

Erlangen AI Hub Seminar – 11/11/2025

## Linear orbits of compact Lie groups and machine learning

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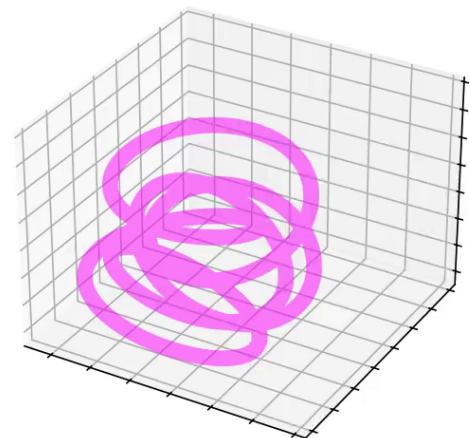
Raphaël Tinarrage – IST Austria



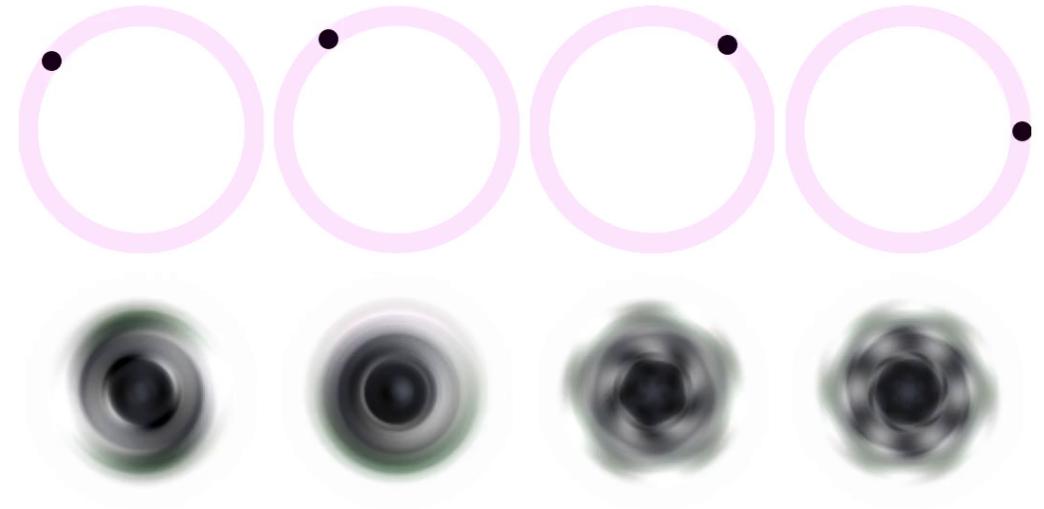
Rotations of  $m \times m$  RGB image



Embedding in  $\mathbb{R}^{m \times m \times 3}$



Projection in eigenplanes



Eigenvalues of the point cloud's covariance matrix:

311.2, 311.2, 221.3, 221.3, 82.3, 82.3, 79.4, 79.4, ...

In these eigenplanes, the orbit is close to

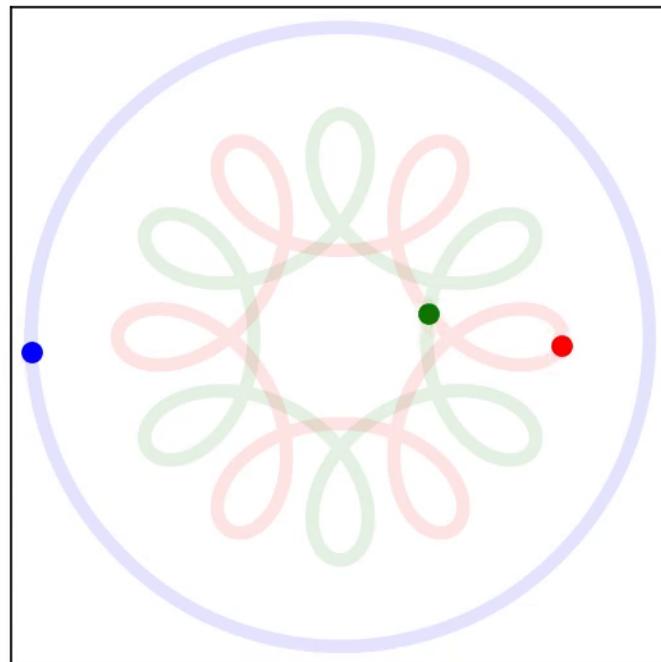
$$\theta \mapsto \begin{pmatrix} \mu_1 \cos \omega_1 \theta \\ \mu_1 \sin \omega_1 \theta \\ \mu_2 \cos \omega_2 \theta \\ \mu_2 \sin \omega_2 \theta \\ \vdots \\ \mu_k \cos \omega_k \theta \\ \mu_k \sin \omega_k \theta \end{pmatrix} = \begin{pmatrix} \cos \omega_1 \theta & -\sin \omega_1 \theta \\ \sin \omega_1 \theta & \cos \omega_1 \theta \\ & & \cos \omega_2 \theta & -\sin \omega_2 \theta \\ & & \sin \omega_2 \theta & \cos \omega_2 \theta \\ & & & & \ddots \\ & & & & \cos \omega_k \theta & -\sin \omega_k \theta \\ & & & & \sin \omega_k \theta & \cos \omega_k \theta \end{pmatrix} \begin{pmatrix} \mu_1 \\ 0 \\ \mu_2 \\ 0 \\ \vdots \\ \mu_k \\ 0 \end{pmatrix}$$

In 1975, Roger Broucke found several periodic orbits.

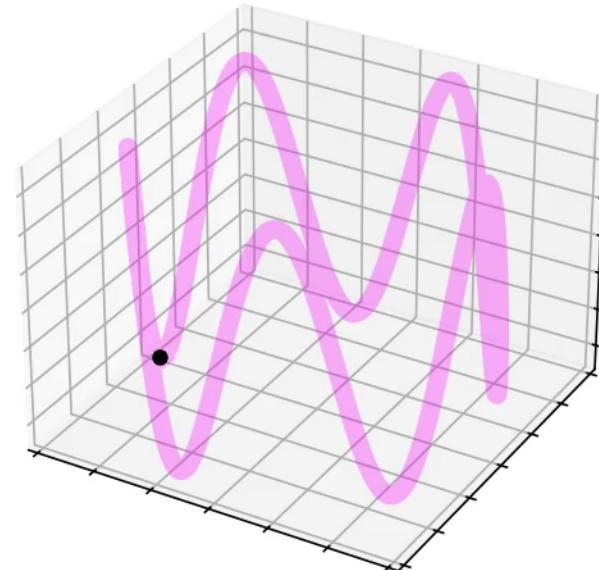
Let  $x_1(t)$ ,  $x_2(t)$ ,  $x_3(t)$  be the three bodies, and define  $z(t) = (x_1(t), x_2(t), x_3(t)) \in \mathbb{R}^6$ .

## Orbit A3

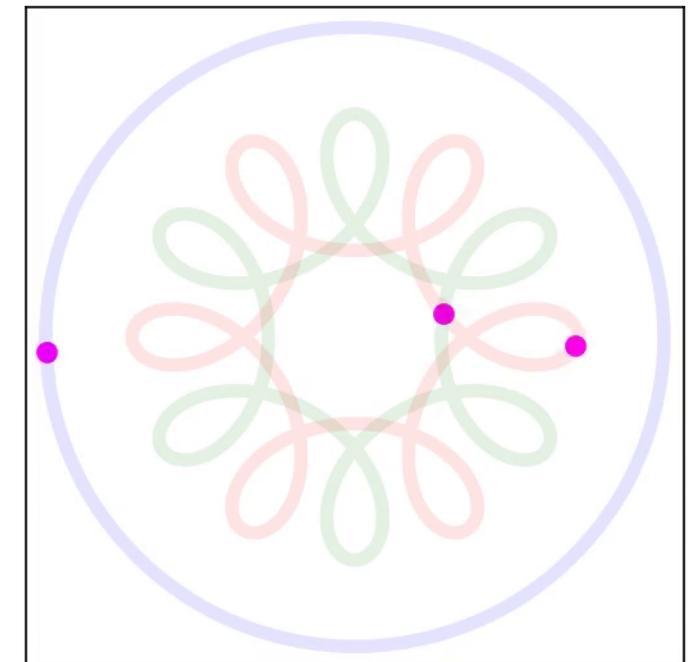
Trajectory of  $x_1, x_2, x_3$   
(found by integration)



Trajectory of  $z$



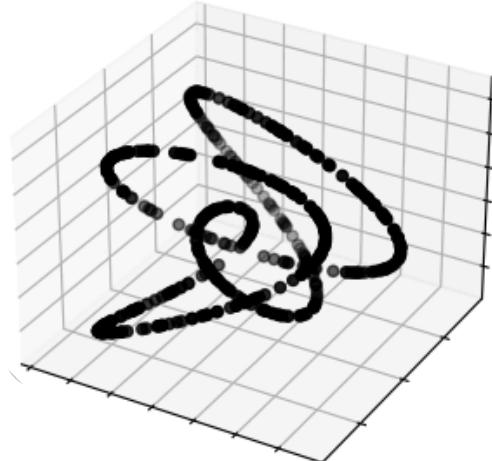
Reconstructed orbit of  $\text{SO}(2)$



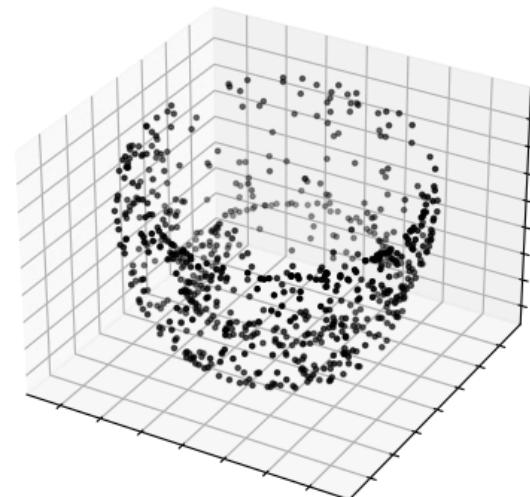
**Input:** A point cloud  $X = \{x_1, \dots, x_N\} \subset \mathbb{R}^n$ .

