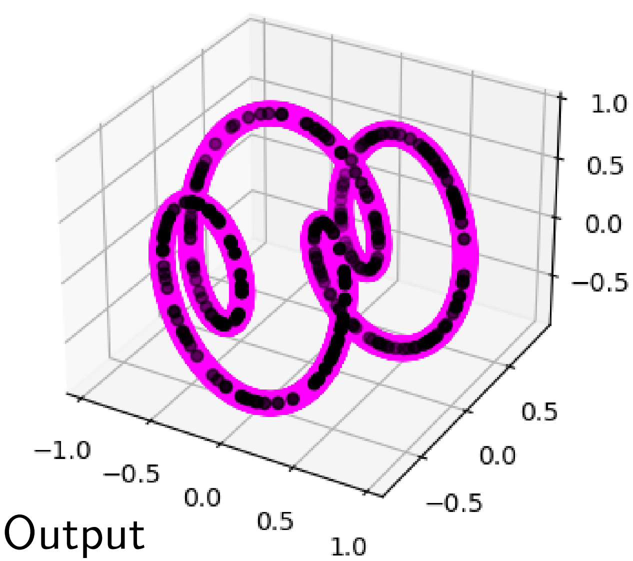
It is an orbit of $\mathrm{SO}(2)$ for the representation $\phi\colon \mathrm{SO}(2) \to \mathrm{M}_4(\mathbb{R})$ defined as

$$t \mapsto \mathrm{diag}\left(\begin{pmatrix} \cos t & -(1/2)\sin t \\ 2\sin t & \cos t \end{pmatrix}, \begin{pmatrix} \cos 4t & -\sin 4t \\ \sin 4t & \cos 4t \end{pmatrix} \right).$$

We expect the algorithm to output a faithful approximation of ϕ and $\mathcal{O}$.



Input



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Example: Let $X \subset \mathbb{R}^4$ be a 300-sample of (with potentially noise and anomalous points)

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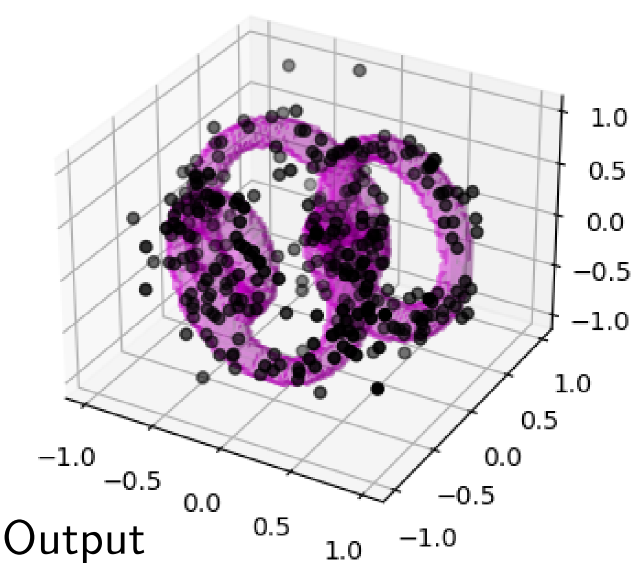

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Main idea: Estimate the pushforward Lie algebra $\mathfrak{h} = \mathrm{d}\phi(\mathfrak{g})$ to deduce $\mathcal{O}$ through

$$\mathcal{O} \;=\; \phi(G)\cdot x \;=\; \exp(\mathfrak{h})\cdot x \;=\; \left\{\exp(A)x \mid A \in \mathfrak{h}\right\},$$

where x is any element of $\mathcal{O}$. The algebra $\mathfrak{h}$ is found as a Lie subalgebra of $\mathfrak{sym}(\mathcal{O})$.

$$\begin{array}{ccccccc}
G & \xrightarrow{\quad\phi\quad} & \phi(G) & \subset & \mathrm{Sym}(\mathcal{O}) & \subset & \mathrm{GL}_n(\mathbb{R}) \\
\uparrow{\scriptstyle\exp} & & \uparrow{\scriptstyle\exp} & & \uparrow{\scriptstyle\exp} & & \uparrow{\scriptstyle\exp} \\
\mathfrak{g} & \xrightarrow{\quad\mathrm{d}\phi\quad} & \mathfrak{h} & \subset & \mathfrak{sym}(\mathcal{O}) & \subset & \mathfrak{gl}_n(\mathbb{R})
\end{array}$$

Symmetry group:
$\mathrm{Sym}(\mathcal{O}) = \{P \in \mathrm{GL}_n(\mathbb{R}) \mid P\mathcal{O} = \mathcal{O}\}$

Symmetry algebra:
$\mathfrak{sym}(\mathcal{O}) = \{P \in \mathfrak{gl}_n(\mathbb{R}) \mid \exp(P) \in \mathrm{Sym}(\mathcal{O})\}$

Step 1: Orthonormalization Apply dimension reduction and orthonormalization.

Step 2: Lie-PCA Diagonalize the Lie-PCA operator $\Lambda\colon \mathrm{M}_n(\mathbb{R}) \to \mathrm{M}_n(\mathbb{R})$.

Step 3: Closest Lie algebra Estimate $\widehat{\mathfrak{h}}$ through an optimization program over $\mathrm{O}(n)$.

Step 4: Generate the orbit Deduce $\widehat{\mathcal{O}}_x = \exp(\widehat{\mathfrak{h}})\cdot x$ and check that it is close to X.

Step 1: Orthonormalization

We wish to normalize the orbit $\mathcal{O}$ so as to make ϕ an orthogonal representation,

i.e., such that ϕ takes values in $\mathrm{O}(n)$,

i.e., such that $\mathcal{O}$ lies in a sphere of a certain radius.

Fact: there exists a positive-definite matrix M such that the conjugated representation $M\phi M^{-1}$ is orthogonal. Orbits are obtained by left translation by M.

We find M as the square root of the Moore-Penrose pseudo-inverse of the **covariance matrix**:

$$M = \sqrt{\Sigma[X]^{+}} \qquad \text{where} \qquad \Sigma[X] = \tfrac{1}{N}\textstyle\sum_{i=1}^{N} x_i x_i^{\top}.$$

Example: With $M = \frac{1}{\sqrt{2}}\mathrm{diag}\big(1, 1/2, 1, 1\big)$,

$$\phi\colon t \mapsto \mathrm{diag}\left(\begin{pmatrix} \cos t & -(1/2)\sin t \\ 2\sin t & \cos t \end{pmatrix}, \begin{pmatrix} \cos 4t & -\sin 4t \\ \sin 4t & \cos 4t \end{pmatrix} \right)$$

$$M\phi M^{-1}\colon t \mapsto \mathrm{diag}\left(\begin{pmatrix} \cos t & \sin t \\ \sin t & \cos t \end{pmatrix}, \begin{pmatrix} \cos 4t & -\sin 4t \\ \sin 4t & \cos 4t \end{pmatrix} \right)$$

$$\mathcal{O} = \big\{ (\cos t, 2\sin t, \cos 4t, \sin 4t) \mid t \in [0, 2\pi) \big\}.$$

$$M\mathcal{O} = \big\{ \tfrac{1}{\sqrt{2}}(\cos t, \sin t, \cos 4t, \sin 4t) \mid t \in [0, 2\pi) \big\}.$$

Step 1: Orthonormalization

Dimension reduction: In addition, we apply Principal Component Analysis to X.
Let ϵ be parameter, and $\Pi_{\Sigma[X]}^{\geq \epsilon}$ be the projection matrix on the subspace of $\mathbb{R}^n$ spanned by the eigenvectors of $\Sigma[X]$ of eigenvalue greater than ϵ. We set $X \leftarrow \Pi_{\Sigma[X]}^{\geq \epsilon} X$.

