Seminário PMA - 28/05/2024

DETECTION OF REPRESENTATION ORBITS OF COMPACT LIE GROUPS FROM POINT CLOUDS

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The idea of symmetry in the late XIX century






Bernhard Riemann 1826 - 1866 | Sophus Lie 1842 – 1899 | Wilhelm Killing 1847 - 1923 | Felix Klein 1849 – 1925 | Élie Cartan 1869 - 1951 | Hermann Weyl 1885 – 1955

1872, F. Klein, Vergleichende Betrachtungen über neuere geometrische Forschungen:
Non-Euclidean geometries should be studied through their symmetries (*Erlangen program*).

Winter 1873, S. Lie:
A *Lie group* is a manifold equipped with a group structure. A Lie group posseses a *Lie algebra*, which allows to work infinitesimally (Lie group–Lie algebra correspondence).

1913, E. Cartan, Theorem of the highest weight:
The irreducible representations of Lie groups are classified by their highest weights.

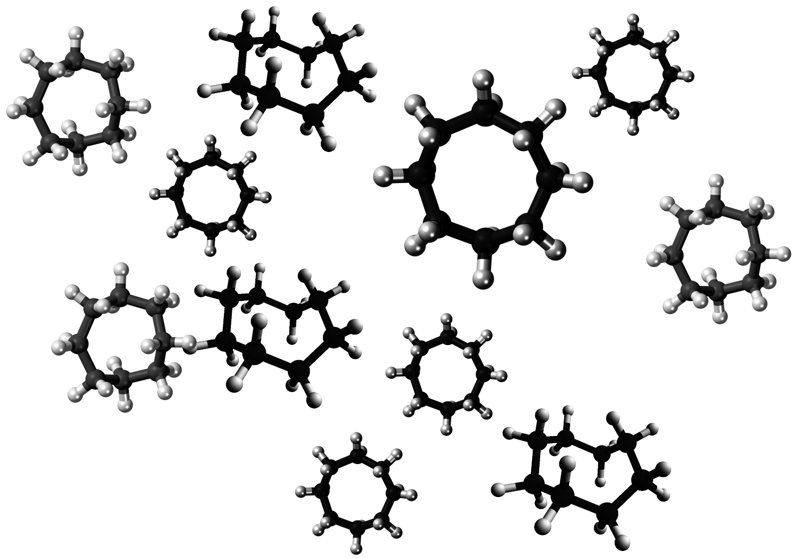
1935, V. Fock, Zur theorie des wasserstoffatoms:
Description of the hydrogen atom through $\mathrm{SO}(4)$-symmetry on top of the Schrödinger equation.

1939, Myers–Steenrod theorem:
The isometry group of a Riemannian manifold is a Lie group.

Symmetries in datasets

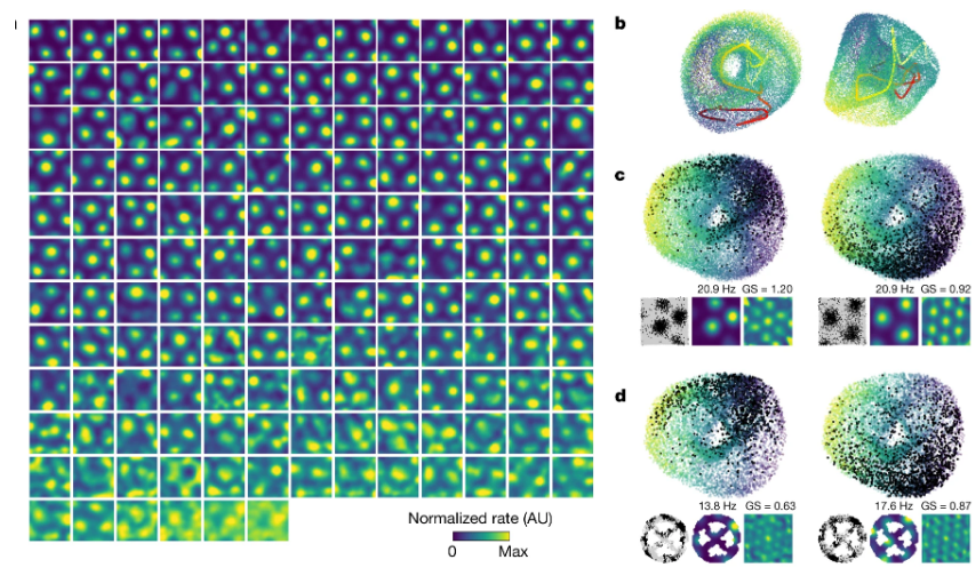
(1) Certain real-life experiments exhibit symmetric objects.

[Martin, Thompson, Coutsias & Watson, Topology of cyclo-octane energy landscape, 2010]



The space of conformation of $\mathrm{C_8H_{16}}$ molecules is the union of **a Klein bottle and a sphere**.

[Richard J. Gardner et al, Toroidal topology of population activity in grid cells, 2022]

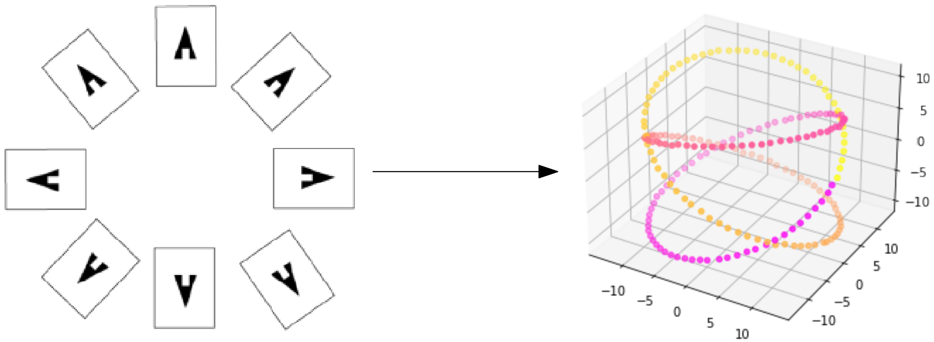


The firing matrix of grid cells in rat brains shows the connecivity of a **torus**.

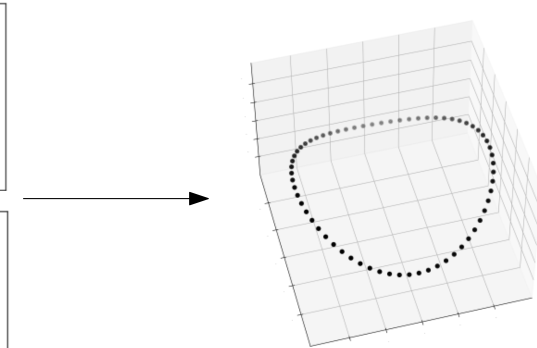
Symmetries in datasets

(1) Certain real-life experiments exhibit symmetric objects.

(2) Euclidean transformations are governed by Lie group representations.



$\mathrm{SO}(2)$



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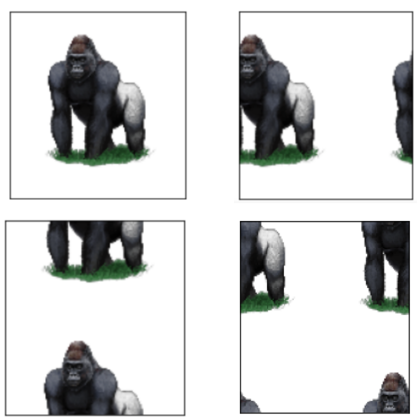
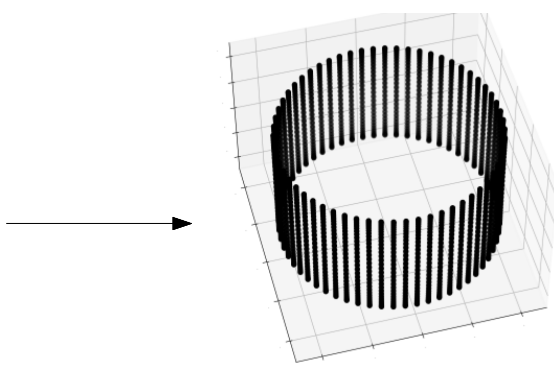




$\mathrm{SO}(2) \times \mathrm{SO}(2) \simeq T^2$

The $n \times m$-images can be embedded in $\mathbb{R}^{n \times m}$.

After applying permutations of the pixels, the embedded images lie on an **orbit of a Lie group representation.**

Symmetries in datasets

(1) Certain real-life experiments exhibit symmetric objects.

(2) Euclidean transformations are governed by Lie group representations.

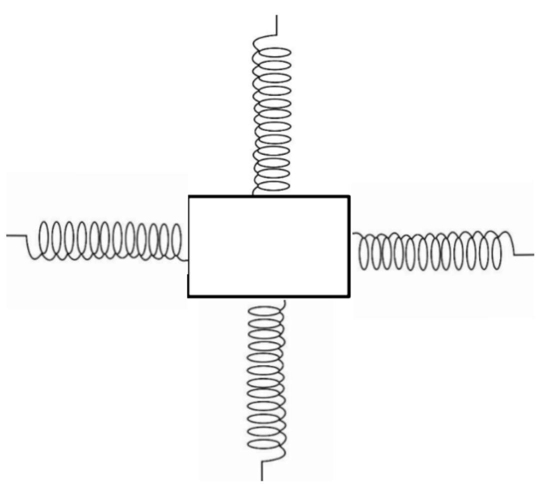
(3) Symmetries in Hamiltonian systems yield conservation laws.

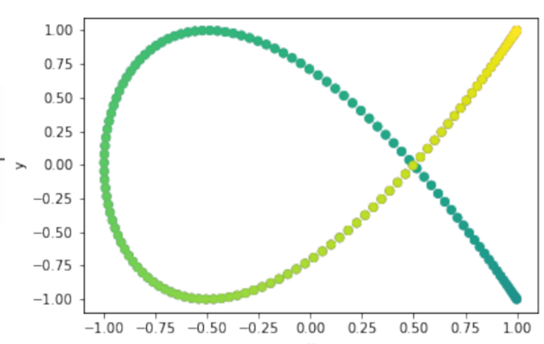
Hamiltonian's systems follow the equations $$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial \mathbf{q}} \qquad \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \frac{\partial H}{\partial \mathbf{p}}.$$

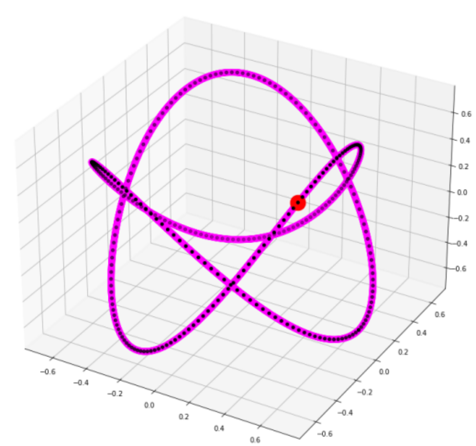
Let ω be the canonical symplectic form in $\mathbb{R}^{2n}$. A *symplectomorphism* is a Lie group representation $L : G \to \mathrm{GL}_{2n}(\mathbb{R})$ on $\mathbb{R}^{2n}$ that preserves the the system's dynamics, i.e. $L(g)^*\omega = \omega \ \forall g \in G$.