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

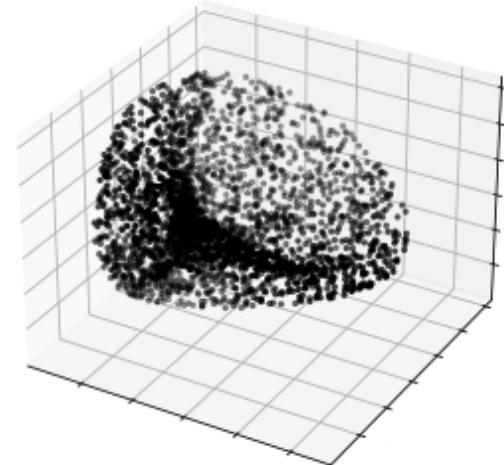
Orbit of  $\text{SO}(2)$  in  $\mathbb{R}^6$



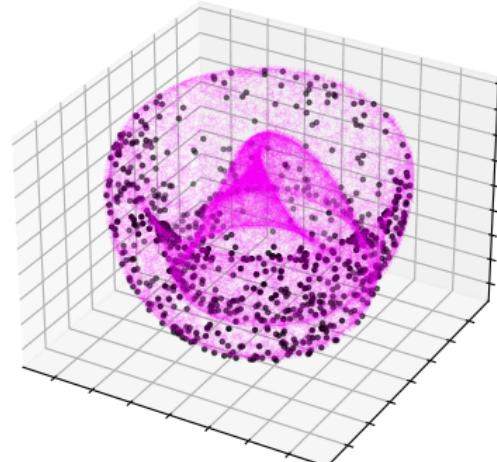
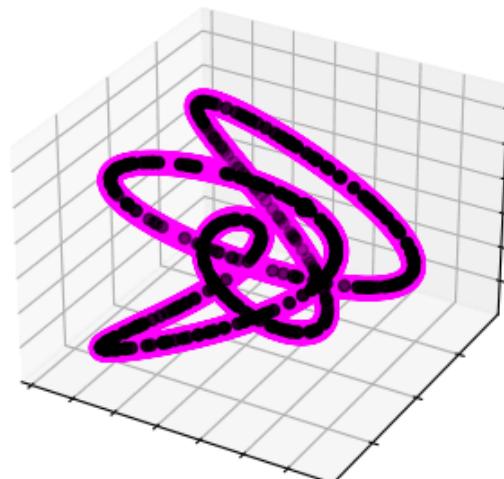
Orbit of  $T^2$  in  $\mathbb{R}^6$



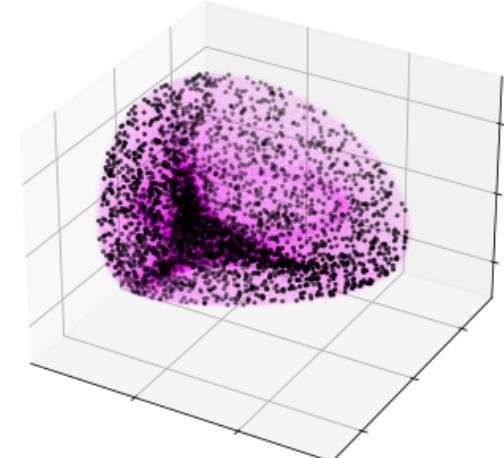
Orbit of  $\text{SO}(3)$  in  $\mathbb{R}^9$



**Input:**



**Output:**



A **Lie group** is a smooth manifold endowed with a group operation, and such that  $(g, h) \mapsto gh^{-1}$  is smooth.

- $\mathrm{GL}_n(\mathbb{R})$     general linear group: the  $n \times n$  invertible matrices.
- $\mathrm{O}(n)$     orthogonal group: the  $n \times n$  orthogonal matrices ( $A^\top = A^{-1}$ ).
- $\mathrm{SO}(n)$     special orthogonal group: the  $n \times n$  orthogonal matrices with determinant +1.
- $\mathrm{U}(n)$     unitary group:  $n \times n$  (complex) unitary matrices ( $A^* = A^{-1}$ ).
- $\mathrm{SU}(n)$     special unitary group:  $n \times n$  (complex) unitary matrices with determinant +1.
- $T^d$      $d$ -torus: the product  $\mathrm{SO}(2) \times \cdots \times \mathrm{SO}(2)$ .

A (real) **representation** of dimension  $n$  is a smooth homomorphism  $\phi: G \rightarrow \mathrm{GL}_n(\mathbb{R})$ .

- If  $G$  is a matrix group, the natural embedding  $G \rightarrow \mathrm{GL}_n(\mathbb{R})$  is a representation.
- For  $G = \mathrm{SO}(2)$  and  $\omega \in \mathbb{Z}$ , one has  $\theta \mapsto \begin{pmatrix} \cos \omega\theta & -\sin \omega\theta \\ \sin \omega\theta & \cos \omega\theta \end{pmatrix}$ .

A representation  $\phi: G \rightarrow \mathrm{GL}_n(\mathbb{R})$  is **irreducible** (irrep) if no non-trivial subspace  $V \subset \mathbb{R}^n$  is stabilized.

**Fact:** Every representation  $\phi$  is equivalent to a sum of irreps. That is, one has a decomposition  $\mathbb{R}^n = V_1 \oplus \cdots \oplus V_k$ , irreps  $\phi_i: G \rightarrow V_i$  and a change of basis  $A \in \mathrm{GL}_n(\mathbb{R})$  such that

$$A\phi A^{-1} = \phi_1 \oplus \cdots \oplus \phi_k.$$

Irreps can be explicitly enumerated:

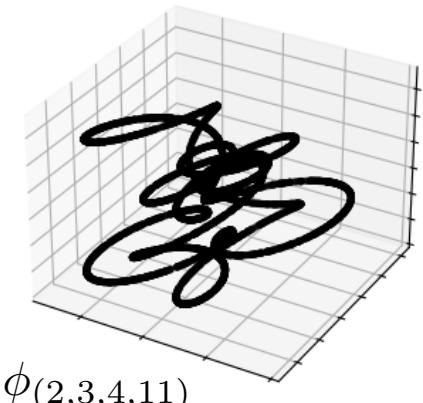
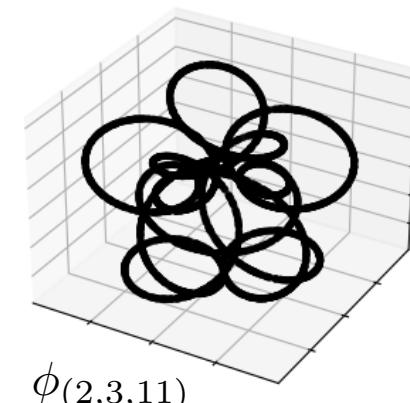
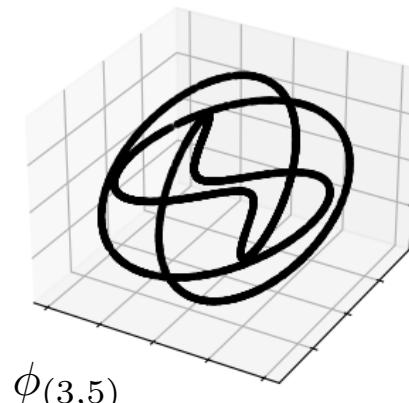
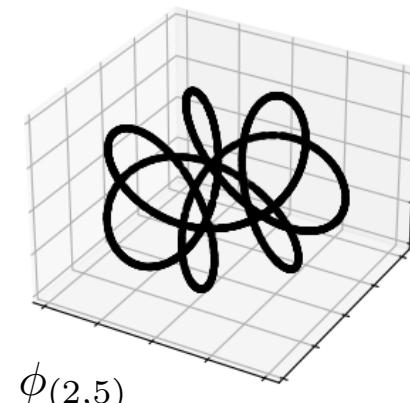
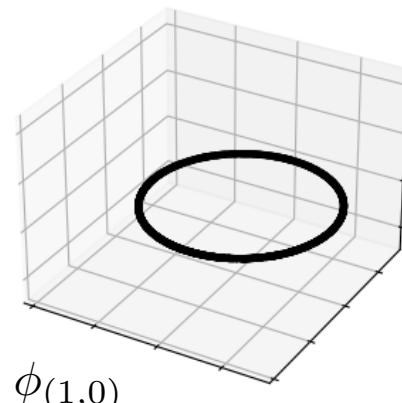
- $\mathrm{SO}(2)$       the  $\theta \mapsto R(\omega\theta)$  for  $\omega \in \mathbb{Z} \setminus \{0\}$ , where  $R(\theta) \mapsto \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$ .
- $T^d$       the  $(\theta_i)_{i=1}^d \mapsto R(\sum_{i=1}^d \omega_i \theta_i)$  for  $(\omega_i)_{i=1}^d \in \mathbb{Z}^d \setminus \{0\}$ .
- $\mathrm{SO}(3)$       one irrep in  $\mathbb{R}^n$  for  $n$  odd.
- $\mathrm{SU}(2)$       one irrep in  $\mathbb{R}^n$  for  $n$  odd or  $n \equiv 0 \pmod{4}$ .