This has the effect of:

- reducing the computational cost of the next steps,
- avoiding numerical errors, when computing the pseudo-inverse of $\Sigma[X]$,
- ensuring that we will estimate non-trivial representations.

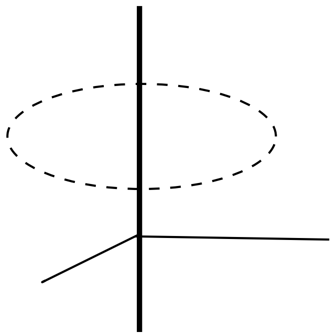
Intrinsic/extrinsic symmetries: For a Riemannian manifold $\mathcal{M}$ isometrically embedded in $\mathbb{R}^n$,

- $\mathrm{Isom}(\mathcal{M})$: the set of diffeomorphisms $\mathcal{M} \to \mathcal{M}$ that preserve the metric,
- $\mathrm{Sym}(\mathcal{M}) = \{P \in \mathrm{GL}_n(\mathbb{R}) \mid P\mathcal{M} = \mathcal{M}\}$.

By restricting the action of the matrices P to $\mathcal{M}$, we obtain a group homomorphism

$$\mathrm{Sym}(\mathcal{M}) \to \mathrm{Isom}(\mathcal{M}).$$

It may not be injective, since certain matrices P may act trivially on $\mathcal{M}$.
This is avoided by projecting $\mathcal{M}$ into the subspace is spans.



Step 2: Lie-PCA

We wish to estimate $\mathfrak{sym}(\mathcal{O}) = \{P \in \mathfrak{gl}_n(\mathbb{R}) \mid \exp(P) \in \mathrm{Sym}(\mathcal{O})\}$.

A solution has been proposed in [Cahill, Mixon, Parshall, **Lie PCA: Density estimation for symmetric manifolds**, Applied and Computational Harmonic Analysis, 2023].

Lie-PCA operator: $\Lambda\colon \mathrm{M}_n(\mathbb{R}) \to \mathrm{M}_n(\mathbb{R})$ is defined as

$$\Lambda(A) = \frac{1}{N} \sum_{1 \leq i \leq N} \widehat{\Pi}\big[\mathrm{N}_{x_i} X\big] \cdot A \cdot \Pi\big[\langle x_i \rangle\big]$$

where
- $\widehat{\Pi}\big[\mathrm{N}_{x_i} X\big]$ estimation of projection matrices on the normal spaces $\mathrm{N}_{x_i}\mathcal{O}$,
- $\Pi\big[\langle x_i \rangle\big]$'s are the projection matrices on the lines $\langle x_i \rangle$.

In practice, we find $\widehat{\Pi}\big[\mathrm{N}_{x_i} X\big]$ via local PCA.

Facts: (1) Λ is symmetric. (2) The kernel of Λ is approximately $\mathfrak{sym}(\mathcal{O})$.

We can find $\mathfrak{sym}(\mathcal{O})$ as the subspace spanned by the bottom eigenvectors of Λ.

Example: Eigenvalues of Λ on the sample X of $\mathcal{O} = \big\{(\cos t, \sin t, \cos 4t, \sin 4t) \mid t \in [0, 2\pi)\big\}$:

$$0.001,\ 0.102,\ 0.109,\ 0.112,\ 0.135,\ 0.145,\ 0.156,\ 0.212,$$
$$0.212,\ 0.233,\ 0.236,\ 0.247,\ 0.249,\ 0.259,\ 0.296,\ 0.296.$$

Step 2: Lie-PCA

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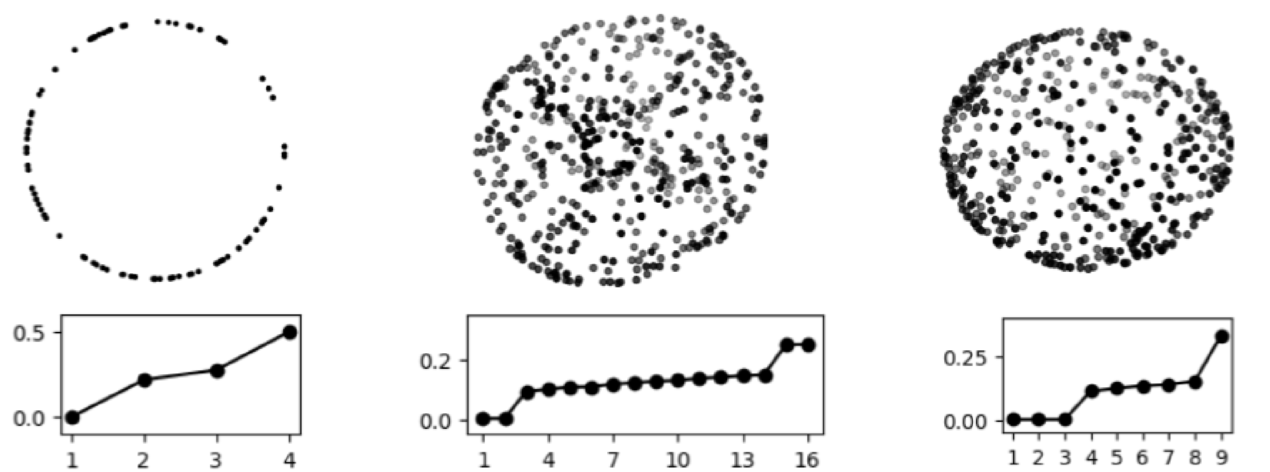
X

Example: eigenvalues of Λ



$\mathrm{Sym}(S^1) = \mathrm{SO}(2)$ $\mathrm{Sym}(T^2) = T^2$ $\mathrm{Sym}(S^2) = \mathrm{SO}(3)$

Step 2: Lie-PCA

Derivation of Lie-PCA: Based on the fact that

$$\mathfrak{sym}(\mathcal{O}) = \left\{A \in \mathrm{M}_n(\mathbb{R}) \mid \forall x \in \mathcal{O}, Ax \in \mathrm{T}_x\mathcal{O}\right\}$$

where $\mathrm{T}_x\mathcal{O}$ denotes the tangent space of $\mathcal{O}$ at x. In other words,

$$\mathfrak{sym}(\mathcal{O}) = \bigcap_{x\in\mathcal{O}} S_x\mathcal{O} \quad \text{where} \quad S_x\mathcal{O} = \{A \in \mathrm{M}_n(\mathbb{R}) \mid Ax \in \mathrm{T}_x\mathcal{O}\},$$