Emmy Noether
1882 - 1935

Noether's theorem (1915):
If H is invariant under the action of G, then the moment mapping is conserved.





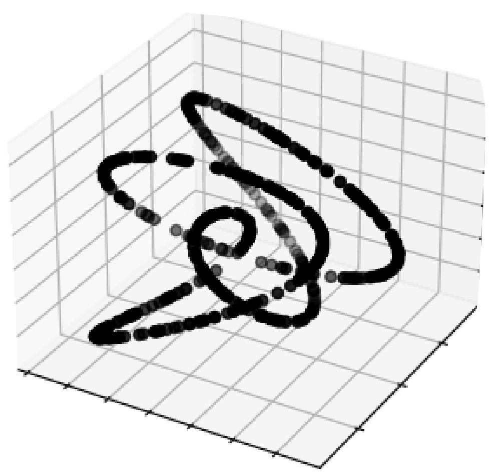
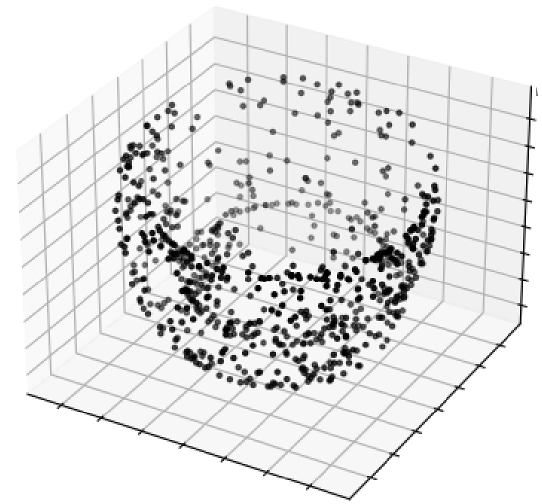
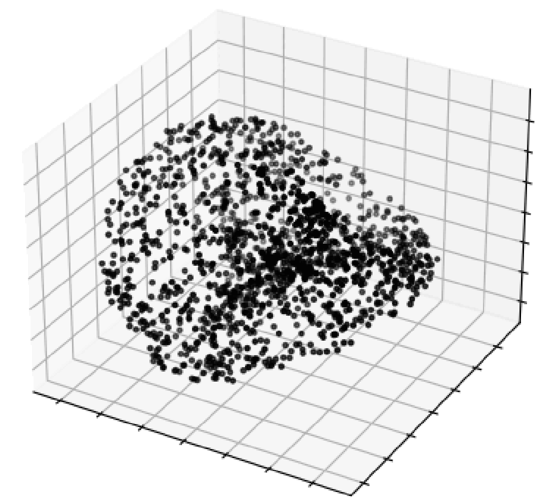


Input: A point cloud $X = \{x_1 \ldots, x_N\} \subset \mathbb{R}^n$.

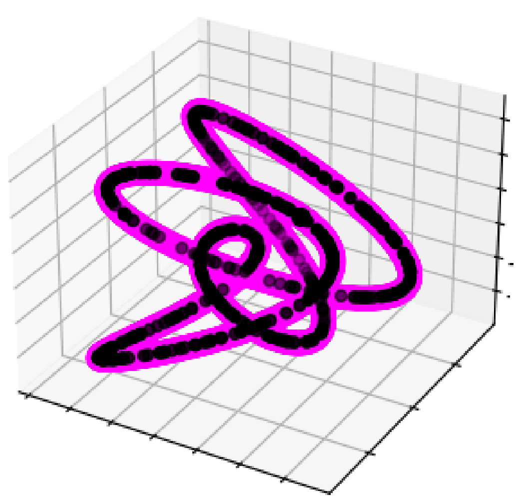
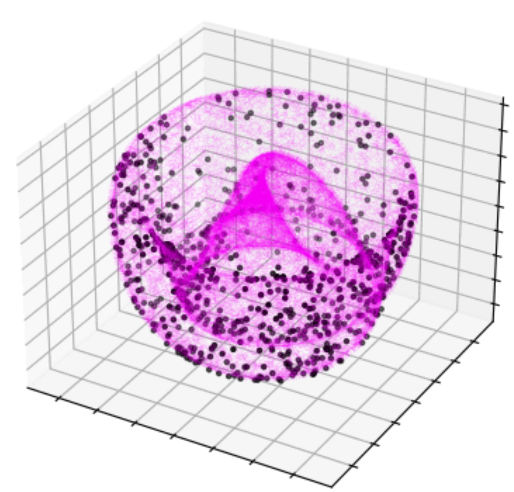
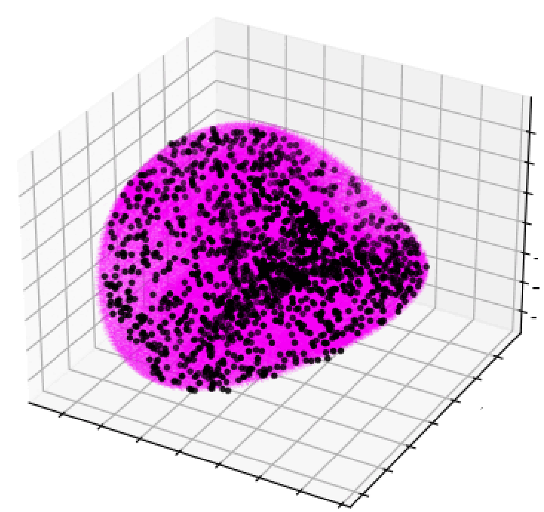
Output: A compact Lie group G, a representation ϕ of it in $\mathbb{R}^n$, and an orbit $\mathcal{O}$ close to X.

Orbit of $\mathrm{SO}(2)$ in $\mathbb{R}^6$ | Orbit of T^2 in $\mathbb{R}^6$ | Orbit of $\mathrm{SU}(2)$ in $\mathbb{R}^7$

Input:

Output:

1. Lie group - Lie algebra correspondence
2. Closest Lie algebra problem
3. Examples
4. Proof of robustness

Definition: A *Lie group* is a group G that is also a smooth manifold, and such that the multiplication map $(g,h) \mapsto gh$ and the inverse map $g \mapsto g^{-1}$ are smooth.

Example: Given $n \in \mathbb{N}$ positive, on has the *matrix groups*

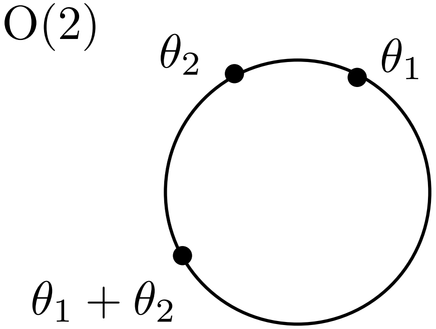
- $\mathrm{O}(n)$ orthogonal group: the set of orthogonal $n \times n$ matrices $(A^\top = A^{-1})$
- $\mathrm{SO}(n)$ special orthogonal group: set of orthogonal $n \times n$ matrices of determinant $+1$
- $\mathrm{Sp}(2n,\mathbb{C})$ symplectic group: the set of complex sympletic $n \times n$ matrices
- $\mathrm{U}(n)$ unitary group: the set of complex unitary $n \times n$ matrices $(A^* = A^{-1})$
- $\mathrm{SU}(n)$ special unitary group: the set of complex unitary $n \times n$ matrices of determinant $+1$

Products of Lie groups are Lie groups:

- T^n n-torus: the product $\mathrm{SO}(2) \times \cdots \times \mathrm{SO}(2)$

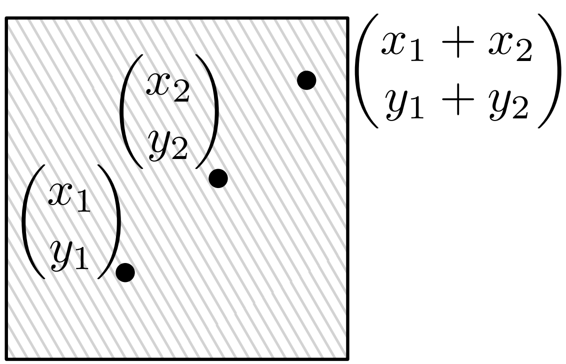
Group structure on $\mathrm{SO}(2)$
(the circle)

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



Group structure on T^2
(Pac-Man's world)

$$\begin{pmatrix} \cos x & -\sin x & 0 & 0 \\ \sin x & \cos x & 0 & 0 \\ 0 & 0 & \cos y & -\sin y \\ 0 & 0 & \sin y & \cos y \end{pmatrix}$$



Definition: A *representation* of a group G in $\mathbb{R}^n$ is a smooth group morphism $G \to \mathrm{GL}_n(\mathbb{R})$ (the $n \times n$ invertible matrices).
In other words, it is an immersion of G in a matrix space, that preserves the algebraic structure.