The **orbit** of  $x_0 \in \mathbb{R}^n$  under a representation  $\phi: G \rightarrow \mathrm{GL}_n(\mathbb{R})$  is  $\mathcal{O} = \{\phi(g)x_0 \mid g \in G\}$ .

Example: Orbits of  $\mathrm{SO}(2)$  in  $\mathbb{R}^{2k}$ .

Let us write  $\phi \simeq \phi_{\omega_1} \oplus \cdots \oplus \phi_{\omega_k}$ . The orbit is made of the points

$$\phi(\theta)x_0 = \begin{pmatrix} \cos \omega_1 \theta & -\sin \omega_1 \theta \\ \sin \omega_1 \theta & \cos \omega_1 \theta \\ & \ddots \\ & & \cos \omega_2 \theta & -\sin \omega_2 \theta \\ & & \sin \omega_2 \theta & \cos \omega_2 \theta \\ & & & \ddots \\ & & & & \cos \omega_k \theta & -\sin \omega_k \theta \\ & & & & \sin \omega_k \theta & \cos \omega_k \theta \end{pmatrix} x_0$$



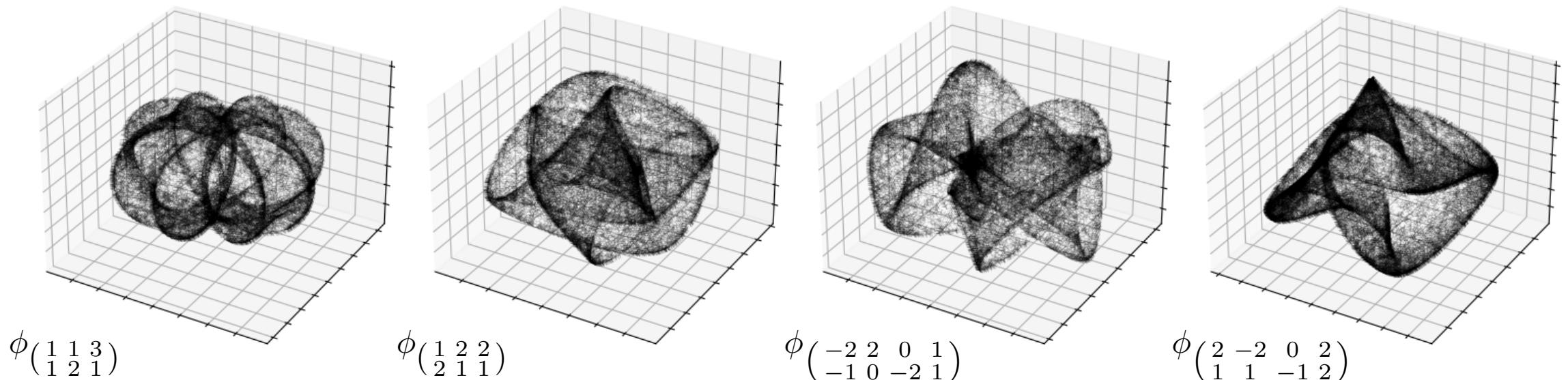
The **orbit** of  $x_0 \in \mathbb{R}^n$  under a representation  $\phi: G \rightarrow \mathrm{GL}_n(\mathbb{R})$  is  $\mathcal{O} = \{\phi(g)x_0 \mid g \in G\}$ .

Example: Orbits of  $T^2$  in  $\mathbb{R}^{2k}$ .

Let us write

$$\phi \simeq \phi \begin{pmatrix} \omega_1^{(1)} \\ \omega_1^{(2)} \end{pmatrix} \oplus \cdots \oplus \phi \begin{pmatrix} \omega_k^{(1)} \\ \omega_k^{(2)} \end{pmatrix}$$

One builds the integer matrix of weights  $\begin{pmatrix} \omega_1^{(1)} & \dots & \omega_k^{(1)} \\ \omega_1^{(2)} & \dots & \omega_k^{(2)} \end{pmatrix}$ .



The **orbit** of  $x_0 \in \mathbb{R}^n$  under a representation  $\phi: G \rightarrow \mathrm{GL}_n(\mathbb{R})$  is  $\mathcal{O} = \{\phi(g)x_0 \mid g \in G\}$ .

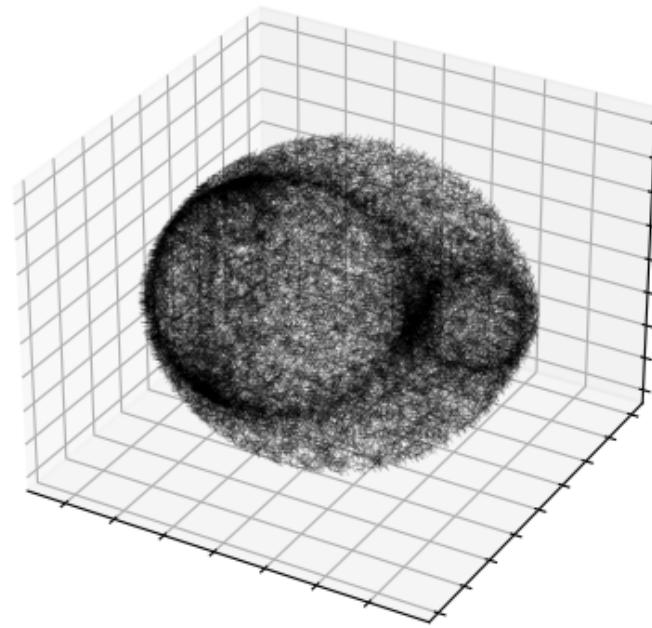
Example: Orbits of  $\mathrm{SO}(3)$  and  $\mathrm{SU}(2)$  in  $\mathbb{R}^n$ .

$\mathrm{SO}(3)$  has a finite number of (equivalence classes) of representations in  $\mathbb{R}^n$ : one for each decomposition

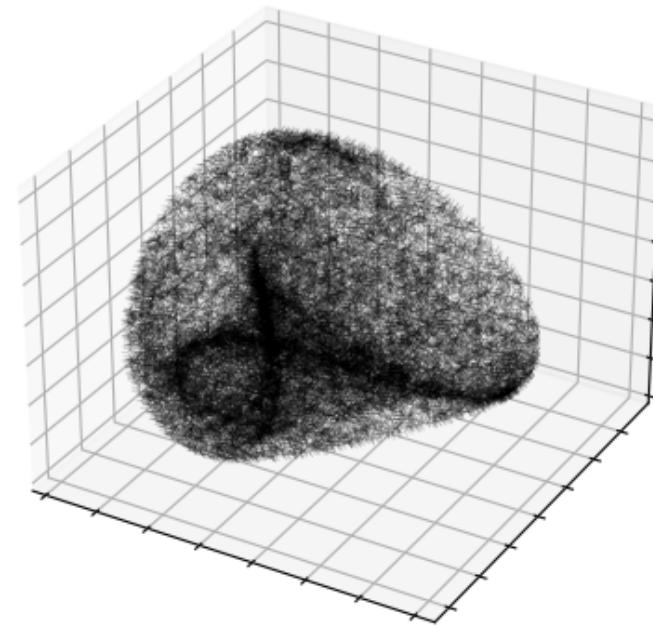
$$n = \omega_1 + \cdots + \omega_k$$

where the  $\omega_i$  are odd.

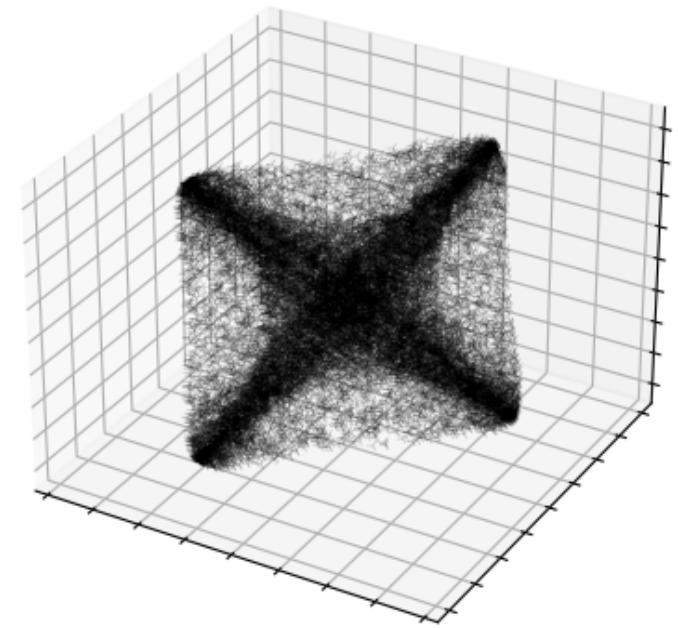
For  $\mathrm{SU}(2)$ , one can also use multiples of 4.



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



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



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

Say we observe an orbit  $\mathcal{O}$  of a representation  $\phi_1: G \rightarrow \mathrm{GL}_n(\mathbb{R})$ , and we want to find  $\phi_1$ .