Using only the point cloud $X = \{x_1, \ldots, x_N\}$, we consider

$$\bigcap_{i=1}^{N} S_{x_i}\mathcal{O} = \ker\left(\sum_{i=1}^{N} \Pi\big[(S_{x_i}\mathcal{O})^\perp\big]\right),$$

Besides, the authors show that

$$\Pi\big[(S_{x_i}\mathcal{O})^\perp\big](A) = \Pi\big[\mathrm{N}_{x_i}\mathcal{O}\big] \cdot A \cdot \Pi\big[\langle x_i\rangle\big].$$

One naturally puts

$$\Lambda(A) = \frac{1}{N}\sum_{i=1}^{N} \widehat{\Pi}\big[\mathrm{N}_{x_i}X\big] \cdot A \cdot \Pi\big[\langle x_i\rangle\big]$$

where $\widehat{\Pi}\big[\mathrm{N}_{x_i}X\big]$ is an estimation of $\Pi\big[\mathrm{N}_{x_i}\mathcal{O}\big]$ computed from the observation X.

Step 3: Closest Lie algebra

We will suppose that $\mathrm{Sym}(\mathcal{O}) \simeq G$ (hence $\mathfrak{sym}(\mathcal{O}) = \mathfrak{h}$). General case studied in our paper.

In the original Lie-PCA, the authors propose to estimate $\mathfrak{sym}(\mathcal{O})$ as $\langle A_1, \dots, A_d \rangle$, the linear subspace of $\mathrm{M}_n(\mathbb{R})$ spanned by the $d = \dim G$ bottom eigenvectors of Λ.
But:

(1) $\langle A_1, \dots, A_d \rangle$ may not be closed under Lie bracket $[A, B] = AB - BA$.

(2) $\langle A_1, \dots, A_d \rangle$ may not be a Lie algebra derived from G:

$$A_1 = \begin{pmatrix} 0 & -2.3 & 0 & 0 \\ 2.3 & 0 & 0 & 0 \\ 0 & 0 & 0 & -5.5 \\ 0 & 0 & 5.5 & 0 \end{pmatrix} \overset{?}{\approx} \begin{pmatrix} 0 & -2 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -5 \\ 0 & 0 & 5 & 0 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -3 \\ 0 & 0 & 3 & 0 \end{pmatrix}$$

Solution: Project $\langle A_1, \dots, A_d \rangle$ to the closest Lie algebra derived from G

$$\arg\min \left\| \Pi\left[\langle A_i \rangle_{i=1}^d\right] - \Pi\left[\widehat{\mathfrak{h}}\right] \right\| \quad \text{s.t.} \quad \widehat{\mathfrak{h}} \in \mathcal{G}(G, \mathfrak{so}(n)),$$

where
- $\Pi\left[\langle A_i \rangle_{i=1}^d\right]$ and $\Pi\left[\widehat{\mathfrak{h}}\right]$ are projection matrices, seen as operators on $\mathrm{M}_n(\mathbb{R})$,
- $\left\| \Pi\left[\langle A_i \rangle_{i=1}^d\right] - \Pi\left[\widehat{\mathfrak{h}}\right] \right\|$ is the distance on the Grassmannian of d-planes in $\mathrm{M}_n(\mathbb{R})$,
- $\mathcal{G}(G, \mathfrak{so}(n))$, the set of Lie subalgebras of $\mathfrak{so}(n)$ coming from an almost-faithful representation of G in $\mathbb{R}^n$

Step 3: Closest Lie algebra

Reformulation: The minimization program

$$\arg\min \left\| \Pi\left[\langle A_i\rangle_{i=1}^d\right] - \Pi\left[\widehat{\mathfrak{h}}\right] \right\| \quad \text{s.t.} \quad \widehat{\mathfrak{h}} \in \mathcal{G}(G, \mathfrak{so}(n)),$$

is equivalent to

$$\arg\min \left\| \Pi\left[\langle A_i\rangle_{i=1}^d\right] - \Pi\left[\langle O \mathrm{diag}(B_i^k)_{k=1}^p O^\top\rangle_{i=1}^d\right] \right\| \quad \text{s.t.} \quad \begin{cases} (B^1, \dots, B^p) \in \mathfrak{orb}(G, n), \\ O \in \mathrm{O}(n). \end{cases}$$

where $\mathfrak{orb}(G,n)$ is a choice of representatives in the moduli space of orbit-equivalence of almost-faithful representation of G in $\mathbb{R}^n$.

This program splits into $|\mathfrak{orb}(G,n)|$ minimization problems over $\mathrm{O}(n)$.

In practice, we perform the minimizations via by gradient descent (package `Pymanopt`).

Example: We still consider $\mathcal{O} = \left\{(\cos t, \sin t, \cos 4t, \sin 4t) \mid t \in [0, 2\pi)\right\}$. The representations of $\mathrm{SO}(2)$ on $\mathbb{R}^4$ take the form

$$\phi_u \oplus \phi_v(t) = \mathrm{diag}\left(\begin{pmatrix} \cos ut & -\sin ut \\ \sin ut & \cos ut \end{pmatrix}, \begin{pmatrix} \cos vt & -\sin vt \\ \sin vt & \cos vt \end{pmatrix} \right).$$

Result of minimization:

Weights	$(0,1)$	$(1,2)$	$(1,3)$	$(1,4)$	$(2,3)$	$(3,4)$
Costs	0.004	0.002	0.002	$\mathbf{4.29 \times 10^{-5}}$	0.006	0.008

Step 3: Closest Lie algebra

Reformulation: The minimization program

$$\arg\min \left\| \Pi\left[\langle A_i\rangle_{i=1}^d\right] - \Pi\left[\widehat{\mathfrak{h}}\right] \right\| \quad \text{s.t.} \quad \widehat{\mathfrak{h}} \in \mathcal{G}(G, \mathfrak{so}(n)),$$

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We only implemented the algorithm for $G = \mathrm{SO}(2)$, T^d, $\mathrm{SO}(3)$ and $\mathrm{SU}(2)$.

Step 4: Generate the orbit

We have calculated a representation $\widehat{\phi}\colon G \to \mathrm{SO}(n)$ and pushforward Lie algebra $\widehat{\mathfrak{h}}$.
We now exponentiate it: let $x \in X$ arbitrary and

$$\widehat{\mathcal{O}}_x = \exp\left(\widehat{\mathfrak{h}}\right) \cdot x = \left\{ \exp(A)x \mid A \in \widehat{h} \right\}.$$

In practice, it is enough to compute

$$\widehat{\mathcal{O}}_x = \left\{ \exp(A)x \mid A \in \mathfrak{h}, \|A\| \leq \delta \times \mathrm{diam}(G) \right\}$$

where $\mathrm{diam}(G)$ is the diameter of G (endowed with a bi-invariant Riemannian structure) and δ is a Lispchitz constant for $\widehat{\phi}$.