Example: Of course, matrix Lie groups come with a canonical representation, since they are already included in a matrix space.

$$\mathrm{O}(n) \hookrightarrow \mathrm{GL}_n(\mathbb{R})$$
$$\mathrm{SO}(n) \hookrightarrow \mathrm{GL}_n(\mathbb{R})$$

$$\mathrm{Sp}(2n, \mathbb{C}) \hookrightarrow \mathrm{GL}_n(\mathbb{C}) \hookrightarrow \mathrm{GL}_{2n}(\mathbb{R})$$
$$\mathrm{U}(n) \hookrightarrow \mathrm{GL}_n(\mathbb{C}) \hookrightarrow \mathrm{GL}_{2n}(\mathbb{R})$$
$$\mathrm{SU}(n) \hookrightarrow \mathrm{GL}_n(\mathbb{C}) \hookrightarrow \mathrm{GL}_{2n}(\mathbb{R})$$

However, more sophisticated representations exist.

$$\begin{tikzcd} & \mathrm{SO}(2) \arrow[dl] \arrow[dr] & \\ \mathrm{GL}_2(\mathbb{R}) & & \mathrm{GL}_2(\mathbb{R}) \end{tikzcd}$$

$$\theta \mapsto \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \qquad\qquad \begin{pmatrix} \cos 3\theta & -\sin 3\theta \\ \sin 3\theta & \cos 3\theta \end{pmatrix}$$

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$$\begin{tikzcd} & \mathrm{SO}(2) \arrow[dl] \arrow[d] \arrow[dr] & \\ \mathrm{GL}_4(\mathbb{R}) & \mathrm{GL}_4(\mathbb{R}) & \mathrm{GL}_4(\mathbb{R}) \end{tikzcd}$$

$$\theta \mapsto \begin{pmatrix} \cos\theta & -\sin\theta & 0 & 0 \\ \sin\theta & \cos\theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} \cos 2\theta & -\sin 2\theta & 0 & 0 \\ \sin 2\theta & \cos 2\theta & 0 & 0 \\ 0 & 0 & \cos 5\theta & -\sin 5\theta \\ 0 & 0 & \sin 5\theta & \cos 5\theta \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos\theta & -\sin\theta \\ 0 & 0 & \sin\theta & \cos\theta \end{pmatrix}$$

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However, more sophisticated representations exist.

Definition: Two representations $\phi_1, \phi_2 \colon G \to \mathrm{GL}_n(\mathbb{R})$ are *equivalent* if there exists $A \in \mathrm{GL}_n(\mathbb{R})$ such that $\phi_2 = A\phi_1 A^{-1}$.

They are "equal up to a change of coordinates'.

Proposition: Representations of $\mathrm{SO}(2)$ in $\mathbb{R}^{2n}$ are classified by $\mathbb{Z}^n/\mathfrak{S}_n$ (tuples up to permutation).
More precisely, to $(\omega_1, \ldots, \omega_n) \in \mathbb{Z}^n$ is associated a representation $\phi_{(\omega_1,\ldots,\omega_n)} \colon \mathrm{SO}(2) \to \mathrm{GL}_{2n}(\mathbb{R})$.

$$\phi_{(\omega_1,\ldots,\omega_n)}(\theta) = \begin{pmatrix} R(\omega_1\theta) & & & \\ & R(\omega_2\theta) & & \\ & & \ddots & \\ & & & R(\omega_n\theta) \end{pmatrix} \quad \text{where} \quad R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

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Proposition: Representations of $\mathrm{SO}(2)$ in $\mathbb{R}^{2n}$ are classified by $\mathbb{Z}^n/\mathfrak{S}_n$ (tuples up to permutation). More precisely, to $(\omega_1, \ldots, \omega_n) \in \mathbb{Z}^n$ is associated a representation $\phi_{(\omega_1,\ldots,\omega_n)} \colon \mathrm{SO}(2) \to \mathrm{GL}_{2n}(\mathbb{R})$.

Proposition: Representations of T^2 in $\mathbb{R}^{2n}$ are classified by $(\mathbb{Z}^n)^2/\mathfrak{S}_n$ ($2 \times n$ matrix up to permutation of the columns).

More generally, the equivalence classes representations are studied through combinations of *irreducible representations*.

Orbits

Definition: Let $G \to \mathrm{GL}_n(\mathbb{R})$ be a representation of G in $\mathbb{R}^n$, and $x_0 \in \mathbb{R}^n$ a point. The *orbit* of x_0 under the action of G is $\mathcal{O} = \{\phi(g)x_0 \mid g \in G\}$.

Example: Orbits of $\mathrm{SO}(2)$ are "circles". For instance, the orbit of $(1,0)$ under the representation

- $$\mathrm{SO}(2) \longrightarrow \mathrm{GL}_2(\mathbb{R})$$
  $$\theta \longmapsto \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

is $\mathcal{O} = \left\{ \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \mid \theta \in \mathbb{R} \right\}$

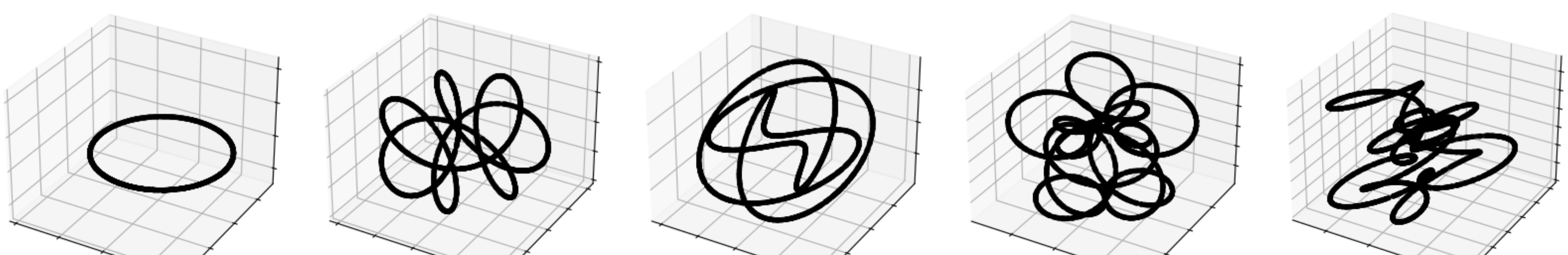
The orbit of $(1,0,1,0)$ under the representation

- $$\mathrm{SO}(2) \longrightarrow \mathrm{GL}_4(\mathbb{R})$$
  $$\theta \longmapsto \begin{pmatrix} \cos\theta & -\sin\theta & 0 & 0 \\ \sin\theta & \cos\theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

is $\mathcal{O} = \left\{ \begin{pmatrix} \cos\theta \\ \sin\theta \\ 1 \\ 0 \end{pmatrix} \mid \theta \in \mathbb{R} \right\}$

- $$\mathrm{SO}(2) \longrightarrow \mathrm{GL}_4(\mathbb{R})$$
  $$\theta \longmapsto \begin{pmatrix} \cos 2\theta & -\sin 2\theta & 0 & 0 \\ \sin 2\theta & \cos 2\theta & 0 & 0 \\ 0 & 0 & \cos 5\theta & -\sin 5\theta \\ 0 & 0 & \sin 5\theta & \cos 5\theta \end{pmatrix}$$

is $\mathcal{O} = \left\{ \begin{pmatrix} \cos 2\theta \\ \sin 2\theta \\ \cos 5\theta \\ \sin 5\theta \end{pmatrix} \mid \theta \in \mathbb{R} \right\}$



$\phi_{(1,0)}$ $\phi_{(2,5)}$ $\phi_{(3,5)}$ $\phi_{(2,3,11)}$ $\phi_{(2,3,4,11)}$

Definition: Let $G \to \mathrm{GL}_n(\mathbb{R})$ be a representation of G in $\mathbb{R}^n$, and $x_0 \in \mathbb{R}^n$ a point. The *orbit* of x_0 under the action of G is $\mathcal{O} = \{\phi(g)x_0 \mid g \in G\}$.

Example: Orbits of $\mathrm{SO}(2)$ are "circles".

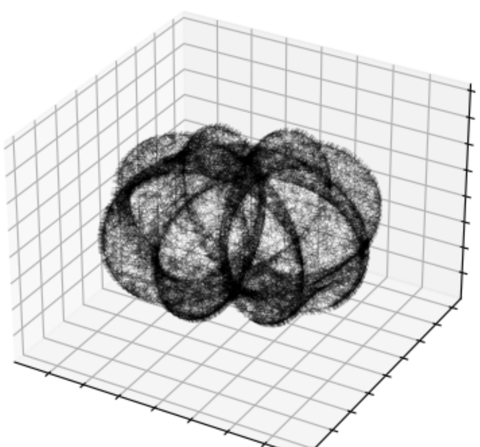
Example: Orbits of T^2 are "tori". For instance, the orbit of $(1,0,1,0,1,0)$ under the representation

- $T^2 \longrightarrow \mathrm{GL}_6(\mathbb{R})$

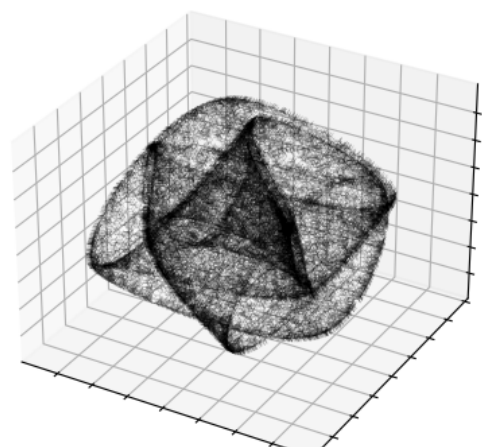
$$\theta \longmapsto \begin{pmatrix} \cos\theta & -\sin\theta & 0 & 0 & 0 & 0 \\ \sin\theta & \cos\theta & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos\theta & -\sin\theta & 0 & 0 \\ 0 & 0 & \sin\theta & \cos\theta & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos 3\theta & -\sin 3\theta \\ 0 & 0 & 0 & 0 & \sin 3\theta & \cos 3\theta \end{pmatrix}$$

$$\mu \longmapsto \begin{pmatrix} \cos\mu & -\sin\mu & 0 & 0 & 0 & 0 \\ \sin\mu & \cos\mu & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos 2\mu & -\sin 2\mu & 0 & 0 \\ 0 & 0 & \sin 2\mu & \cos 2\mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos\mu & -\sin\mu \\ 0 & 0 & 0 & 0 & \sin\mu & \cos\mu \end{pmatrix}$$

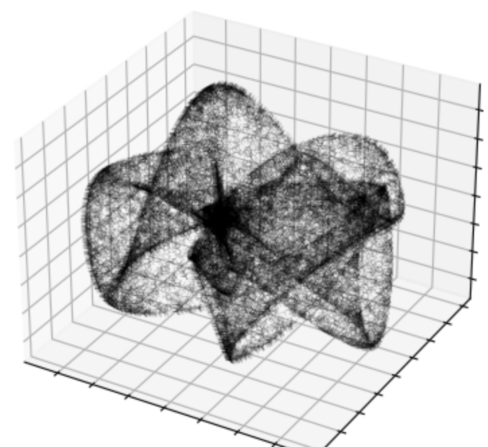
is $$\mathcal{O} = \left\{ \begin{pmatrix} \cos\theta + \cos\mu \\ \sin\theta + \sin\mu \\ \cos\theta + \cos 2\mu \\ \sin\theta + \sin 2\mu \\ \cos 3\theta + \cos\mu \\ \sin 3\theta + \sin\mu \end{pmatrix} \;\middle|\; (\theta,\mu) \in \mathbb{R}^2 \right\}$$