Identifiability problem: another representation  $\phi_2$  may generate  $\mathcal{O}$ .

$$\begin{aligned} \phi_1: \theta &\mapsto \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} & \phi_2: \theta &\mapsto \begin{pmatrix} \cos 2\theta & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix} \end{aligned}$$

The representations are said **orbit-equivalent** if there exists a  $A \in \mathrm{GL}_n(\mathbb{R})$  such that for all  $x_0 \in \mathbb{R}^n$ ,

$$\underbrace{\{A\phi_1(g)A^{-1}x_0 \mid g \in G\}}_{\text{orbit of } x_0 \text{ under } A\phi_1 A^{-1}} = \underbrace{\{\phi_2(g)x_0 \mid g \in G\}}_{\text{orbit of } x_0 \text{ under } \phi_2}.$$

The orbit-equivalence classes of representations of:

- $\mathrm{SO}(2)$  in  $\mathbb{R}^{2k}$  are the (non-negative, non-decreasing) primitive  $k$ -tuples of integers.
- $T^d$  in  $\mathbb{R}^{2k}$  are the primitive lattices in  $\mathbb{Z}^k$  of rank  $\leq d$ .

For  $\mathrm{SO}(3)$  and  $\mathrm{SU}(2)$ , equivalence and orbit-equivalence coincide.

A Lie group  $G$  admits a **Lie algebra**, denoted  $\mathfrak{g}$ . It is a vector space endowed with a **Lie bracket**  $\mathfrak{g} \times \mathfrak{g} \rightarrow \mathfrak{g}$ .

For  $G \subset M_n(\mathbb{R})$ ,  $\mathfrak{g}$  is the tangent space of  $G$  at identity, and the bracket is the commutator  $[A, B] = AB - BA$ .

- $GL_n(\mathbb{R}) \quad \mathfrak{gl}(n)$  is the set of  $n \times n$  matrices.
- $SO(n) \quad \mathfrak{so}(n)$  is the set of  $n \times n$  skew-symmetric matrices.
- $T^n \quad t^n$  is the set of  $2n \times 2n$  skew-symmetric matrices that are  $2 \times 2$  block-diagonal.

One has an **exponential map**  $\exp: \mathfrak{g} \rightarrow G$ . Is it surjective when  $G$  is connected and compact.

Given a representation  $\phi: G \rightarrow \mathrm{GL}_n(\mathbb{R})$ , one builds the **derived homomorphism**  $d\phi$ :

$$\begin{array}{ccc} G & \xrightarrow{\phi} & \mathrm{GL}_n(\mathbb{R}) \\ \exp \uparrow & & \uparrow \exp \\ \mathfrak{g} & \xrightarrow{d\phi} & \mathfrak{gl}(n) \end{array}$$

We call  $d\phi(\mathfrak{g})$  the **pushforward** Lie algebra. It is a subalgebra of  $\mathfrak{gl}(n)$ .

**Fact:** Two representations  $\phi_1, \phi_2$  are orbit-equivalent iff there exists  $A \in \mathrm{GL}_n(\mathbb{R})$  such that

$$A d\phi_1(\mathfrak{g}) A^{-1} = d\phi_2(\mathfrak{g}).$$

Moduli space of Lie algebras: This is an invitation to work in

$$\mathcal{G}^{\mathrm{Lie}}(d, \mathfrak{gl}(n)) \diagup \mathrm{GL}_n(\mathbb{R})$$

where  $\mathcal{G}^{\mathrm{Lie}}(d, \mathfrak{gl}(n))$  is the Grassmannian of  $d$ -dimensional Lie subalgebras of  $\mathfrak{gl}(n)$ , acted upon by  $\mathrm{GL}_n(\mathbb{R})$ .

Denote  $\mathfrak{h} = \mathbf{d}\phi(\mathfrak{g})$ . There exists a intermediate space between  $\mathbf{d}\phi(\mathfrak{g}) \subset \mathfrak{gl}(n)$ .

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

**Symmetry group:**

$$\text{Sym}(\mathcal{O}) = \{P \in \text{GL}_n(\mathbb{R}) \mid P\mathcal{O} = \mathcal{O}\}$$

**Symmetry algebra:**

$$\mathfrak{sym}(\mathcal{O}) = \{P \in \mathfrak{gl}(n) \mid \exp(P) \in \text{Sym}(\mathcal{O})\}$$

Good news:  $\mathfrak{sym}(\mathcal{O})$  can be estimated from a finite sample of  $\mathcal{O}$ .

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

Temporary hypothesis: We will suppose that  $\mathbf{d}\phi(\mathfrak{g}) = \mathfrak{sym}(\mathcal{O})$ .

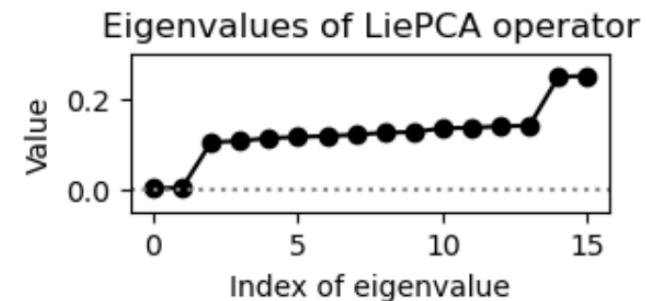
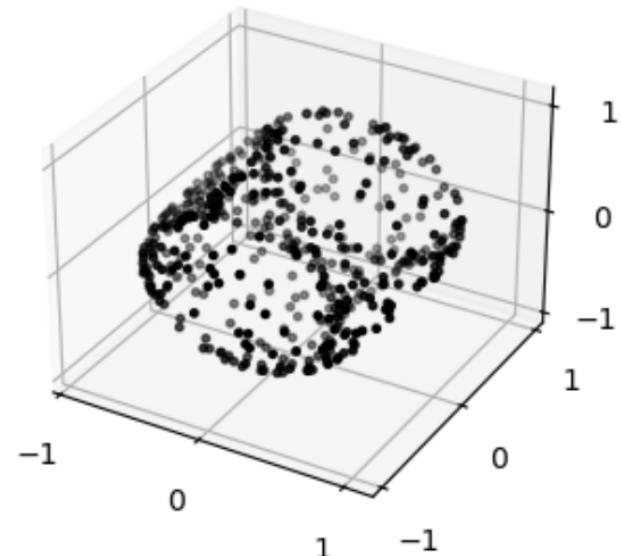
LiePCA operator: Say we observe  $X = \{x_1, \dots, x_N\} \subset \mathbb{R}^n$ , assumed close to  $\mathcal{O}$ .

Define  $\Lambda: M_n(\mathbb{R}) \rightarrow M_n(\mathbb{R})$  as 
$$\Lambda(A) = \frac{1}{N} \sum_{1 \leq i \leq N} \widehat{\Pi}[N_{x_i} X] \cdot A \cdot \Pi[\langle x_i \rangle]$$

where

- $\widehat{\Pi}[N_{x_i} X]$  are estimations of projection matrices onto the normal spaces  $N_{x_i} \mathcal{O}$ ,
- $\Pi[\langle x_i \rangle]$  are projection matrices on the lines  $\langle x_i \rangle$ .

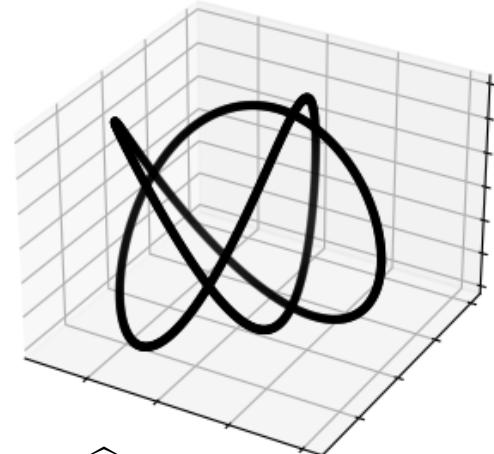
Lemma:  $\ker \Lambda \approx \mathfrak{sym}(\mathcal{O})$ .



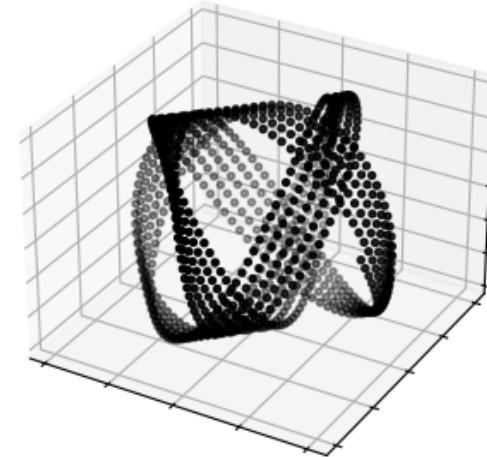
Define  $\widehat{\mathfrak{h}}$  as the subspace of  $\mathfrak{gl}(n)$  spanned by the  $d$  bottom eigenvectors of  $\Lambda$ .

What can go wrong:  $\widehat{\mathfrak{h}}$  is estimated as if it were a vector subspace.