Hausdorff distance: As a sanity check, we compute the one-sided Hausdorff distance

$$\mathrm{d_H}\left(X | \widehat{\mathcal{O}}_x\right).$$

Wasserstein distance: Hausdorff distance is not suited when X has anomalous points. In this case, we consider

$$\mu_{\widehat{\mathcal{O}}} = \frac{1}{N}\sum_{i=1}^{N} \mu_{\widehat{\mathcal{O}}_{x_i}}$$

with $\mu_{\widehat{\mathcal{O}}_{x_i}}$ uniform measure on $\widehat{\mathcal{O}}_{x_i}$ (pushforward of Haar measure on G)

and compute the Wasserstein distance $\mathrm{W}_2\left(\mu_X, \mu_{\widehat{\mathcal{O}}}\right)$.

Toy examples

Rep of $\mathrm{SO}(2)$ with noise: Let X be a 300-sample of

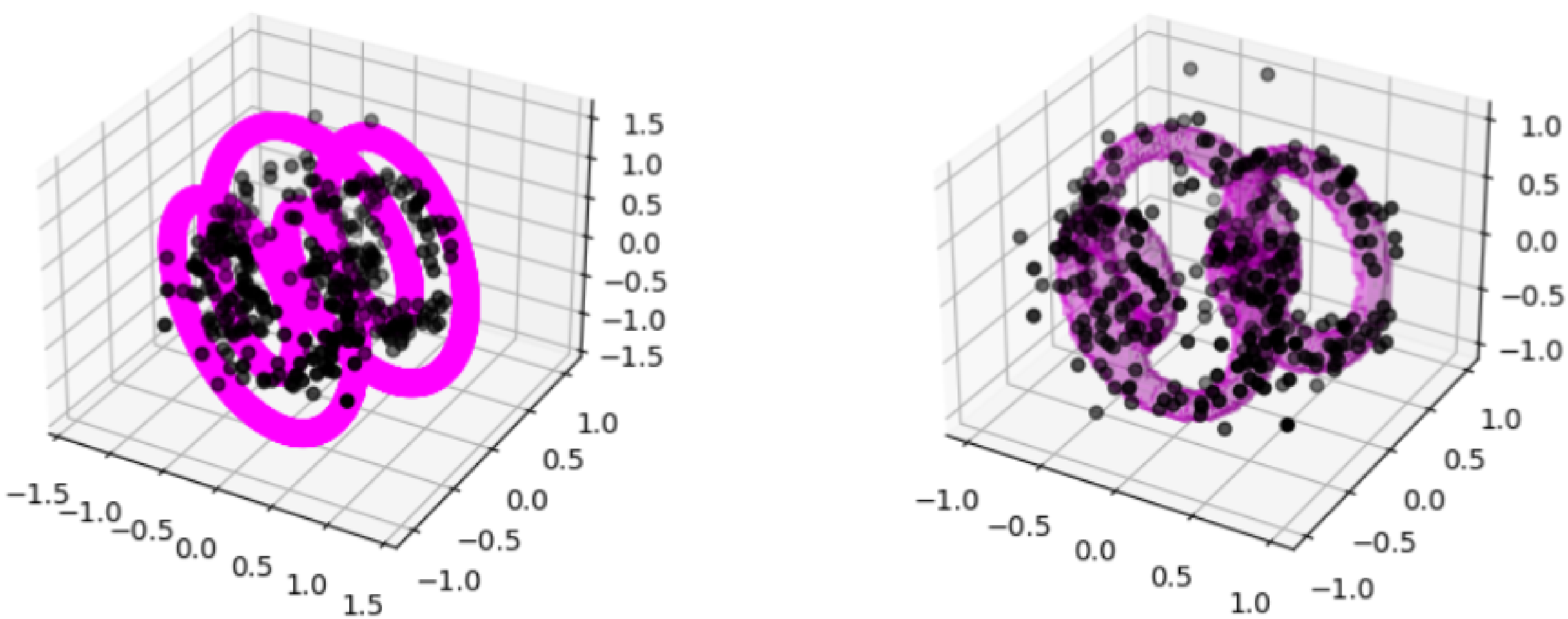
$$\mathcal{O} = \left\{(\cos t, 2\sin t, \cos 4t, \sin 4t) \mid t \in [0, 2\pi)\right\}$$

to which we add an additive Gaussian noise ($\sigma = 0.03$) and 30 points uniformly in $[-1,1]^4$.

The algorithm, with $G = \mathrm{SO}(2)$, retrieves successfully the representation $\phi_1 \oplus \phi_4$.

However, with an arbitrary $x \in X$, we obtain the Hausdorff distance $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}_x\big) \approx 1.128$.

On the other hand, the Wasserstein distance is $\mathrm{W}_2\big(\mu_X, \mu_{\widehat{\mathcal{O}}}\big) \approx 0.392$.



To visualize $\mu_{\widehat{\mathcal{O}}}$, we consider a Gaussian kernel density estimator $f\colon \mathbb{R}^4 \to [0, +\infty)$ (bandwidth 0.1) and represent the sublevel set $f^{-1}([0.5, +\infty))$.

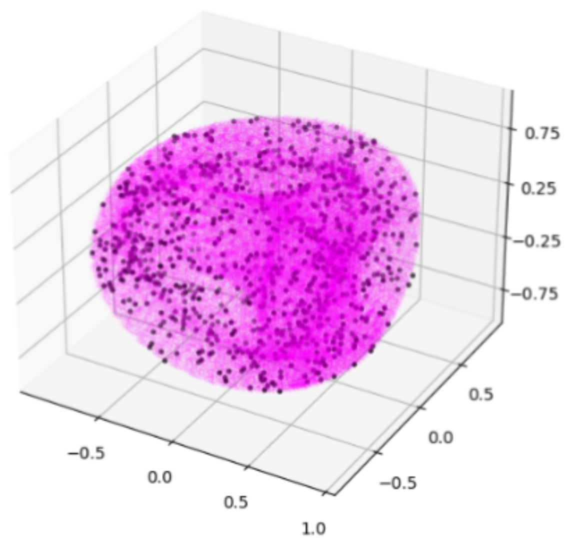
Toy examples

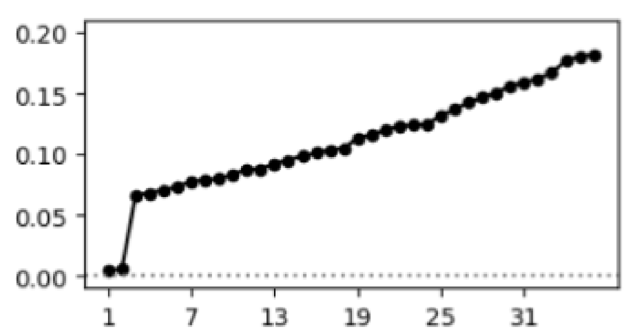
Rep of T^2 in $\mathbb{R}^6$: Let X be a uniform 750-sample of an orbit of the representation $\phi_{(1,1)} \oplus \phi_{(1,2)} \oplus \phi_{(2,1)}$ of the torus T^2 in $\mathbb{R}^6$.