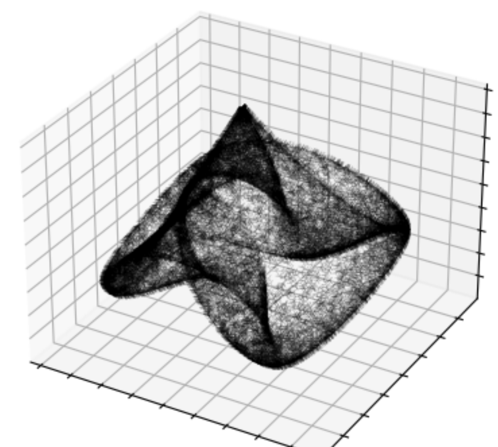
$\phi_{\begin{pmatrix}1&1&3\\1&2&1\end{pmatrix}}$



$\phi_{\begin{pmatrix}1&2&2\\2&1&1\end{pmatrix}}$



$\phi_{\begin{pmatrix}-2&2&0&1\\-1&0&-2&1\end{pmatrix}}$



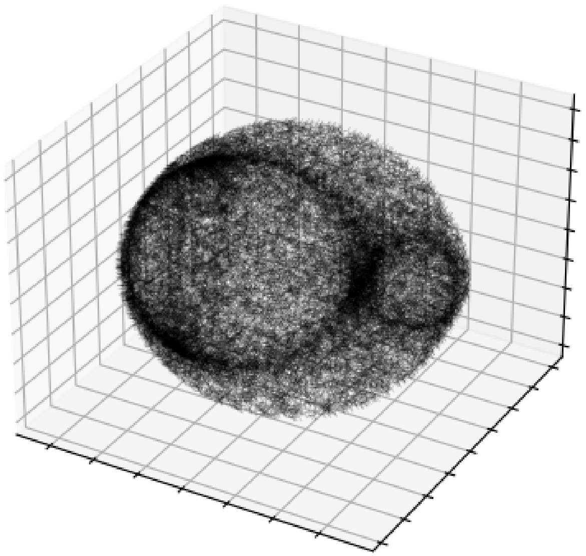
$\phi_{\begin{pmatrix}2&-2&0&2\\1&1&-1&2\end{pmatrix}}$

Definition: Let $G \to \mathrm{GL}_n(\mathbb{R})$ be a representation of G in $\mathbb{R}^n$, and $x_0 \in \mathbb{R}^n$ a point. The *orbit* of x_0 under the action of G is $\mathcal{O} = \{\phi(g)x_0 \mid g \in G\}$.

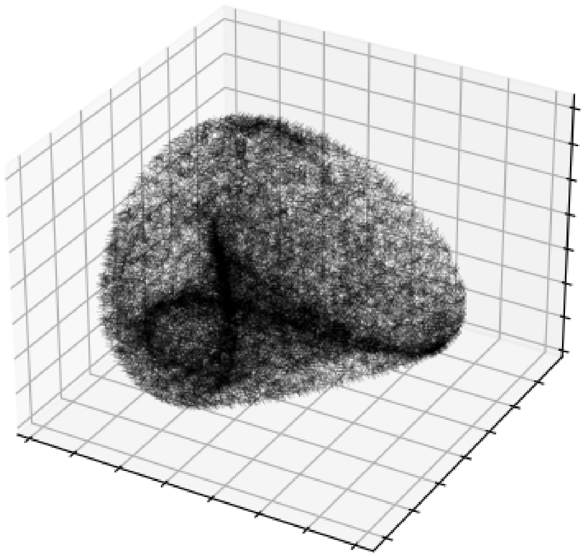
Example: Orbits of $\mathrm{SO}(2)$ are "circles".

Example: Orbits of T^2 are "tori".

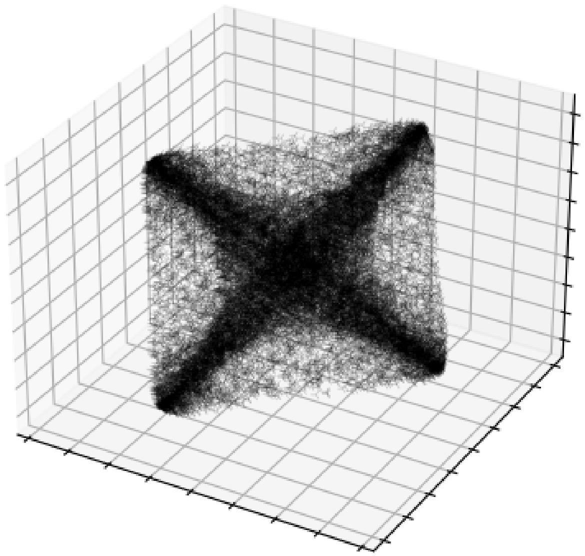
Example: Orbits of $\mathrm{SO}(3)$ and $\mathrm{SU}(2)$ are "spheres".



$\psi_{(5)}$ in $\mathbb{R}^5$



$\psi_{(3,4)}$ in $\mathbb{R}^7$



$\psi_{(8)}$ in $\mathbb{R}^8$

Let G be a Lie group, $0 \in G$ the identity element and $\mathfrak{g} = \mathrm{T}_0 G$ the tangent space.

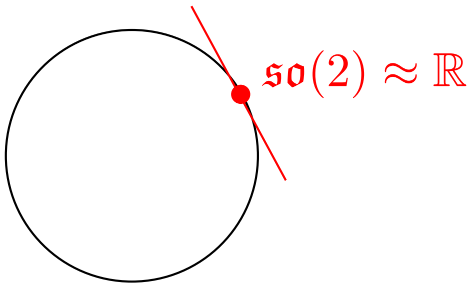
There exists an **exponential map**, denoted $\exp\colon \mathfrak{g} \to G$. It is smooth. When G is connected and compact, it is surjective.

Remark: Any compact Lie group admits a (bi-invariant) Riemannian metric for which the Lie-exponential and Riemann-exponential coincide.

Example: In the case of matrix groups, the exponential map is simply the matrix exponential.

- $\mathrm{SO}(2) = \left\{ \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix} \mid t \in \mathbb{R} \right\} \xleftarrow{\quad\exp\quad} \mathfrak{so}(2) = \left\{ \begin{pmatrix} 0 & -t \\ t & 0 \end{pmatrix} \mid t \in \mathbb{R} \right\}$

One has $\exp \begin{pmatrix} 0 & -t \\ t & 0 \end{pmatrix} = \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix}$



- $\mathrm{SO}(3) = \left\{ A \in \mathrm{GL}_3(\mathbb{R}) \mid A^\top = A^{-1}, \det A = 1 \right\} \xleftarrow{\quad\exp\quad} \mathfrak{so}(3) = \langle X_1, X_2, X_3 \rangle$ where

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \qquad X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \qquad X_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Caution: In general, $\exp(t_1 X_1 + t_2 X_2 + t_3 X_2) \neq \exp(t_1 X_1) \exp(t_2 X_2) \exp(t_3 X_3)$.

Actually, the Lie algebra $\mathfrak{g}$ of a Lie group G admits an algebraic structure, called **Lie bracket**.

It is a bilinear map $\mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ that satisfies the Jacobi identity.

It is denoted $[A, B]$, where $A, B \in \mathfrak{g}$.

Example: In the case of matrix groups, the Lie bracket is simply the commutator

$$[A, B] = AB - BA.$$

For instance, in $\mathrm{SO}(3)$, one has $[X_1, X_2] = X_3$, $[X_2, X_3] = X_1$ and $[X_1, X_3] = -X_2$, where

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \qquad X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \qquad X_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Remark: The Lie algebra contains a lot of information regarding the Lie group.
For instance, for simply connected Lie groups G_1 and G_2, one has $\mathfrak{g}_1 \simeq \mathfrak{g}_2 \implies G_1 \simeq G_2$.

Lie algebras allow to study representations from an infinitesimal viewpoint.

Proposition: Given a representation $\phi\colon G \to \mathrm{GL}_n(\mathbb{R})$, there exists a morphism $\mathrm{d}\phi\colon \mathfrak{g} \to \mathfrak{gl}_n(\mathbb{R})$ of Lie algebras, called **derived representation**, such that the following diagram commutes

$$\begin{tikzcd} G \arrow[r, "\phi"] & \mathrm{GL}_n(\mathbb{R}) \\ \mathfrak{g} \arrow[u, "\exp"] \arrow[r, "\mathrm{d}\phi"] & \mathfrak{gl}_n(\mathbb{R}) \arrow[u, "\exp"'] \end{tikzcd} \quad = n \times n \text{ matrices}$$

Remark: In practice, we prefer to work with **orthogonal representations**, i.e., such that $\phi(G) \subset \mathrm{SO}(n)$. In this case, the diagram reads

$$\begin{tikzcd} G \arrow[r, "\phi"] & \mathrm{SO}(n) \\ \mathfrak{g} \arrow[u, "\exp"] \arrow[r, "\mathrm{d}\phi"] & \mathfrak{so}(n) \arrow[u, "\exp"'] \end{tikzcd} \quad = \text{skew-symmetric } n \times n \text{ matrices}$$

The image $\mathrm{d}\phi(\mathfrak{g}) \subset \mathfrak{so}(n)$ is called the **push-forward Lie algebra**. It will play a key role in our problem.