- It may not be a Lie algebra ( $A, B \in \widehat{\mathfrak{h}} \implies AB - BA \in \widehat{\mathfrak{h}}$ ).
- It may not come from a compact Lie group.
- We still do not know what is the representation.



exact  $\widehat{\mathfrak{h}}$



inexact  $\widehat{\mathfrak{h}}$

We wish to find the Lie algebra closest to  $\widehat{\mathfrak{h}}$ . The problem reads

$$\min \left\{ d(\widehat{\mathfrak{h}}, V) \mid V \in \mathcal{G}^{\text{Lie}}(d, \mathfrak{gl}(n)) \right\}.$$

Remember that  $d\phi(\mathfrak{g}) \subset \mathfrak{sym}(\mathcal{O})$  and  $\ker \Lambda \approx \mathfrak{sym}(\mathcal{O})$  (LiePCA operator).

Case  $d\phi(\mathfrak{g}) = \mathfrak{sym}(\mathcal{O})$ : We compute the span  $\widehat{\mathfrak{h}}$  of bottom eigenvectors of  $\Lambda$ , and solve

$$\min \left\{ d(\widehat{\mathfrak{h}}, V) \mid V \in \mathcal{G}^{\text{Lie}}(d, \mathfrak{gl}(n)) \right\}.$$

Case  $d\phi(\mathfrak{g}) \subset \mathfrak{sym}(\mathcal{O})$ : We consider instead

$$\min \left\{ \sum_{i=1}^d \|\Lambda(A_i)\|^2 \mid \langle A_1, \dots, A_d \rangle = V \in \mathcal{G}^{\text{Lie}}(d, \mathfrak{gl}(n)) \right\}$$

**Tentative implementation:** Let us embed  $\mathcal{G}^{\text{Lie}}(d, \mathfrak{gl}(n)) \hookrightarrow M_{n^2}(\mathbb{R})$ , the  $n^2 \times n^2$  matrices, via  $V \mapsto \text{proj}[V]$ .

$$\min \text{tr}(\Lambda^2 P) \quad \text{such that} \quad \begin{cases} P \text{ is a } n^2 \times n^2 \text{ matrix,} \\ P^2 = P, \\ P^\top = P, \\ \text{rank}(P) = d, \\ \forall i, j \in [1 \dots, d], \quad P(Pe_i \cdot Pe_j - Pe_j \cdot Pe_i) = Pe_i \cdot Pe_j - Pe_j \cdot Pe_i. \end{cases}$$

Fix  $G$  and let  $\mathcal{G}(G, \mathfrak{gl}(n))$  be the  $d$ -dimensional Lie subalgebras of  $\mathfrak{gl}(n)$  that are pushforward of  $\mathfrak{g}$ .

The set  $\mathcal{G}(G, \mathfrak{gl}(n)) / \mathrm{GL}_n(\mathbb{R})$  is in correspondence with the orbit-equivalence classes of reps of  $G$  in  $\mathbb{R}^n$ .

Let  $\mathfrak{orb}(G, n)$  denote a choice of representatives.

**Lemma:** The optimization problem is equivalent to

$$\min \sum_{i=1}^d \left\| \Lambda(A \mathrm{diag}(B_i^k)_{k=1}^p A^{-1}) \right\|^2 \quad \text{such that} \quad \begin{cases} (B^1, \dots, B^p) \in \mathfrak{orb}(G, n), \\ A \in \mathrm{GL}_n(\mathbb{R}), \end{cases}$$

Any representation  $\phi: G \rightarrow \mathrm{GL}_n(\mathbb{R})$ , up to a change of basis, decomposes as  $\phi = \phi_1 \oplus \dots \oplus \phi_p$ .

By denoting  $B^i = d\phi_i(\mathfrak{g})$ , the element  $d\phi(\mathfrak{g})$  of  $\mathfrak{orb}(G, n)$  is associated to  $(B^1, \dots, B^p)$ .

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**Orthonormalization trick:** After a pre-processing step, we can reduce the program to  $A \in \mathrm{O}(n)$ .

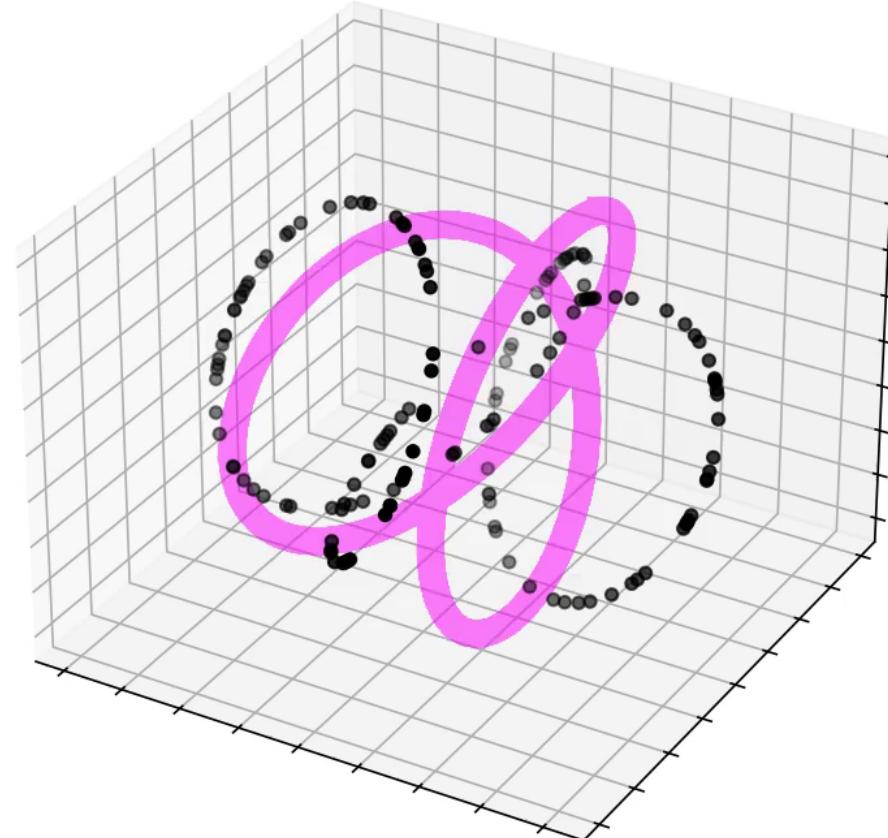
# Closest Lie algebra

9/15 (4/6)

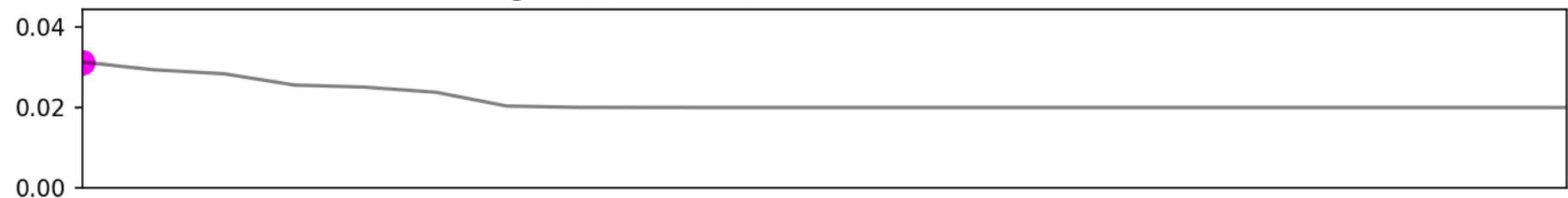
$\text{SO}(2)$ -orbit in  $\mathbb{R}^4$

Rep	Score
(1,2)	+1 : 0.020 -1 : 0.001
(1,3)	+1 : 0.017 -1 : $1 \times 10^{-5}$
(1,4)	+1 : 0.014 -1 : $4 \times 10^{-4}$
(2,3)	+1 : 0.020 -1 : 0.004
(3,4)	+1 : 0.022 -1 : 0.005

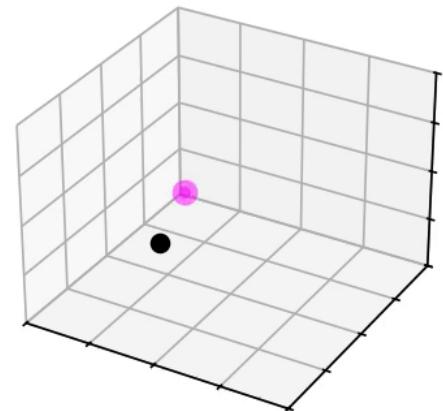
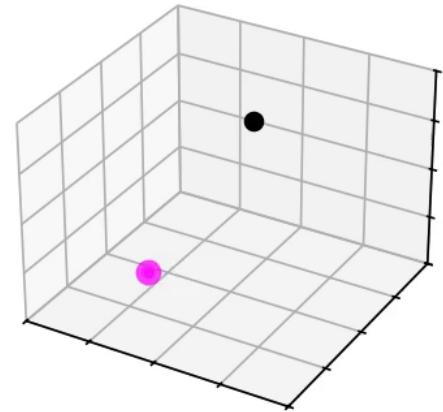
Generated orbit -  $d_H(X | \widehat{\mathcal{O}}_x) = 1.164$