We apply the algorithm with $G = T^2$ on X, and restrict the representations to those with weights at most 2.

The algorithm's output is $\begin{pmatrix} 0 & 1 & 1 \\ 2 & -2 & 1 \end{pmatrix}$, that is, the representation $\phi_{(0,2)} \oplus \phi_{(1,-2)} \oplus \phi_{(1,1)}$.
Moreover, $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}_x\big) \approx 0.071$.

Type	$\begin{pmatrix} 0 & 1 & 1 \\ 2 & -2 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 2 \\ -2 & 2 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 2 \\ 2 & -2 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & -2 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & -2 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 2 \\ 2 & -2 & 1 \end{pmatrix}$
Costs	$\mathbf{0.036}$	0.136	0.198	0.233	0.244	0.312
Type	$\begin{pmatrix} 0 & 1 & 2 \\ 1 & -2 & -2 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 2 \\ 1 & -2 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 2 & 2 \\ -2 & -2 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 1 \\ -2 & -1 & 2 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 2 \\ 1 & -2 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & -2 & 1 \end{pmatrix}$
Costs	0.331	0.348	0.388	0.447	0.457	0.472





Eigenvalues of Lie-PCA operator

Toy examples

The irreps of $\mathrm{SU}(2)$ and $\mathrm{SO}(3)$ in $\mathbb{R}^n$ are parametrized by the partitions of n.

Orthogonal group in $\mathbb{R}^9$: Let X be a 3000-sample of the 3×3 special orthogonal matrices.

Fact: $\mathrm{SO}(3)$ acts transitively on itself.

The algorithm yields:

Representation	$(3,5)$	$(3,3,3)$	$(4,5)$	(8)	(5)	(7)
Cost	$\mathbf{2 \times 10^{-5}}$	$\mathbf{4 \times 10^{-5}}$	0.001	0.001	0.03	0.004
Representation	(9)	$(3,3)$	$(3,4)$	$(4,4)$	(3)	(4)
Cost	0.004	0.006	0.007	0.009	0.011	0.013

Representation $(3,5)$: we get $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}_x\big) \approx 2.658$.
In comparison, $\mathrm{d_H}\big(\widehat{\mathcal{O}}_x|X\big) \approx 0.543$.
This indicates that the representation is not transitive on X.

Representation $(3,3,3)$: $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}_x\big) \approx 0.061$.

Toy examples

The irreps of $\mathrm{SU}(2)$ and $\mathrm{SO}(3)$ in $\mathbb{R}^n$ are parametrized by the partitions of n.

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This indicates that the representation is not transitive on X.

action $\mathrm{SO}(3) \to \mathrm{SO}(3)$ by conjugation (not transitive)

Representation $(3,3,3)$: $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}_x\big) \approx 0.061$.

action $\mathrm{SO}(3) \to \mathrm{SO}(3)$ by translation (transitive)

This is a case where $\dim G < \dim \mathrm{Sym}(\mathcal{O})$.

1. Lie theory
2. Applications of the algorithm
3. Description of the algorithm
4. Proof of robustness
5. Conclusion

Measure-theoretic point of view

Input: $X = \{x_1 \dots, x_N\} \subset \mathbb{R}^n$ and G compact Lie group

Model: X sampled close to an orbit $\mathcal{O}$ of a representation $\phi \colon G \to \mathbb{R}^n$

Step 1: **Orthonormalization** via $X \leftarrow \sqrt{\Sigma[X]^+} \cdot \Pi_{\Sigma[X]}^{\geq \epsilon} \cdot X$.

with $\Sigma[X]$ covariance matrix, and $\Pi_{\Sigma[X]}^{\geq \epsilon}$ projection on eigenvectors $> \epsilon$.

Step 2: **Diagonalize** the operator $\Lambda \colon A \mapsto \frac{1}{N} \sum_{i=1}^{N} \widehat{\Pi}\left[\mathrm{N}_{x_i} X\right] \cdot A \cdot \Pi\left[\langle x_i \rangle\right]$

where $A \in \mathrm{M}_n(\mathbb{R})$, and $\widehat{\Pi}\left[\mathrm{N}_{x_i} X\right]$ estimation of projection on normal space of X.

Step 3: **Solve** $\arg\min_{\widehat{h}} \left\| \Pi\left[\langle A_i \rangle_{i=1}^{d}\right] - \Pi\left[\widehat{\mathfrak{h}}\right] \right\|$ with $(A_i)_{i=1}^{d}$ bottom eigenvectors of Λ

where $\widehat{h} \in \mathcal{G}(\mathfrak{g}, \mathfrak{so}(n))$ Grassmann variety of Lie subalgebras pushforward of G.

Step 4: **Output** $\widehat{\mathcal{O}}_x = \left\{ \exp(A)x \mid A \in \widehat{h} \right\}$

where $x \in X$ is an arbitrary point.

Goal: Show that $\widehat{\mathcal{O}}_x$ is close to $\mathcal{O}$

Measure-theoretic point of view

Input: $X = \{x_1 \ldots, x_N\} \subset \mathbb{R}^n$ and G compact Lie group

μ measure on $\mathbb{R}^n$. E.g., μ_X empirical measure on X

Model: X sampled close to an orbit $\mathcal{O}$ of a representation $\phi\colon G \to \mathbb{R}^n$

$\mu_{\mathcal{O}}$ uniform measure on $\mathcal{O}$

Step 1: **Orthonormalization** via $X \leftarrow \sqrt{\Sigma[X]^+} \cdot \Pi^{\geq \epsilon}_{\Sigma[X]} \cdot X$.

$$\mu \leftarrow \sqrt{\Sigma[\mu]^+} \cdot \Pi^{\geq \epsilon}_{\Sigma[\mu]} \cdot \mu.$$

Step 2: **Diagonalize** the operator $\Lambda\colon A \mapsto \frac{1}{N} \sum_{i=1}^N \widehat{\Pi}\big[\mathrm{N}_{x_i} X\big] \cdot A \cdot \Pi\big[\langle x_i \rangle\big]$

$$\Lambda[\mu]\colon A \mapsto \int_{i=1}^N \widehat{\Pi}\big[\mathrm{N}_{x_i} X\big] \cdot A \cdot \Pi\big[\langle x_i \rangle\big] \mathrm{d}\mu$$

Step 3: **Solve** $\arg\min_{\widehat{h}} \big\|\Pi\big[\langle A_i \rangle_{i=1}^d\big] - \Pi\big[\widehat{\mathfrak{h}}\big]\big\|$ with $(A_i)_{i=1}^d$ bottom eigenvectors of Λ

$\arg\min_{\widehat{h}} \big\|\Pi\big[\langle A_i \rangle_{i=1}^d\big] - \Pi\big[\widehat{\mathfrak{h}}\big]\big\|$ with $(A_i)_{i=1}^d$ bottom eigenvectors of $\Lambda[\mu]$

Step 4: **Output** $\widehat{\mathcal{O}}_x = \big\{ \exp(A)x \mid A \in \widehat{h} \big\}$

$$\mu_{\widehat{\mathcal{O}}_x} = \exp(\widehat{\mathfrak{h}}) \cdot \mu$$

Goal: Show that $\widehat{\mathcal{O}}_x$ is close to $\mathcal{O}$

Show that $\mathrm{W}_2\big(\mu_{\widehat{\mathcal{O}}_x}, \mu_{\mathcal{O}}\big)$ "$\leq$" $\mathrm{W}_2(\mu, \mu_{\mathcal{O}})$

Measure-theoretic point of view

Why working with Wasserstein and not Hausdorff?