1. Lie group - Lie algebra correspondence
2. Closest Lie algebra problem
3. Examples
4. Proof of robustness

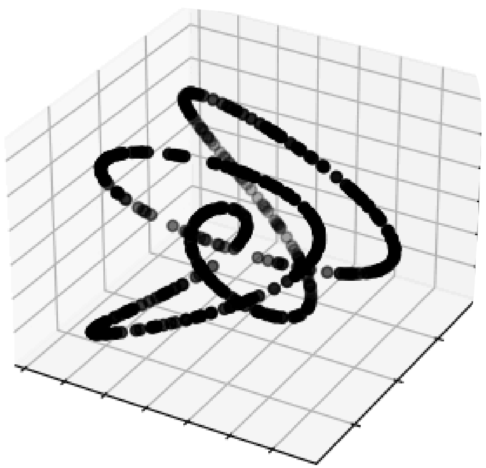
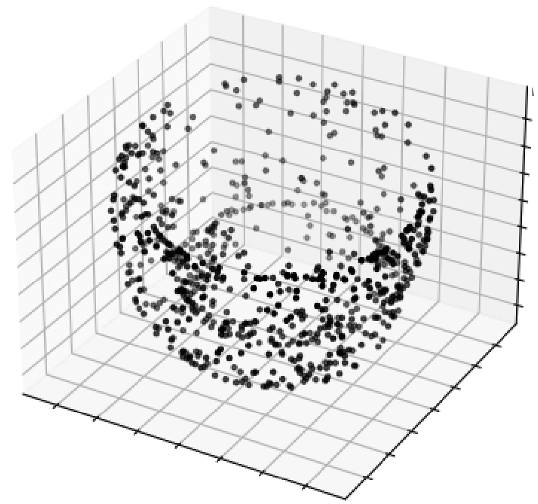
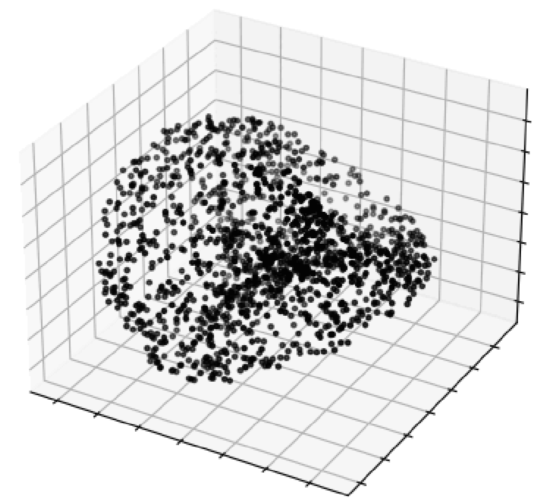
Formulation of our problem - infinitesimal viewpoint

Input: A point cloud $X = \{x_1 \ldots, x_N\} \subset \mathbb{R}^n$.

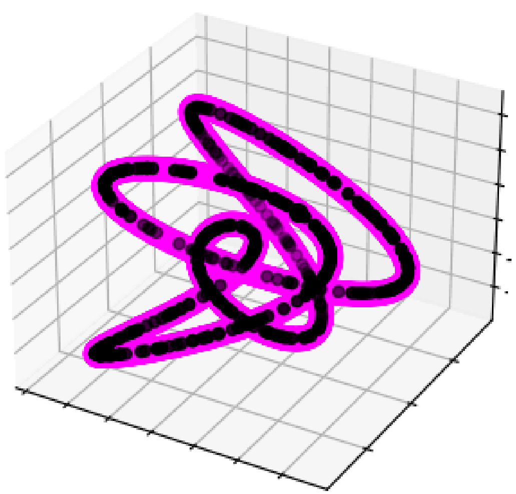
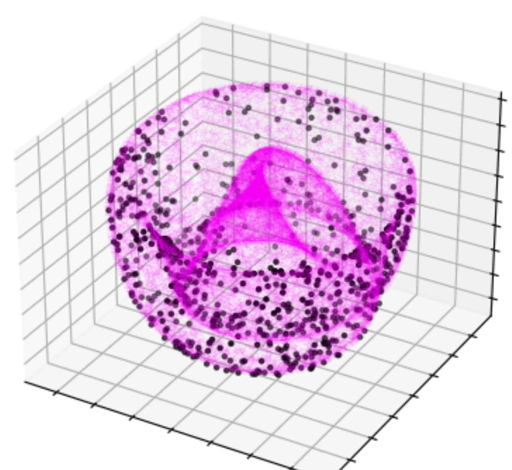
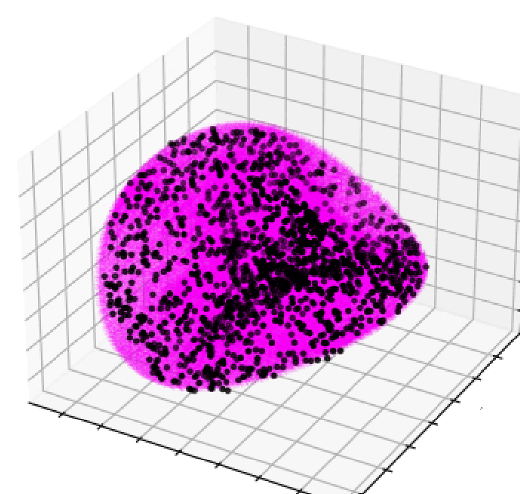
Output: An orthogonal representation ϕ of a compact Lie group G in $\mathbb{R}^n$, and an orbit $\mathcal{O}$ close to X.

Orbit of $\mathrm{SO}(2)$ in $\mathbb{R}^6$ | Orbit of T^2 in $\mathbb{R}^6$ | Orbit of $\mathrm{SU}(2)$ in $\mathbb{R}^7$

Input:

Output:

Input: A point cloud $X = \{x_1 \ldots, x_N\} \subset \mathbb{R}^n$.

Output: An orthogonal representation ϕ of a compact Lie group G in $\mathbb{R}^n$, and an orbit $\mathcal{O}$ close to X.

Idea: Obtain the best orbit $\mathcal{O}$ via mean squared error.

Problem: It is unclear how to compute the projection of X on $\mathcal{O}$.

Input: A point cloud $X = \{x_1 \dots, x_N\} \subset \mathbb{R}^n$.

Output: An orthogonal representation ϕ of a compact Lie group G in $\mathbb{R}^n$, and an orbit $\mathcal{O}$ close to X.

Idea: Obtain the best orbit $\mathcal{O}$ via mean squared error.

Problem: It is unclear how to compute the projection of X on $\mathcal{O}$.

Other idea: Instead of estimating the representation ϕ, aim for the push-forward algebra $\mathfrak{h} = \mathrm{d}\phi(\mathfrak{g})$. Then $\mathcal{O}$ is obtained by exponentiating it:

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

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

[Cahill, Mixon & Parshall, Lie PCA: Density estimation for symmetric manifolds, 2023]

Lie-PCA is a recently developed algorithm allowing to estimate $\mathfrak{h}$ from X.
The output, denoted $\widehat{\mathfrak{h}} = \mathrm{span}\{\widehat{\mathfrak{h}}_1, \dots, \widehat{\mathfrak{h}}_d\}$, is a d-dimensional linear subspace of $\mathfrak{so}(n)$.

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

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

We define $\widehat{\mathfrak{h}}$ as the subspace spanned by the bottom eigenvectors $\widehat{\mathfrak{h}}_1, \ldots, \widehat{\mathfrak{h}}_d$ of Λ.

Definition of Lie-PCA

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

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We define $\widehat{\mathfrak{h}}$ as the subspace spanned by the bottom eigenvectors $\widehat{\mathfrak{h}}_1, \dots, \widehat{\mathfrak{h}}_d$ of Λ.

Derivation of Lie-PCA: Based on the fact that $\mathfrak{sym}(\mathcal{O}) = \big\{A \in \mathrm{M}_n(\mathbb{R}) \mid \forall x \in \mathcal{O}, Ax \in \mathrm{T}_x\mathcal{O}\big\}$, where $\mathrm{T}_x\mathcal{O}$ denotes the tangent space of $\mathcal{O}$ at x. In other words,

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

Using only the point cloud $X = \{x_1, \dots, x_N\}$, 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.

Other idea: Instead of estimating the representation ϕ, aim for the push-forward algebra $\mathfrak{h} = \mathrm{d}\phi(\mathfrak{g})$. Then $\mathcal{O}$ is obtained by exponentiating it.

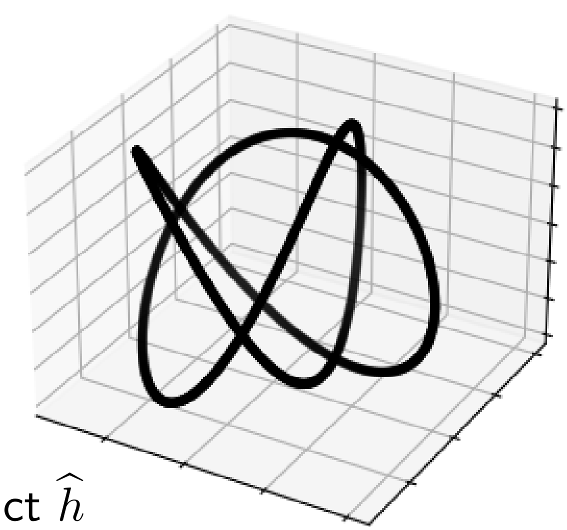
$$\begin{tikzcd} G \arrow[r, "\phi"] & \mathrm{SO}(n) \\ \mathfrak{g} \arrow[u, "\exp"] \arrow[r, "\mathrm{d}\phi"] & \mathfrak{so}(n) \arrow[u, "\exp"'] \end{tikzcd}$$

Definition of orbit: $\mathcal{O} = \{\phi(g)x \mid g \in G\}$

From the Lie algebra: $\mathcal{O} = \{\exp(h)x \mid h \in \mathfrak{h}\}$

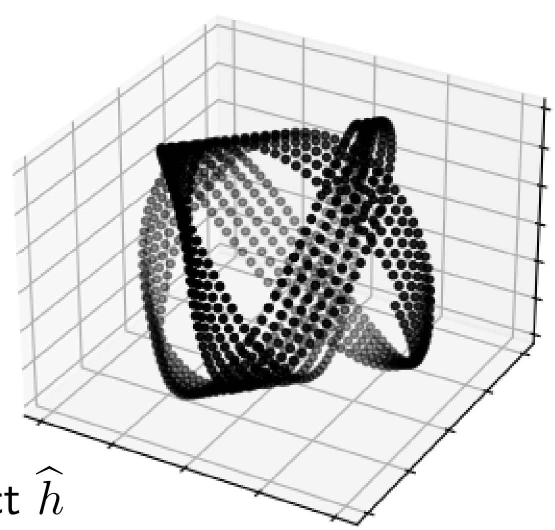
Via Lie-PCA, we get $\widehat{\mathfrak{h}}$, a d-dimensional linear subspace of $\mathfrak{so}(n)$. It is an estimation of $\mathfrak{h}$.