Weights (1, 2) - Determinant +1 - Final cost 2.00e-02



Lie algebra



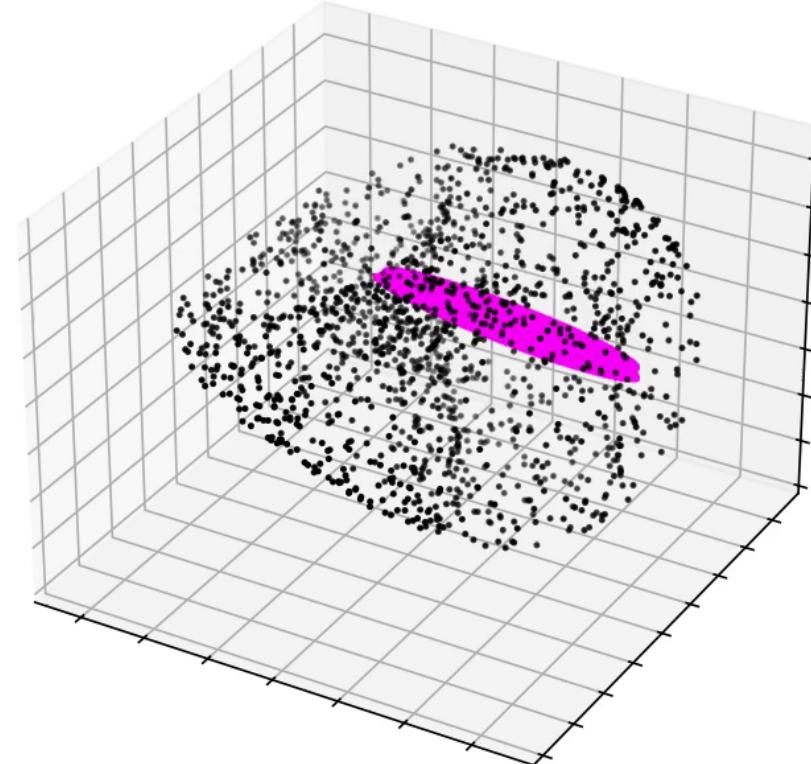
# Closest Lie algebra

9/15 (5/6)

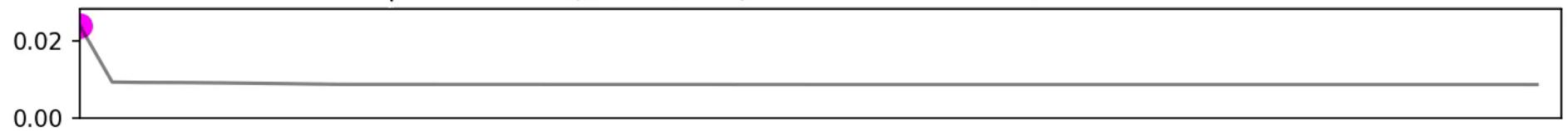
$SU(2)$ -orbit in  $\mathbb{R}^7$

Rep	Score
(3)	+1 : 0.008
(4)	+1 : 0.013
(5)	+1 : 0.003
(3,3)	+1 : 0.003
(3,4)	+1 : $3 \times 10^{-5}$
(7)	+1 : 0.005

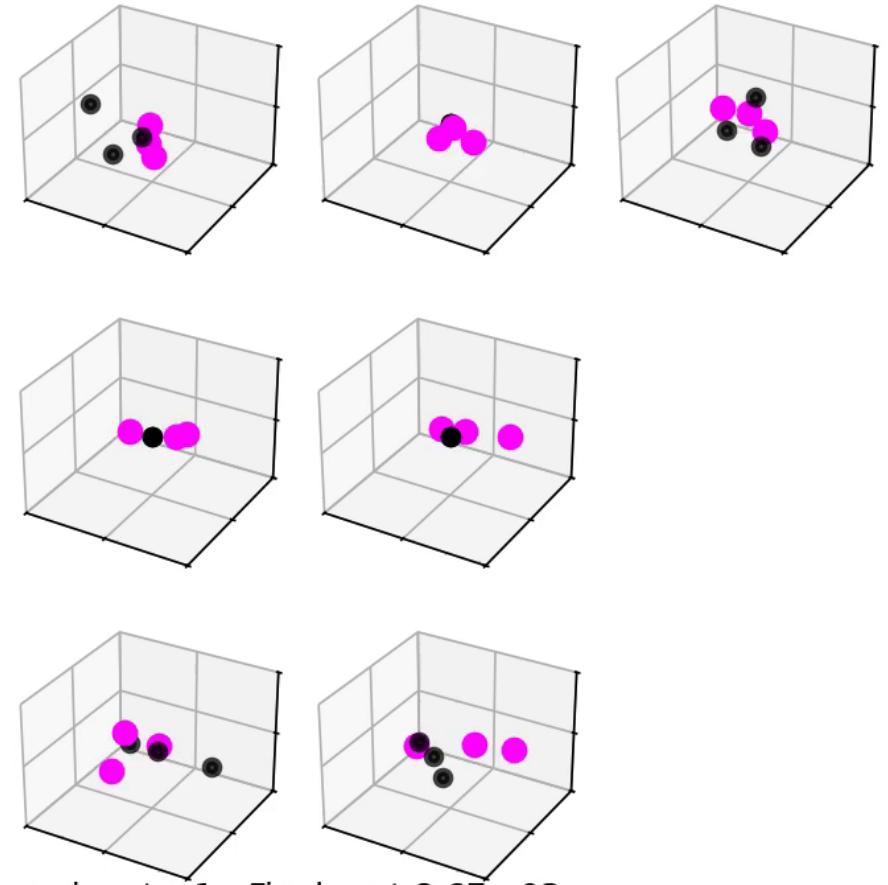
Generated orbit -  $d_H(X | \widehat{\mathcal{O}}_x) = 1.739$



Representation (1, 1, 1, 1, 3) - Determinant +1 - Final cost 8.67e-03



Lie algebra



Reformulation of the optimization program:

$$\min \left\{ d(\hat{\mathfrak{h}}, V) \mid V \in \mathcal{G}^{\text{Lie}}(d, \mathfrak{gl}(n)) \right\}.$$

reduces to:

- $\text{SO}(2)$  two-sided orthogonal Procrustes problem  $\longrightarrow$  reduction of skew-symmetric matrix
- $T^d$  simultaneous reduction of  $d$  skew-symmetric matrices  $\longrightarrow$  optimization over  $\text{O}(n)$
- $\text{SO}(3), \text{SU}(2)$  no reduction found

**Fact:** If  $G$  is compact, for every representation  $G \rightarrow \mathrm{GL}_n(\mathbb{R})$ , there exists  $M$  positive-definite such that

$$\forall g \in G, M\phi(g)M^{-1} \in \mathrm{O}(n).$$

Given an orbit  $\mathcal{O} = G \cdot x_0$ , consider the Haar measure  $\mu_G$ , and define the **covariance matrix**

$$\Sigma[\mathcal{O}] = \int_G (\phi(g)x_0)(\phi(g)x_0)^\top d\mu_G(g).$$

$M$  is found as the square root of the Moore-Penrose pseudo-inverse:

$$M[\mathcal{O}] = \sqrt{\Sigma[\mathcal{O}]^+}.$$

Given a sample  $X$ , we build  $\Sigma[X] = \frac{1}{N} \sum_{i=1}^N x_i x_i^\top$  and  $M[X] = \sqrt{\Sigma[X]^+}$ .

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

$$\phi: t \mapsto \mathrm{diag}\left(\begin{pmatrix} \cos t & -(1/2)\sin t \\ 2\sin t & \cos t \end{pmatrix}, \begin{pmatrix} \cos 4t & -\sin 4t \\ \sin 4t & \cos 4t \end{pmatrix}\right), \quad \mathcal{O} = \{(\cos t, 2\sin t, \cos 4t, \sin 4t) \mid t \in [0, 2\pi]\}.$$

$$M\phi M^{-1}: t \mapsto \mathrm{diag}\left(\begin{pmatrix} \cos t & \sin t \\ \sin t & \cos t \end{pmatrix}, \begin{pmatrix} \cos 4t & -\sin 4t \\ \sin 4t & \cos 4t \end{pmatrix}\right), \quad M\mathcal{O} = \left\{\frac{1}{\sqrt{2}}(\cos t, \sin t, \cos 4t, \sin 4t) \mid t \in [0, 2\pi]\right\}.$$

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

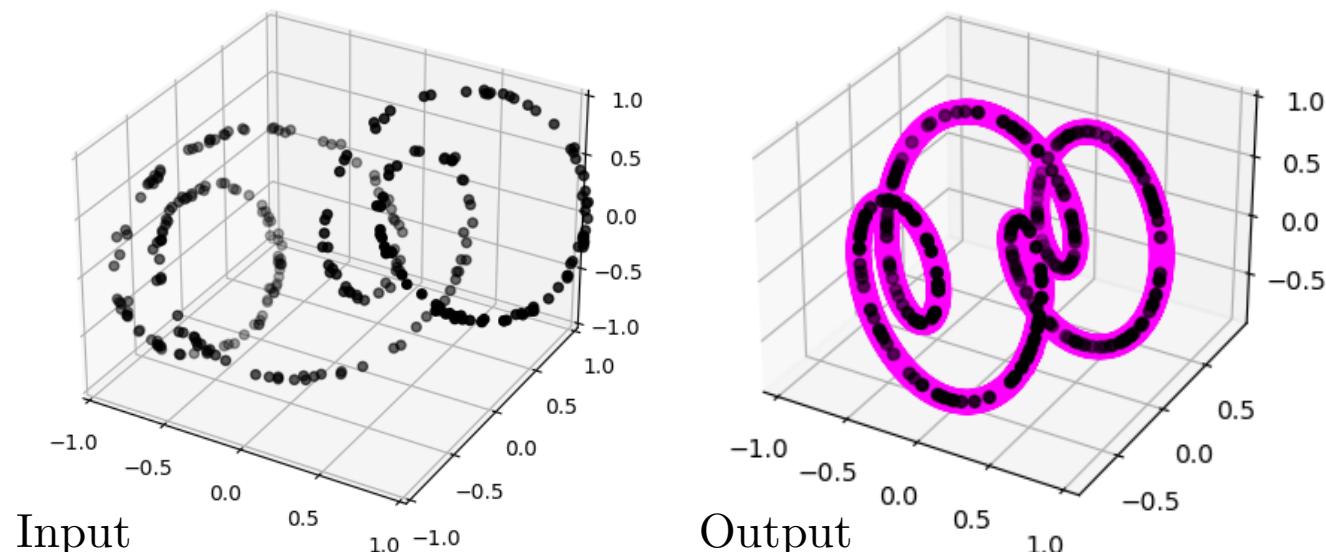
**Output:** A representation  $\phi$  of  $G$  in  $\mathbb{R}^n$ , and an orbit  $\mathcal{O}$  close to  $X$ .