- Natural formalism for Lie groups (averaging with the Haar measure)
- Allows noise and anomalous points
- Local PCA is not stable in Hausdorff

Remark: We aim for an explicit bound $\mathrm{W}_2(\mu_{\widehat{\mathcal{O}}_x}, \mu_{\mathcal{O}})$ " $\leq$ " $\mathrm{W}_2(\mu, \mu_{\mathcal{O}})$. This is different from other statistical formalisms. In particular, no law of large numbers / concentration.

Robustness

Theorem: Let G be a compact Lie group of dimension d, $\mathcal{O}$ an orbit of an almost-faithful representation $\phi\colon G \to \mathbb{R}^n$, potentially non-orthogonal, and l its dimension. Let $\mu_{\mathcal{O}}$ be the uniform measure on $\mathcal{O}$, and $\mu_{\widetilde{\mathcal{O}}}$ that on the orthonormalized orbit.

Besides, let $X \subset \mathbb{R}^n$ be a finite point cloud and μ_X its empirical measure. Let $\widehat{\phi}$, $\widehat{\mathfrak{h}}$ and $\mu_{\widehat{\mathcal{O}}}$ be the output of the algorithm. Under technical assumptions, it holds that $\widehat{\phi}$ is equivalent to ϕ, and

$$\|\Pi\big[\widehat{h}\big] - \Pi\big[\mathfrak{sym}(\mathcal{O})\big]\|_{\mathrm{F}} \leq 9d\frac{\rho}{\lambda}\left(r + 4\left(\frac{\widetilde{\omega}}{r^{l+1}}\right)^{1/2}\right)$$

$$\mathrm{W}_2\big(\mu_{\widehat{\mathcal{O}}}, \mu_{\widetilde{\mathcal{O}}}\big) \leq \frac{1}{\sqrt{2}}\frac{\mathrm{W}_2(\mu_X, \mu_{\mathcal{O}})}{\sigma_{\min}} + 3\sqrt{dn}\left(\frac{\rho}{\lambda}\right)^{1/2}\left(r + 4\left(\frac{\widetilde{\omega}}{r^{l+1}}\right)^{1/2}\right)^{1/2}$$

where

- $\rho = \left(16l(l+2)6^l\right)^{\frac{\max(\mathrm{vol}(\widetilde{\mathcal{O}}),\mathrm{vol}(\widetilde{\mathcal{O}})^{-1})}{\min(1,\mathrm{reach}(\widetilde{\mathcal{O}}))}}$
- $\sigma_{\max}^2$, $\sigma_{\min}^2$ the top and bottom nonzero eigenvalues of the covariance matrix $\Sigma[\mu_{\mathcal{O}}]$
- $\widetilde{\omega} = 4(n+1)^{3/2}\left(\frac{\sigma_{\max}^3}{\sigma_{\min}^3}\right)\left(\omega(\upsilon + \omega)\right)^{1/2}$ with $\omega = \frac{\mathrm{W}_2(\mu_{\mathcal{O}}, \mu_X)}{\sigma_{\min}}$ and $\upsilon = \left(\frac{\mathbb{V}\big[\|\mu_{\mathcal{O}}\|\big]}{\sigma_{\min}^2}\right)^{1/2}$
- r is the radius of local PCA (estimation of tangent spaces)
- λ the bottom nonzero eigenvalue of the ideal Lie-PCA operator $\Lambda_{\mathcal{O}}$

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bias-variance trade-off when estimating tangent spaces

$$\lesssim \left(r + \left(\frac{\mathrm{W}_2(\mu_X, \mu_{\mathcal{O}})^{1/2}}{r^{l+1}}\right)^{1/2}\right)^{1/2}$$

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- $\rho = \left(16l(l+2)6^l\right)\frac{\max(\mathrm{vol}(\widetilde{\mathcal{O}}), \mathrm{vol}(\widetilde{\mathcal{O}})^{-1})}{\min(1, \mathrm{reach}(\widetilde{\mathcal{O}}))}$
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- r is the radius of local PCA (estimation of tangent spaces)
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Robustness

Technical assumptions: Define the quantities

$$\omega = \frac{\mathrm{W}_2(\mu_{\mathcal{O}}, \mu_X)}{\sigma_{\min}}, \qquad \upsilon = \left(\frac{\mathbb{V}\left[\|\mu_{\mathcal{O}}\|\right]}{\sigma_{\min}^2}\right)^{1/2},$$

$$\widetilde{\omega} = 4(n+1)^{3/2}\left(\frac{\sigma_{\max}^3}{\sigma_{\min}^3}\right)\left(\omega(\upsilon+\omega)\right)^{1/2}, \qquad \rho = \left(16l(l+2)6^l\right)\frac{\max(\mathrm{vol}(\widetilde{\mathcal{O}}), \mathrm{vol}(\widetilde{\mathcal{O}})^{-1})}{\min(1, \mathrm{reach}(\widetilde{\mathcal{O}}))},$$

$$\gamma = \left(4(2d+1)\sqrt{2}\right)^{-1} \cdot \lambda \cdot \Gamma(G, n, \omega_{\max}) \quad \text{(rigidity constant of Lie subalgebras)}$$

Suppose that ω is small enough, so as to satisfy

$$\omega < \left(\left(\upsilon^2 + \frac{1}{2}\right)^{1/2} - \upsilon\right) \Big/ \left(3(n+1)\frac{\sigma_{\max}^2}{\sigma_{\min}^2}\right), \qquad \widetilde{\omega} \leq \min\left\{\left(\frac{1}{6\rho}\right)^{3(l+1)}, \frac{\gamma^{l+3}}{16}, \left(\frac{\gamma}{(6\rho)^2}\right)^{l+1}\right\}.$$

Choose two parameters ϵ and r in the following nonempty sets:

$$\epsilon \in \left((2\upsilon+\omega)\omega\sigma_{\min}^2,\ \frac{1}{2}\sigma_{\min}^2\right], \qquad r \in \left[(6\rho)^2 \cdot \widetilde{\omega}^{1/(l+1)},\ (6\rho)^{-1}\right] \cap \left[(4/\gamma)^{2/(l+1)} \cdot \widetilde{\omega}^{1/(l+1)},\ \gamma\right].$$

Moreover, we suppose that

- the minimization problems are computed exactly,
- $\mathfrak{sym}(\mathcal{O})$ is spanned by matrices whose spectra come from primitive integral vectors of coordinates at most $\omega_{\max}$,
- $G = \mathrm{Sym}(\mathcal{O})$.