Problem: The subspace $\widehat{\mathfrak{h}}$ is estimated as if it were a linear subspace. It may not be a Lie algebra (for $A, B \in \widehat{\mathfrak{h}}$, we must have $AB - BA \in \widehat{\mathfrak{h}}$).



exact $\widehat{h}$

Exponentiating a non-Lie algebra, or a Lie algebra not coming from a compact Lie group, may yield large errors



inexact $\widehat{h}$

We wish to project $\widehat{\mathfrak{g}}$ on the closest Lie algebra. We work in $\mathfrak{so}(n)$, the set of skew-symmetric $n \times n$ matrices. It has dimension $n(n+1)/2$. It is endowed with the Frobenius inner product and norm

$$\langle A, B\rangle = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{i,j}b_{i,j} \qquad \text{and} \qquad \|A\| = \sqrt{\sum_{i=1}^{n}\sum_{j=1} a_{i,j}}.$$

Stiefel variety of Lie algebras

Treat the d-dimensional subspaces of $\mathfrak{so}(n)$ as $n(n-1)/2 \times d$ matrices

$\mathcal{V}^{\mathsf{Lie}}(d, \mathfrak{so}(n))$ is defined as the **set of d-frames** $(A_1, \ldots, A_d)$ of $\mathfrak{so}(n)$ (i.e., normalized and pairwise orthogonal) with the Lie algebra condition: $\forall i, j \in [1, \ldots, n]$, $A_iA_j - A_jA_i \in \langle A_1, \ldots, A_d\rangle$.

The problem is

$$\min\left\{\sum_{i=1}^{d} \|\widehat{\mathfrak{h}}_i - A_i\|^2 \mid (A_1, \ldots, A_d) \in \mathcal{V}^{\mathsf{Lie}}(d, \mathfrak{so}(n))\right\}$$

Grassmannian variety of Lie algebras

Treat the d-dimensional subspaces of $\mathfrak{so}(n)$ as $n(n-1)/2 \times n(n-1)/2$ matrices

$\mathcal{G}^{\mathsf{Lie}}(d, \mathfrak{so}(n))$ is defined as the **set of orthogonal projection matrices** of rank d on $\mathfrak{so}(n)$ with the Lie algebra condition: $\forall i, j \in [1, \ldots, n]$, $P(Pe_i \cdot Pe_j - Pe_j \cdot Pe_i) = Pe_i \cdot Pe_j - Pe_j \cdot Pe_i$ where $(e_1, \ldots, e_{n(n+1)/2})$ is an orthonormal basis of $\mathfrak{so}(n)$.

The problem is

$$\min\left\{\|\mathsf{proj}[\widehat{\mathfrak{h}}] - P\| \mid P \in \mathcal{G}^{\mathsf{Lie}}(d, \mathfrak{so}(n))\right\}$$

Written explicitely in matrix form, this reads:

Stiefel variety of Lie algebras

$$\min \sum_{i=1}^{d} \|\widehat{\mathfrak{h}}_i - A_i\|^2 \text{ such that } \begin{cases} \forall i \in [1\ldots,d], & A_i \text{ is a } (n \times n)\text{-matrix}, \\ \forall i \in [1\ldots,d], & A^\top = -A, \\ \forall i,j \in [1\ldots,d], & \sum_{k=1}^{d} \langle A_k, A_iA_j - A_jA_i\rangle^2 = \|A_iA_j - A_jA_i\|^2. \end{cases}$$

Grassmannian variety of Lie algebras

$$\min \|\mathrm{proj}[\widehat{\mathfrak{h}}] - P\| \text{ such that } \begin{cases} P \text{ is a } \big(n(n+1)/2 \times n(n+1)/2\big)\text{-matrix}, \\ P^2 = P, \\ P^\top = P, \\ \mathrm{rank}(P) = d, \\ \forall i,j \in [1\ldots,d],\ P(Pe_i \cdot Pe_j - Pe_j \cdot Pe_i) = Pe_i \cdot Pe_j - Pe_j \cdot Pe_i. \end{cases}$$

Problem: (1) These programs seem intractable (they contain the classification of Lie algebras)
(2) Actually, a Lie algebra in $\mathfrak{so}(n)$ may not even come from a compact Lie group.

Idea: Fix a compact Lie group G, and restrict the Stiefel $\mathcal{V}^{\mathsf{Lie}}(d, \mathfrak{so}(n))$ and the Grassmannian $\mathcal{G}^{\mathsf{Lie}}(d, \mathfrak{so}(n))$ to the Lie algebras that are push-forward of G.

From now on, G is a fixed compact Lie group of dimension d.

Stiefel variety of pushforward Lie algebras of G

$\mathcal{V}(G, \mathfrak{so}(n))$ is defined as the set of $(A_1, \ldots, A_d) \in \mathcal{V}^{\mathsf{Lie}}(d, \mathfrak{so}(n))$ for which there exists an orthogonal representation $\phi\colon G \to \mathrm{SO}(n)$ such that $\mathrm{d}\phi(\mathfrak{g})$ is spanned by $(A_1, \ldots, A_d)$.

Lemma: Seen as a subset of the $n(n+1)/2 \times d$ matrices, the connected components of $\mathcal{V}(G, \mathfrak{so}(n))$ are in correspondence with the **orbit-equivalence classes** of orthogonal representations of G in $\mathbb{R}^n$.

Definition: We say that two representations $\phi, \phi' : G \to \mathrm{GL}_n(\mathbb{R})$ are *orbit-equivalent* if there exists a matrix $M \in \mathrm{M}_n(\mathbb{R})$ such that $\mathrm{d}\phi(\mathfrak{g}) = M\mathrm{d}\phi'(\mathfrak{g})M^{-1}$. In particular, their orbits are conjugated. We shall denote by $\mathfrak{orb}(G, n)$ a set of representatives of the orbit-equivalence classes.

Grassmannian variety of pushforward Lie algebras of G

$\mathcal{G}(G, \mathfrak{so}(n))$ is defined as the set consisting of those elements $P \in \mathcal{G}^{\mathrm{Lie}}(d, \mathfrak{so}(n))$ for which there exists an orthogonal representation $\phi\colon G \to \mathrm{SO}(n)$ such that P is the projection matrix on $\mathrm{d}\phi(\mathfrak{g})$.

Lemma: Seen as a subset of the $n(n+1)/2 \times n(n+1)/2$ matrices, the connected components of $\mathcal{G}(G, \mathfrak{so}(n))$ are also in correspondence with the orbit-equivalence of G in $\mathbb{R}^n$.

From now on, G is a fixed compact Lie group of dimension d.

Stiefel variety of pushforward Lie algebras of G

$\mathcal{V}(G, \mathfrak{so}(n))$ is defined as the set of $(A_1, \ldots, A_d) \in \mathcal{V}^{\mathsf{Lie}}(d, \mathfrak{so}(n))$ for which there exists an orthogonal representation $\phi\colon G \to \mathrm{SO}(n)$ such that $\mathrm{d}\phi(\mathfrak{g})$ is spanned by $(A_1, \ldots, A_d)$.

Lemma: Seen as a subset of the $n(n+1)/2 \times d$ matrices, the connected components of $\mathcal{V}(G, \mathfrak{so}(n))$ are in correspondence with the **orbit-equivalence classes** of orthogonal representations of G in $\mathbb{R}^n$.

Definition: We say that two representations $\phi, \phi'\colon G \to \mathrm{GL}_n(\mathbb{R})$ are *orbit-equivalent* if there exists a matrix $M \in \mathrm{M}_n(\mathbb{R})$ such that $\mathrm{d}\phi(\mathfrak{g}) = M\mathrm{d}\phi'(\mathfrak{g})M^{-1}$. In particular, their orbits are conjugated. We shall denote by $\mathfrak{orb}(G, n)$ a set of representatives of the orbit-equivalence classes.

Lemma: For any $(A_1, \ldots, A_d) \in \mathcal{V}(G, \mathfrak{so}(n))$, there exists an integer $p \geq 1$, a p-tuple $(B^1, \ldots, B^p) \in \mathfrak{orb}(G, n)$ and two matrices $O \in \mathrm{O}(n)$ and $P \in \mathrm{O}(d)$ such that, for all $i \in [1 \ldots d]$,

$$A_i = \sum_{j=1}^{d} P_{j,i} O \mathrm{diag}\big(B_j^k\big)_{k=1}^{p} O^\top.$$

In particular, the subspace $\langle A_1, \ldots, A_d \rangle \subset \mathfrak{so}(n)$ is spanned by the matrices

$$O\mathrm{diag}\big(B_1^k\big)_{k=1}^{p} O^\top, \quad O\mathrm{diag}\big(B_2^k\big)_{k=1}^{p} O^\top, \quad \ldots, \quad O\mathrm{diag}\big(B_p^k\big)_{k=1}^{p} O^\top.$$

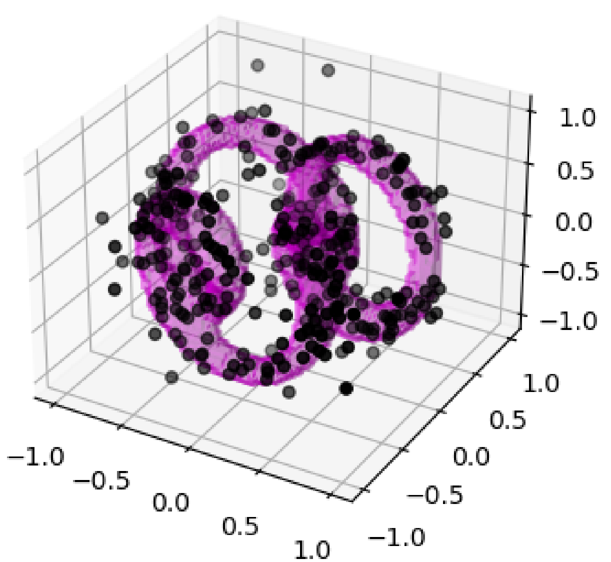
Corollary: The problem $\min\left\{\|\mathrm{proj}[\widehat{\mathfrak{h}}] - P\| \mid P \in \mathcal{G}(G, \mathfrak{so}(n))\right\}$ is equivalent to

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

Remark: This is a discrete-continuous problem.
It splits into N minimization problems over $\mathrm{O}(n)$, where N is the cardinal of $\mathfrak{orb}(G, n)$.

In practice, we perform a gradient descent with line search over $\mathrm{O}(n)$, with QR-retraction.

Remark: To apply this result in practice, one must have access to an explicit description of $\mathfrak{orb}(G, n)$.
We worked out the cases of $\mathrm{SO}(2)$, T^d, $\mathrm{SO}(3)$ and $\mathrm{SU}(2)$.



1. Lie group - Lie algebra correspondence
2. Closest Lie algebra problem
3. Examples
4. Proof of robustness

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.

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.

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.