**Step 1 (Orthonormalization):** Reduce the dimension and orthonormalize the orbit.

**Step 2 (LiePCA):** Diagonalize the operator  $\Lambda: M_n(\mathbb{R}) \rightarrow M_n(\mathbb{R})$ .

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

**Step 4 (Distance to orbit):** Choose a  $x \in X$ , generate  $\widehat{\mathcal{O}}_x = \exp(\widehat{\mathfrak{h}}) \cdot x$  and verify that it is close to  $X$ .



In **Step 4**, we compute the (non-symmetric) Hausdorff distance  $d_H(X | \widehat{\mathcal{O}}_x)$ .

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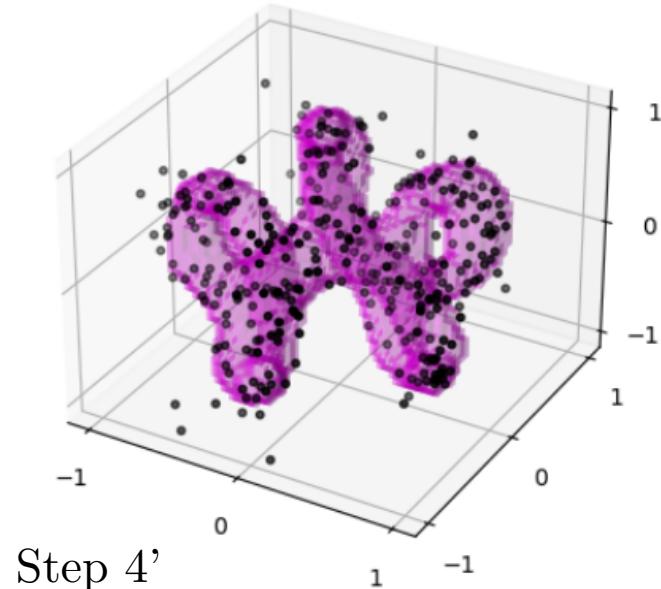
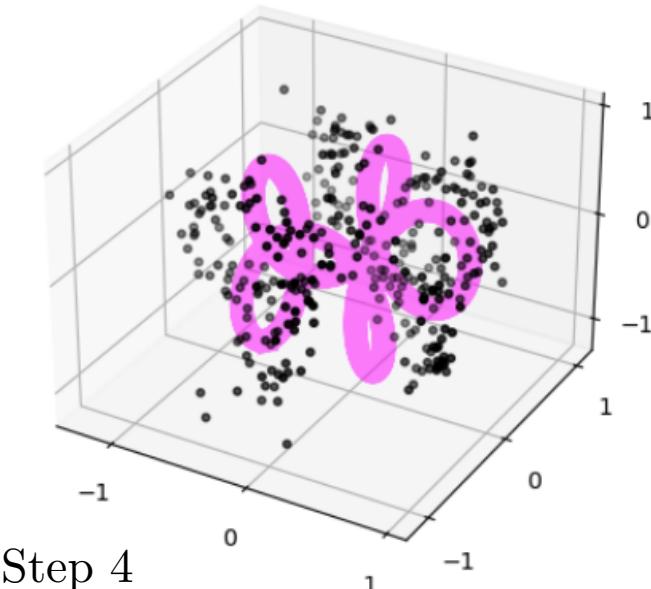
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**Step 4 (Distance to orbit):** Choose a  $x \in X$ , generate  $\widehat{\mathcal{O}}_x = \exp(\widehat{\mathfrak{h}}) \cdot x$  and verify that it is close to  $X$ .

**Step 4' (Distance to noisy orbit):** Build the measure  $\mu_{\widehat{\mathcal{O}}} = \frac{1}{N} \sum_{x \in X} \mu_{\widehat{\mathcal{O}}_x}$  and verify that it is close to  $\mu_X$ .



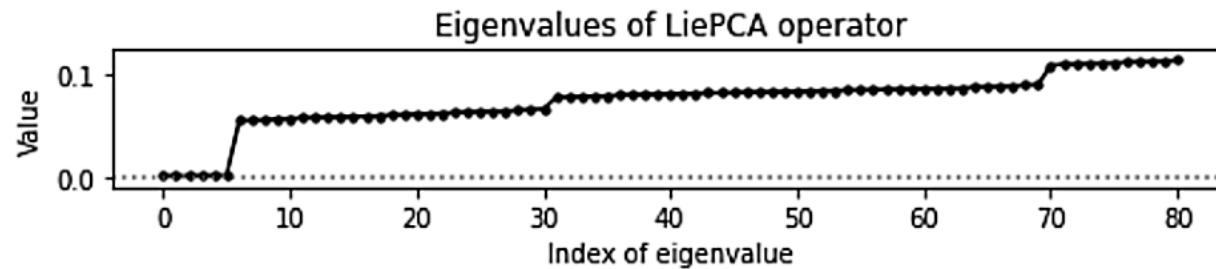
In **Step 4**, we compute the (non-symmetric) Hausdorff distance  $d_H(X | \widehat{\mathcal{O}}_x)$ .

In **Step 4'**, we compute the Wasserstein distance  $W_2(\mu_X, \mu_{\widehat{\mathcal{O}}})$ .

Example: Embed  $\text{SO}(3) \hookrightarrow \mathbb{R}^9$  and sample 3000 points on it.

LiePCA shows a kernel of dimension 6.

This is consistent with  $\text{Isom}(\text{SO}(3)) \simeq \text{SO}(3) \times \text{SO}(3) \times \{\pm 1\}$



We look for an action of  $\text{SO}(3)$  or  $\text{SU}(2)$ . **Step 3** yields

Representation	(3, 5)	(3, 3, 3)	(4, 5)	(8)	(5)	(7)
Cost	<b><math>2 \times 10^{-5}</math></b>	<b><math>4 \times 10^{-5}</math></b>	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

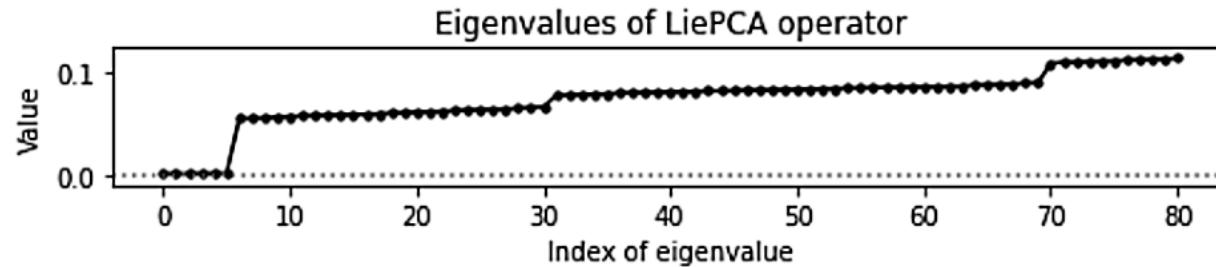
Representation (3, 5):  $d_H(X|\widehat{\mathcal{O}}_x) \approx 2.658$ . However,  $d_H(\widehat{\mathcal{O}}_x|X) \approx 0.543$ .

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

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Representation (3, 5):  $d_H(X|\widehat{\mathcal{O}}_x) \approx 2.658$ . However,  $d_H(\widehat{\mathcal{O}}_x|X) \approx 0.543$ .

action  $\text{SO}(3) \curvearrowright \text{SO}(3)$  by conjugation (not transitive)

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

action  $\text{SO}(3) \curvearrowright \text{SO}(3)$  by translation (transitive)

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

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

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

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

**Step 3:** Solve  $\arg \min \sum_{i=1}^d \|\Lambda(A_i)\|^2$   
with  $(A_i)_{i=1}^d \in \mathcal{V}^{\text{Lie}}(G, \mathfrak{so}(n))$

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

**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.

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

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

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

**Step 1:** Orthonormalization via

$$X \leftarrow \sqrt{\Sigma[X]^+} \cdot \Pi_{\Sigma[X]}^{>\epsilon} \cdot X$$

$$\mu \leftarrow \sqrt{\Sigma[\mu]^+} \cdot \Pi_{\Sigma[\mu]}^{>\epsilon} \cdot \mu$$

**Step 2:** Diagonalize the operator

$$\Lambda: A \mapsto \frac{1}{N} \sum_{i=1}^N \widehat{\Pi}[\mathbf{N}_{x_i} X] \cdot A \cdot \Pi[\langle x_i \rangle]$$

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

**Step 3:** Solve  $\arg \min \sum_{i=1}^d \|\Lambda(A_i)\|^2$   
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$$\arg \min \sum_{i=1}^d \|\Lambda[\mu](A_i)\|^2$$

with  $(A_i)_{i=1}^d \in \mathcal{V}^{\text{Lie}}(G, \mathfrak{so}(n))$

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

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

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

Show that  $W_2(\mu_{\widehat{\mathcal{O}}_x}, \mu_{\mathcal{O}})$  is small

**Theorem:** Under technical assumptions (sufficiently small  $W_2(\mu_X, \mu_{\mathcal{O}})$ ), for a certain choice of parameters, the algorithm outputs a representation  $\widehat{\phi}$  that is orbit-equivalent to  $\phi$ .