Orthonormalization

Ideal covariance matrix: Suppose that $\mathcal{O}$ is an orbit of the representation $\phi\colon G \to \mathrm{M}_n(\mathbb{R})$, and $\mu_{\mathcal{O}}$ the uniform measure on it. With $x_0 \in \mathcal{O}$ an arbitrary point, the covariance matrix can be written

$$\Sigma[\mu_{\mathcal{O}}] = \int \big(\phi(g)x_0\big) \cdot \big(\phi(g)x_0\big)^\top \mathrm{d}\mu_G(g).$$

Now, let $\mathbb{R}^n = \bigoplus_{i=1}^m V_i$ be the decomposition of ϕ into irreps, and denote as $(\Pi\big[V_i\big])_{i=1}^m$ the projection matrices on these subspaces. We can decompose

$$\Sigma[\mu_{\mathcal{O}}] = \sum_{i=1}^m C_i \quad \text{where} \quad C_i = \int \phi_i(g)\Big(\Pi\big[V_i\big](x_0) \cdot \Pi\big[V_i\big](x_0)^\top\Big)\phi_i(g)^\top \mathrm{d}\mu_G(g).$$

If ϕ is orthogonal, then by Schur's lemma, the C_i are homotheties:

$$\Sigma[\mu_{\mathcal{O}}] = \sum_{i=1}^m \sigma_i^2 \Pi\big[V_i\big] \qquad \text{where} \qquad \sigma_i^2 = \frac{\big\|\Pi\big[V_i\big](x_0)\big\|^2}{\dim(V_i)}.$$

This shows that, in general, important quantities are:

- The variance $\mathbb{V}[\|\mu_{\mathcal{O}}\|]$, a measure of *deviation from orthogonality* of $\mathcal{O}$
- The ratio $\sigma_{\max}^2/\sigma_{\min}^2$, a measure of *homogeneity* of $\mathcal{O}$.

Orthonormalization

Proposition: Let $\mathcal{O} \subset \mathbb{R}^n$ be the orbit of a representation, potentially non-orthogonal, $\mu_{\mathcal{O}}$ its uniform measure, $\Pi\big[\langle\mathcal{O}\rangle\big]$ the projection on its span, and $\sigma^2_{\max}, \sigma^2_{\min}$ the top and bottom nonzero eigenvalues of $\Sigma[\mu_{\mathcal{O}}]$.

Besides, let ν be a measure, $\Sigma[\nu]$ its covariance matrix, $\epsilon > 0$ and $\Pi^{\geq\epsilon}_{\Sigma[\nu]}$ the projection on the subspace spanned by eigenvectors with eigenvalue at least ϵ.

If $\mathrm{W}_2(\mu_{\mathcal{O}}, \nu)$ is small enough, then we have the following bound between the pushforward measures after Step 1:

$$\mathrm{W}_2\left(\sqrt{\Sigma[\mu_{\mathcal{O}}]^+}\Pi\big[\langle\mathcal{O}\rangle\big]\mu_{\mathcal{O}},\ \sqrt{\Sigma[\nu]^+}\Pi^{\geq\epsilon}_{\Sigma[\nu]}\nu\right)$$
$$\leq 8(n+1)^{3/2}\left(\frac{\sigma^3_{\max}}{\sigma^3_{\min}}\right)\left(\frac{\mathrm{W}_2(\mu_{\mathcal{O}},\nu)}{\sigma_{\min}}\right)^{1/2}\left(\left(\frac{\mathbb{V}\big[\|\mu_{\mathcal{O}}\|\big]}{\sigma^2_{\min}}\right)^{1/2}+\frac{\mathrm{W}_2(\mu_{\mathcal{O}},\nu)}{\sigma_{\min}}\right)^{1/2}.$$

Proof: Consequence of Davis-Kahan theorem, together with

$$\left\|\Sigma[\mu_{\mathcal{O}}]^{-1/2}-\Sigma[\nu]^{-1/2}\right\|_{\mathrm{op}} \leq \frac{\sqrt{2}}{\sigma^2_{\min}}\cdot\left(2\mathbb{V}\big[\|\mu_{\mathcal{O}}\|\big]^{1/2}+\mathrm{W}_2(\mu_{\mathcal{O}},\nu)\right)^{1/2}\cdot\mathrm{W}_2(\mu_{\mathcal{O}},\nu)^{1/2}.$$

Lie-PCA

Ideal Lie-PCA: Suppose that $\mathcal{O}$ is an orbit of the representation $\phi\colon G \to \mathrm{M}_n(\mathbb{R})$, and $\mu_{\mathcal{O}}$ the uniform measure on it. We define

$$\Lambda_{\mathcal{O}}(A) = \int \Pi\big[\mathrm{N}_x\mathcal{O}\big] \cdot A \cdot \Pi\big[\langle x \rangle\big] \mathrm{d}\mu_{\mathcal{O}}(x).$$

Proposition: Its kernel is eual to $\mathfrak{sym}(\mathcal{O})$. Moreover, when $\mathcal{O} = S^{n-1}$, its nonzero eigenvalues are exactly δ_n and δ_n' where

$$\delta_n = \frac{2(n-1)}{n(n(n+1)-2)} \qquad \text{and} \qquad \delta_n' = \frac{1}{n}.$$

Proof: Show that $\Lambda_{\mathcal{O}}$ is equivariant with respect to the action of G by conjugation:

$$\phi(g)\Lambda(A)\phi(g)^{-1} = \Lambda\Big(\phi(g)A\phi(g)^{-1}\Big)$$

Then use Schur's lemma.

Empirical observation: More generally, the nonzero eigenvalues of $\Lambda_{\mathcal{O}}$ belong to $[1/n^2, 1/n]$ when $\mathcal{O}$ is *homogenous*, i.e., $\sigma^2_{\max}/\sigma^2_{\min} = 1$.

Lie-PCA

Stability: Comparing

$$\Lambda(A) = \sum_{1\leq i\leq N} \widehat{\Pi}\big[\mathrm{N}_{x_i} X\big] \cdot A \cdot \Pi\big[\langle x_i\rangle\big] \qquad \text{and} \qquad \Lambda_{\mathcal{O}}(A) = \int \Pi\big[\mathrm{N}_x \mathcal{O}\big] \cdot A \cdot \Pi\big[\langle x\rangle\big] \mathrm{d}\mu_{\mathcal{O}}(x).$$

amounts to quantifying the quality of normal space estimation. We use local PCA:

$$\widehat{\Pi}\big[\mathrm{N}_{x_i} X\big] = I - \Pi_{x_i}^{l,r}[X],$$

where $\Pi_{x_i}^{l,r}[X]$ is the projection matrix on any l top eigenvectors of the *local covariance matrix* $\Sigma_{x_i}^r[X]$ centered at x_i and at scale r, itself defined as

$$\Sigma_{x_i}^r[X] = \frac{1}{|Y|} \sum_{y\in Y} (y - x_i)(y - x_i)^\top,$$

where $Y = \{y \in X \mid \|y - x_i\| \leq r\}$, the set input points at distance at most r from x_i.