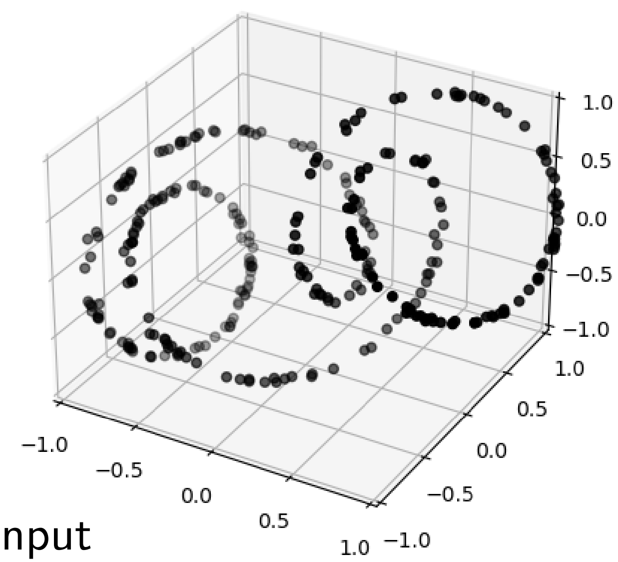
Example: Let $X \subset \mathbb{R}^4$ be a 300-sample of

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

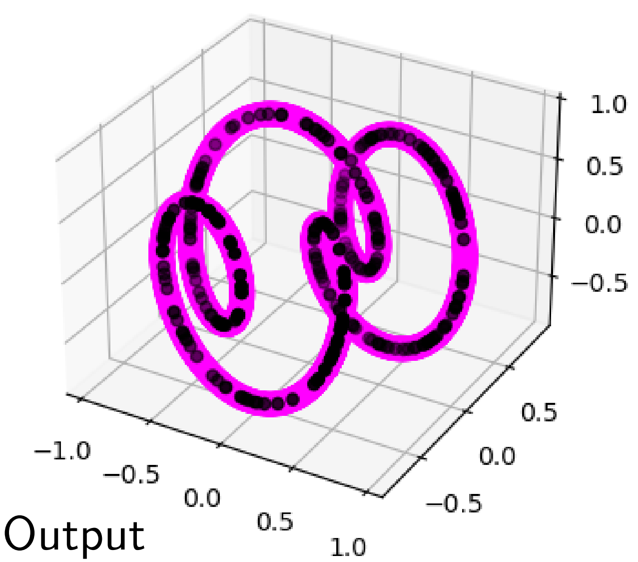
It is an orbit of $\mathrm{SO}(2)$ for the representation $\phi\colon \mathrm{SO}(2) \to \mathrm{M}_4(\mathbb{R})$ defined as

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

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



Input



Output

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

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

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

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

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

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:

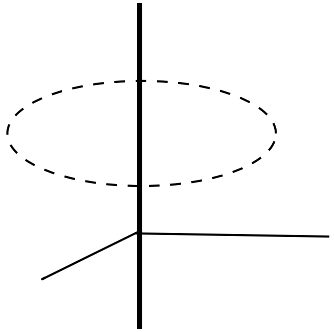
- reducing the computational cost of the next steps,
- avoiding numerical errors, when computing the pseudo-inverse of $\Sigma[X]$,
- ensuring that we will estimate non-trivial representations.

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 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 $\mathrm{W}_2\left(\mu_X, \mu_{\widehat{\mathcal{O}}}\right)$.

Let $G = \mathrm{SO}(2)$, whose dimension is $d = 1$.

In this case, the output $\widehat{h}$ of Lie-PCA is a skew symmetric $n \times n$ matrix. Let us denote it A.

Suppose that n is even. The representations of $\mathrm{SO}(2)$ in $\mathbb{R}^n$ take the form

$$\phi_{(\omega_1,\dots,\omega_{n/2})}(\theta) = \begin{pmatrix} R(\omega_1\theta) & & \\ & \ddots & \\ & & R(\omega_{n/2}\theta) \end{pmatrix} \quad \text{where} \quad R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

and where $(\omega_1,\dots,\omega_{n/2}) \in \mathbb{Z}^{n/2}$. In practice, we fix a maximal frequence $\omega_{\mathsf{max}} \in \mathbb{N}$.

The corresponding pushforward Lie algebra is spanned by the matrix

$$B_{(\omega_1,\dots,\omega_{n/2})} = \begin{pmatrix} L(\omega_1) & & \\ & \ddots & \\ & & L(\omega_{n/2}) \end{pmatrix} \quad \text{where} \quad L(\omega) = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix}$$

In this context, the minimization problem reads

$$\min \left\|\mathsf{proj}[A] - \mathsf{proj}[OB_{(\omega_1,\dots,\omega_{n/2})}O^\top]\right\| \quad \text{s.t.} \quad \begin{cases} (\omega_1,\dots,\omega_{n/2}) \in \mathbb{Z}^{n/2}, \\ O \in \mathrm{O}(n). \end{cases}$$

This is equivalent to

$$\min \left\|A \pm OB_{(\omega_1,\dots,\omega_{n/2})}O^\top\right\| \quad \text{s.t.} \quad \begin{cases} (\omega_1,\dots,\omega_{n/2}) \in \mathbb{Z}^{n/2}, \\ O \in \mathrm{O}(n). \end{cases}$$

We recognize a **two-sided orthogonal Procrustes problem with one transformation**.

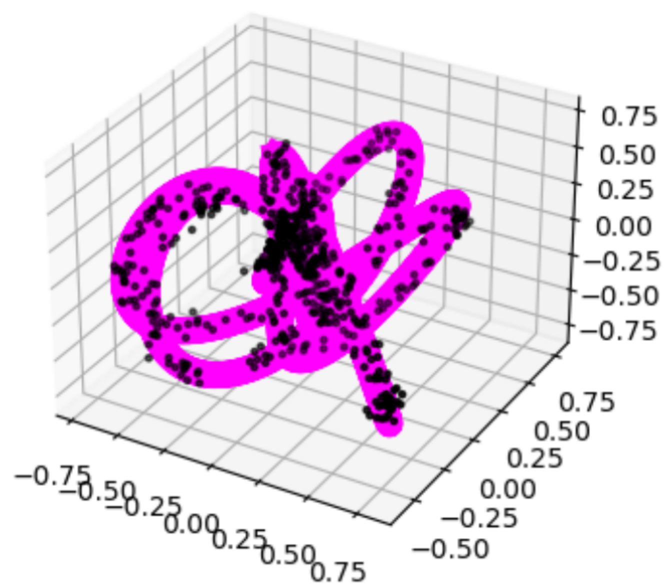
Example: We consider a representation of $\mathrm{SO}(2)$ in $\mathbb{R}^{10}$ with frequencies $(2,4,5,7,8)$ and sample 600 points on one of its orbits, that we corrupt with a Gaussian additive noise of deviation $\sigma = 0.03$.

We perform the minimization over all representations of $\mathrm{SO}(2)$ in $\mathbb{R}^{10}$, with parameter $\omega_{\max} = 10$.

Representation	$(2,4,5,7,8)$	$(2,5,6,8,9)$	$(3,5,7,9,10)$	$(3,6,7,9,10)$	$(3,5,6,8,9)$	$(2,4,5,6,7)$
Cost	$\mathbf{0.028}$	0.032	0.037	0.037	0.038	0.044
Representation	$(3,5,6,9,10)$	$(2,5,7,9,10)$	$(2,3,4,5,6)$	$(2,5,6,9,10)$	$(2,6,7,9,10)$	$(3,5,6,8,10)$
Cost	0.046	0.055	0.057	0.058	0.058	0.058

The correct representation is found.

As a sanity check, we compute the Hausdorff distance between the point cloud and the estimated orbit: $\mathrm{d_H}\big(X \mid \widehat{\mathcal{O}}\big) \approx 0.231$.



Step 3 - Case of T^d

Let $G = T^d$, the torus of dimension d.
In this case, the output $\widehat{h}$ of Lie-PCA is a d-tuple $(A_1, \dots, A_d)$ of skew symmetric $n \times n$ matrices.

The representations of T^d in $\mathbb{R}^n$ take the form

$$\phi_{(\omega_i^j)}(\theta_1, \dots, \theta_d) = \sum_{j=1}^d \phi_{(\omega_1^j, \dots, \omega_{n/2}^j)}(\theta_j)$$

where $(\omega_i^j)_{1 \le i \le n/2}^{1 \le j \le d}$ is a $n/2 \times d$ matrix with integer coefficients.

The push-forward Lie algebra is spanned by

$$B_{(\omega_1^1, \dots, \omega_{n/2}^1)}, \quad B_{(\omega_1^2, \dots, \omega_{n/2}^2)}, \quad \dots, \quad B_{(\omega_1^d, \dots, \omega_{n/2}^d)}.$$

In this context, the minimization problem reads

$$\min \left\| \text{proj}\left[\langle A_i \rangle_{j=1}^d\right] - \text{proj}\left[\langle O B_{(\omega_1^j, \dots, \omega_{n/2}^j)} O^\top \right] \rangle_{j=1}^d) \right\| \quad \text{s.t.} \quad \begin{cases} (\omega_i^j)_{1 \le i \le n/2}^{1 \le j \le d} \in \mathbb{Z}^{n/2 \times d}, \\ O \in \mathrm{O}(n). \end{cases}$$

This is linked to the **simultaneous reduction of a tuple of skew-symmetric matrices**.

Lemma: Denote by $(\rho_i)_{i=1}^d$ the coefficients of an optimal simultaneous reduction of the matrices $(A_i)_{i=1}^d$ in normal form. Then the problem is equivalent to

$$\min_{(\omega_i^j)} \sum_{k=1}^d f\left((\rho_i^k)_{i=1}^{n/2}, \ (\omega_i^k)_{i=1}^{n/2} \right) \qquad \text{where} \qquad f(x,y) = \left\| x/\|x\| - y/\|y\| \right\|^2.$$

We perform the simultaneous reduction via projected gradient descent over $\mathrm{O}(n)$.

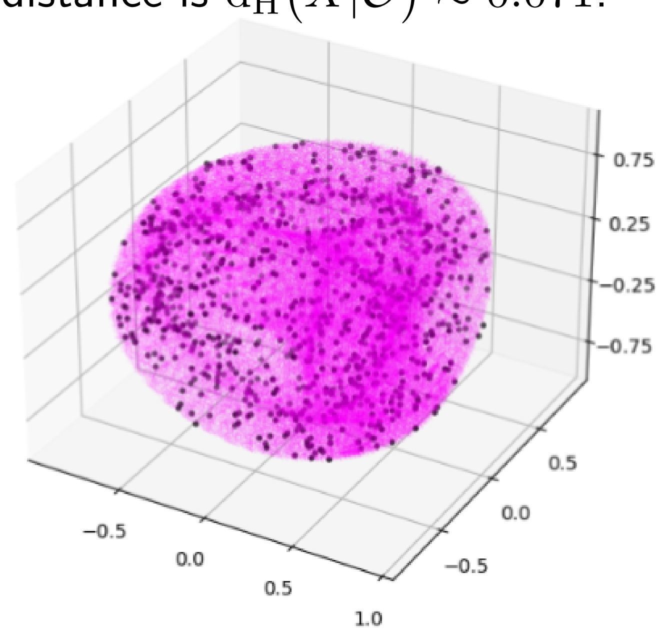
Example: Let X be a uniform 750-sample of an orbit of the representation $\phi_{\left(\begin{smallmatrix}1&1&2\\1&2&1\end{smallmatrix}\right)}$ of the torus T^2 in $\mathbb{R}^6$.