Measure-theoretic formulation: If μ is a measure on $\mathbb{R}^n$, we define its *local covariance matrix* centered at x at scale r as

$$\Sigma_x^r[\mu] = \int_{\mathcal{B}(x,r)} (y - x)(y - x)^\top \frac{d\mu(x)}{\mu(\mathcal{B}(x,r))}.$$

Lie-PCA

Bias-variance tradeoff: Let $\mu_{\mathcal{M}}$ be measure on a submanifold $\mathcal{M} \subset \mathbb{R}^n$ of dimension l, $x \in \mathcal{M}$, ν a measure on $\mathbb{R}^n$ and $y \in \operatorname{supp}(\nu)$. We decompose

$$\left\| \frac{1}{l+2} \Pi\big[\mathrm{T}_x \mathcal{M}\big] - \frac{1}{r^2} \Sigma_y^r[\nu] \right\|_{\mathrm{F}} \leq$$

$$\underbrace{\left\| \frac{1}{l+2} \Pi\big[\mathrm{T}_x \mathcal{M}\big] - \frac{1}{r^2} \Sigma_x^r[\mu_{\mathcal{M}}] \right\|_{\mathrm{F}}}_{\text{consistency}} + \underbrace{\left\| \frac{1}{r^2} \Sigma_x^r[\mu_{\mathcal{M}}] - \frac{1}{r^2} \Sigma_y^r[\mu_{\mathcal{M}}] \right\|_{\mathrm{F}}}_{\text{spatial stability}} + \underbrace{\left\| \frac{1}{r^2} \Sigma_y^r[\mu_{\mathcal{M}}] - \frac{1}{r^2} \Sigma_y^r[\nu] \right\|_{\mathrm{F}}}_{\text{measure stability}}$$

Lemma: If the parameters are chosen correctly, this is

$$\lesssim r + \|x - y\| + \left(\frac{\mathrm{W}_2(\mu, \nu)}{r^{l+1}} \right)^{\frac{1}{2}}.$$

Corollary: We deduce a bound between Lie-PCA operators:

$$\|\Lambda_{\mathcal{O}} - \Lambda\|_{\mathrm{op}} \leq \sqrt{2}\rho \left(r + 4 \left(\frac{\mathrm{W}_2(\mu_{\mathcal{O}}, \mu_X)}{r^{l+1}} \right)^{1/2} \right).$$

Rigidity of Lie subalgebras

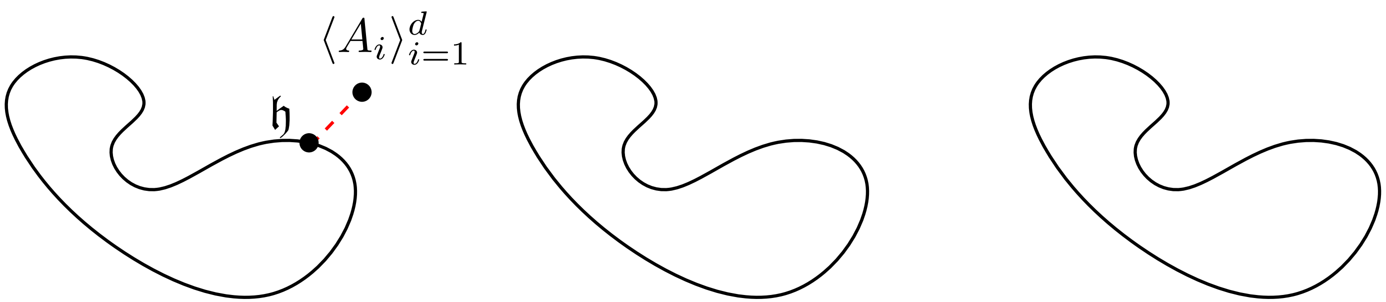
In Step 3, we consider the bottom eigenvectors $A_1, \ldots, A_d$ of Lie-PCA, and solve

$$\arg\min \left\| \Pi\left[\langle A_i \rangle_{i=1}^d\right] - \Pi\left[\widehat{\mathfrak{h}}\right] \right\| \quad \text{s.t.} \quad \widehat{\mathfrak{h}} \in \mathcal{G}(G, \mathfrak{so}(n)),$$

where $\mathcal{G}(G, \mathfrak{so}(n))$ is the subspace of $\mathfrak{so}(n)$ consisting of the Lie subalgebras pushforward of $\mathfrak{g}$ by a representation.

The set $\mathcal{G}(G, \mathfrak{so}(n))$ has many connected components, one for each *orbit-equivalence* class of representations.

Let $\mathfrak{h}$ be the actual subalgebra we are looking for. We want to make sure that the minimizer belongs to the connected component of $\mathfrak{h}$.



The distance from $\langle A_i \rangle_{i=1}^d$ to $\mathfrak{h}$ must be lower than the *reach* of $\mathcal{G}(G, \mathfrak{so}(n))$. In this context, it is related to the *rigidity* of $\mathfrak{h}$.

Lemma: Consider the subset of $\mathcal{G}(G, \mathfrak{so}(n))$ with weights at most $\omega_{\max}$. Then its ridigity satisfies

$$\Gamma(G, n, \omega_{\max}) \geq 4/(n\omega_{\max}^2).$$

1. Lie theory
2. Applications of the algorithm
3. Description of the algorithm
4. Proof of robustness
5. Conclusion

Conclusion

- First algorithm to find the **representation type** (not only a subspace close to the Lie algebra)
- Implementation for $G = \mathrm{SO}(2)$, T^d, $\mathrm{SO}(3)$ and $\mathrm{SU}(2)$
- Can be adapted to other compact Lie group provided an explicit description of its irreps
- Experiments on image analysis, harmonic analysis and physical systems at `https://github.com/HLovisiEnnes/LieDetect`

Limitations:

- Optimizations over $\mathrm{O}(n)$ are computationally expansive and instable
- The algorithm do not handle entangled orbits
- Restricted to **representations** of Lie groups

Next goals:

- Detections of **actions** via the induced representation on space of vector fields

$$\begin{array}{ccc} G & \xrightarrow{\ \ \phi\ \ } & \mathrm{Diff}(\mathcal{M}) \\ \mathrm{exp}\uparrow & & \uparrow\mathrm{exp} \\ \mathfrak{g} & \xrightarrow{\ \ \mathrm{d}\phi\ \ } & \mathscr{X}(\mathcal{M}) \end{array}$$

- Group Equivariant Convolutional Networks