We apply the algorithm with $G = T^2$ on X, and restrict the representations to those with frequencies at most $\omega_{\max} = 2$.

Representation	$\left(\begin{smallmatrix}0&1&1\\2&-2&1\end{smallmatrix}\right)$	$\left(\begin{smallmatrix}1&1&2\\-2&2&-1\end{smallmatrix}\right)$	$\left(\begin{smallmatrix}0&1&2\\2&-2&-1\end{smallmatrix}\right)$	$\left(\begin{smallmatrix}0&1&1\\1&-2&0\end{smallmatrix}\right)$	$\left(\begin{smallmatrix}0&1&1\\1&-2&-1\end{smallmatrix}\right)$	$\left(\begin{smallmatrix}0&1&2\\2&-2&1\end{smallmatrix}\right)$
Cost	$\mathbf{0.036}$	0.136	0.198	0.233	0.244	0.312
Representation	$\left(\begin{smallmatrix}0&1&2\\1&-2&-2\end{smallmatrix}\right)$	$\left(\begin{smallmatrix}0&1&2\\1&-2&-1\end{smallmatrix}\right)$	$\left(\begin{smallmatrix}1&2&2\\-2&-2&1\end{smallmatrix}\right)$	$\left(\begin{smallmatrix}1&1&1\\-2&-1&2\end{smallmatrix}\right)$	$\left(\begin{smallmatrix}0&1&2\\1&-2&0\end{smallmatrix}\right)$	$\left(\begin{smallmatrix}0&1&1\\1&-2&1\end{smallmatrix}\right)$
Cost	0.331	0.348	0.388	0.447	0.457	0.472

The algorithm's output is $\left(\begin{smallmatrix}0&1&1\\2&-2&1\end{smallmatrix}\right)$, i.e., the representation $\phi_{\left(\begin{smallmatrix}0&1&1\\2&-2&1\end{smallmatrix}\right)}$. It is equivalent to $\phi_{\left(\begin{smallmatrix}1&1&2\\1&2&1\end{smallmatrix}\right)}$.

Moreover, the Hausdorff distance is $\mathrm{d_H}\left(X|\widehat{\mathcal{O}}\right) \approx 0.071$.



For $\mathrm{SO}(3)$ and $\mathrm{SU}(2)$, we have found no interesting reduction. We perform the minimization as is.

Example: Let X be a 3000-sample of the 3×3 special orthogonal matrices.

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

The irreps of $\mathrm{SU}(2)$ and $\mathrm{SO}(3)$ in $\mathbb{R}^n$ are parametrized by the partitions of n. 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 the (non-symmetric) Hausdorff distance $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}\big) \approx 2.658$.
In comparison, $\mathrm{d_H}\big(\widehat{\mathcal{O}}|X\big) \approx 0.543$.
This indicates that the representation is not transitive on X.

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

Step 3 - Case of $\mathrm{SO}(3)$ and $\mathrm{SU}(2)$

For $\mathrm{SO}(3)$ and $\mathrm{SU}(2)$, we have found no interesting reduction. We perform the minimization as is.

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

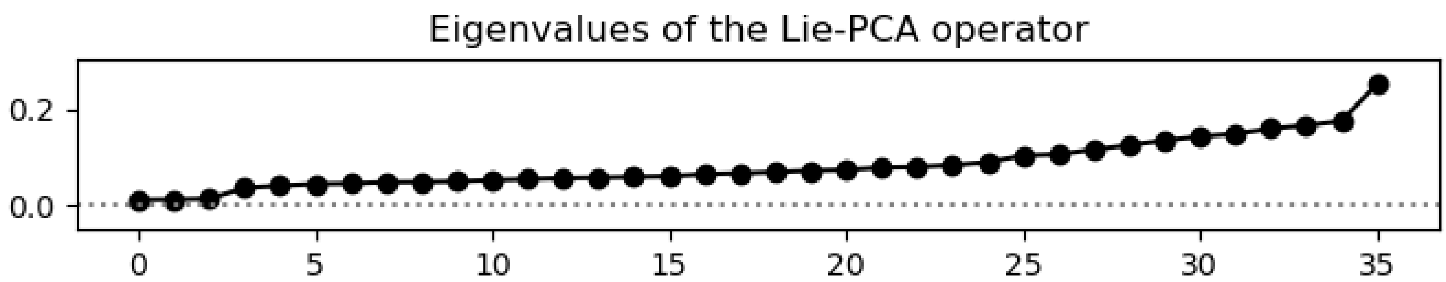
Representation $(3,3,3)$: $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}\big) \approx 0.061$.

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

When the underlying group is unknown, we can guess it from Lie-PCA, or test several candidates.

Example: Let X be a 1500-sample of an orbit of the representation $(1,5)$ of $\mathrm{SU}(2)$ in $\mathbb{R}^6$.

The Lie-PCA operator looks like:



We see a Lie algebra of dimension 3. One expects the torus T^3, $\mathrm{SO}(3)$ or $\mathrm{SU}(2)$.

Representation of $\mathrm{SU}(2)$	$(1,5)$	$(1,1,1,3)$	$(1,1,4)$	$(3,3)$
Cost	$\mathbf{8.6 \times 10^{-5}}$	0.007	0.008	0.015

Representation of T^3	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
Cost	$\mathbf{0.014}$

Representation $(1,5)$: we get the (non-symmetric) Hausdorff distance $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}\big) \approx 0.062$.

Representation $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$: we get the (non-symmetric) Hausdorff distance $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}\big) \approx 0.751$.

1. Lie group - Lie algebra correspondence
2. Closest Lie algebra problem
3. Examples
4. Proof of robustness

Measure-theoretic point of view

Input: $X = \{x_1 \ldots, x_N\} \subset \mathbb{R}^n$ 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 $\Lambda\colon A \mapsto \frac{1}{N}\sum_{i=1}^{N} \widehat{\Pi}\big[\mathrm{N}_{x_i}X\big] \cdot A \cdot \Pi\big[\langle x_i\rangle\big]$

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

Step 3: **Solve** $\arg\min_{\widehat{h}} \left\|\Pi\big[\langle A_i\rangle_{i=1}^d\big] - \Pi\big[\widehat{\mathfrak{h}}\big]\right\|$ 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** $\widehat{\mathcal{O}}_x = \big\{\exp(A)x \mid A \in \widehat{h}\big\}$

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

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

Input: $X = \{x_1 \dots, x_N\} \subset \mathbb{R}^n$ 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** $\arg\min_{\widehat{h}} \left\|\Pi\big[\langle A_i \rangle_{i=1}^d\big] - \Pi\big[\widehat{\mathfrak{h}}\big]\right\|$ with $(A_i)_{i=1}^d$ bottom eigenvectors of Λ

$\arg\min_{\widehat{h}} \left\|\Pi\big[\langle A_i \rangle_{i=1}^d\big] - \Pi\big[\widehat{\mathfrak{h}}\big]\right\|$ 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 $\mathrm{W}_2\big(\mu_{\widehat{\mathcal{O}}_x}, \mu_{\mathcal{O}}\big)$ " $\leq$ " $\mathrm{W}_2(\mu, \mu_{\mathcal{O}})$

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.

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

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

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

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 $\Lambda_{\mathcal{O}}$

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 $\underline{\widehat{\phi} \text{ is equivalent to } \phi}$, and

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

bias-variance trade-off when estimating tangent spaces

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

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 $\Sigma[\mu_{\mathcal{O}}]$
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- r is the radius of local PCA (estimation of tangent spaces)
- λ the bottom nonzero eigenvalue of the ideal Lie-PCA operator $\Lambda_{\mathcal{O}}$

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

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

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 $\mathcal{O}$.

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:

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

Proof: Consequence of Davis-Kahan theorem, together with

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

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 equal 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., $\sigma^2_{\max}/\sigma^2_{\min} = 1$.

Stability: Comparing

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

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

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

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

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

where $Y = \{y \in X \mid \|y - x_i\| \le r\}$, 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

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

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

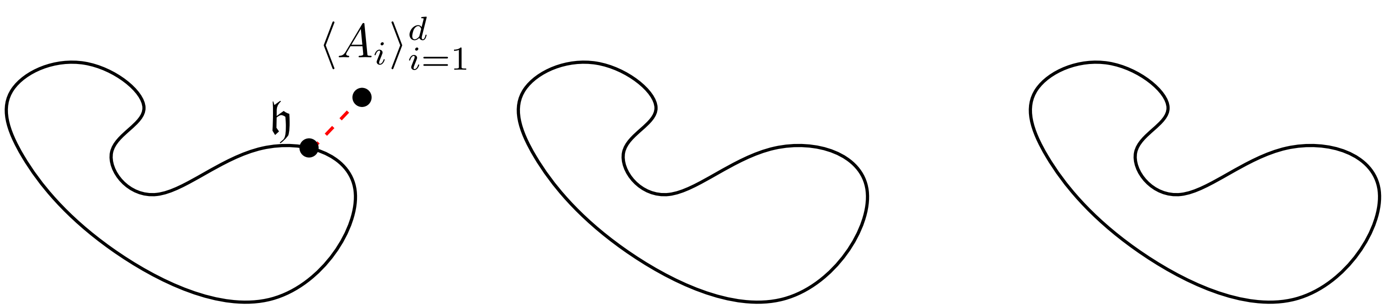
In Step 3, we consider the bottom eigenvectors $A_1, \ldots, A_d$ of Lie-PCA, and solve

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

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

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

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 representations
- 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 does not handle entangled orbits
- Restricted to **representations** of Lie groups

Next goals:

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

$$\begin{tikzcd} G \arrow[r, "\phi"] & \mathrm{Diff}(\mathcal{M}) \\ \mathfrak{g} \arrow[u, "\exp"] \arrow[r, "\mathrm{d}\phi"] & \mathscr{X}(\mathcal{M}) \arrow[u, "\exp"'] \end{tikzcd}$$

- Group Equivariant Convolutional Networks