Let  $l = \dim \mathcal{O}$ . The output measure  $\mu_{\widehat{\mathcal{O}}}$  satisfies

$$W_2(\mu_{\widehat{\mathcal{O}}}, \mu_{\mathcal{O}}) \leq \text{const} \cdot W_2(\mu_X, \mu_{\mathcal{O}})^{1/4(l+3)}.$$

In addition, for all  $x \in X$ , the output orbit  $\widehat{\mathcal{O}}_x$  satisfies

$$d_H(\widehat{\mathcal{O}}_x, \mathcal{O}) \leq \text{const} \cdot d(x, \mathcal{O}) + \text{const} \cdot W_2(\mu_X, \mu_{\mathcal{O}})^{1/4(l+3)}.$$

**Theorem:** Let  $G$  be a compact Lie group of dimension  $d$ ,  $\mathcal{O}$  an orbit of an almost-faithful representation  $\phi: G \rightarrow \mathbb{R}^n$ , potentially non-orthogonal, and  $l$  its dimension. Let  $\mu_{\mathcal{O}}$  be the uniform measure on  $\mathcal{O}$ , and  $\mu_{\tilde{\mathcal{O}}}$  that on the orthonormalized orbit. Let  $X \subset \mathbb{R}^n$  be a finite point cloud and  $\mu_X$  its empirical measure.

Let  $\widehat{\phi}, \widehat{\mathfrak{h}}, \widehat{\mathcal{O}}_x, \mu_{\widehat{\mathcal{O}}}$  be the output of the algorithm. Under technical assumptions,  $\widehat{\phi}$  is orbit-equivalent to  $\phi$ , and

$$\begin{aligned}\|\Pi[\widehat{h}] - \Pi[\mathfrak{sym}(\mathcal{O})]\|_F &\leq 9d \frac{\rho}{\lambda} \left( r + 4 \left( \frac{\widetilde{\omega}}{r^{l+1}} \right)^{1/2} \right) \\ d_H(\widehat{\mathcal{O}}_x, \mathcal{O}) &\leq \sqrt{2} \frac{d(x, \mathcal{O})}{\sigma_{\min}} + 3\sqrt{dn} \left( \frac{\rho}{\lambda} \right)^{1/2} \left( r + 4 \left( \frac{\widetilde{\omega}}{r^{l+1}} \right)^{1/2} \right)^{1/2} \\ W_2(\mu_{\widehat{\mathcal{O}}}, \mu_{\tilde{\mathcal{O}}}) &\leq \frac{1}{\sqrt{2}} \frac{W_2(\mu_X, \mu_{\mathcal{O}})}{\sigma_{\min}} + 3\sqrt{dn} \left( \frac{\rho}{\lambda} \right)^{1/2} \left( r + 4 \left( \frac{\widetilde{\omega}}{r^{l+1}} \right)^{1/2} \right)^{1/2}\end{aligned}$$

where

- $\rho = 16l(l+2)6^l \max(\text{vol}(\tilde{\mathcal{O}}), \text{vol}(\tilde{\mathcal{O}})^{-1}) / \min(1, \text{reach}(\tilde{\mathcal{O}}))$ ,
- $\sigma_{\max}^2, \sigma_{\min}^2$  the top and bottom nonzero eigenvalues of the covariance matrix  $\Sigma[\mu_{\mathcal{O}}]$ ,
- $\widetilde{\omega} = 4(n+1)^{3/2} \left( \frac{\sigma_{\max}^3}{\sigma_{\min}^3} \right) \left( \omega(v+\omega) \right)^{1/2}$  with  $\omega = \frac{W_2(\mu_{\mathcal{O}}, \mu_X)}{\sigma_{\min}}$  and  $v = \left( \frac{\mathbb{V}[\|\mu_{\mathcal{O}}\|]}{\sigma_{\min}^2} \right)^{1/2}$ ,
- $r$  is the radius of local PCA (estimation of tangent spaces),
- $\lambda$  the bottom nonzero eigenvalue of the ideal Lie-PCA operator  $\Lambda_{\mathcal{O}}$ .

**Technical assumptions:** Define the quantities

$$\omega = \frac{W_2(\mu_{\mathcal{O}}, \mu_X)}{\sigma_{\min}}, \quad v = \left( \frac{\mathbb{V}[\|\mu_{\mathcal{O}}\|]}{\sigma_{\min}^2} \right)^{1/2},$$

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

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

Suppose that  $\omega$  is small enough, so as to satisfy

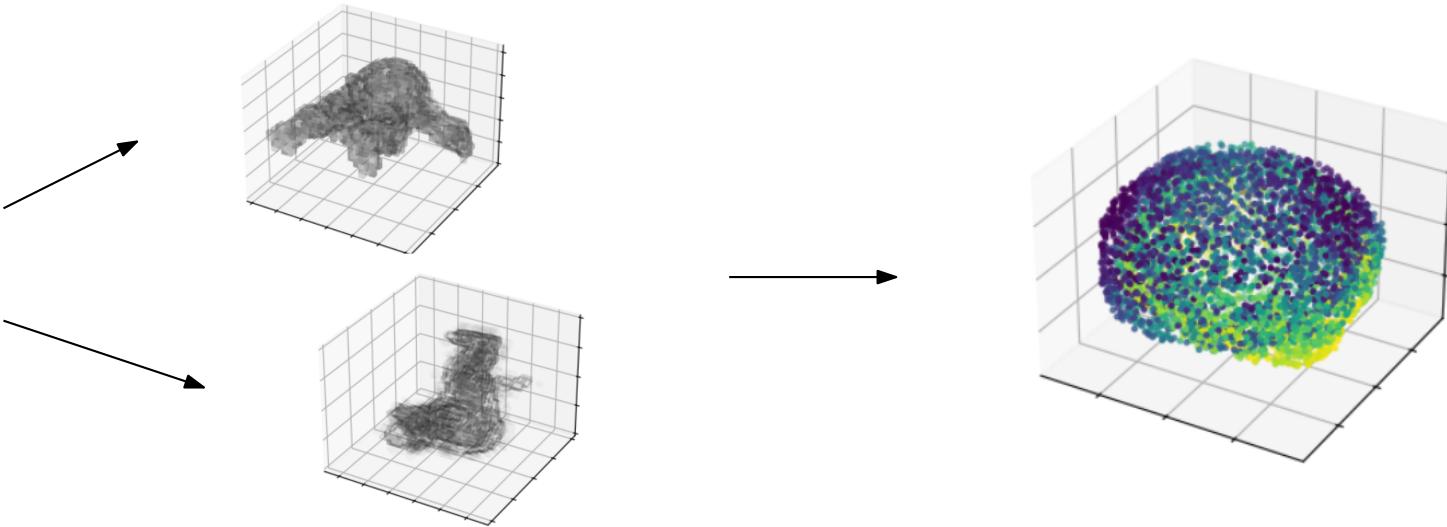
$$\omega < \left( \left( v^2 + \frac{1}{2} \right)^{1/2} - v \right) / \left( 3(n+1) \frac{\sigma_{\max}^2}{\sigma_{\min}^2} \right), \quad \tilde{\omega} \leq \min \left\{ \left( \frac{1}{6\rho} \right)^{3(l+1)}, \frac{\gamma^{l+3}}{16}, \left( \frac{\gamma}{(6\rho)^2} \right)^{l+1} \right\}.$$

Choose two parameters  $\epsilon$  and  $r$  in the following nonempty sets:

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

Moreover, we suppose that

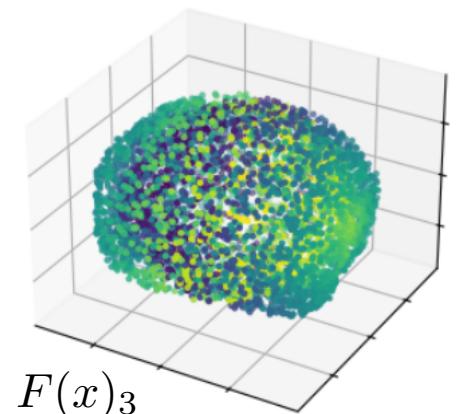
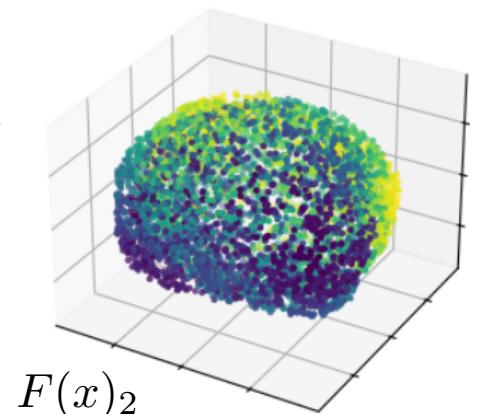
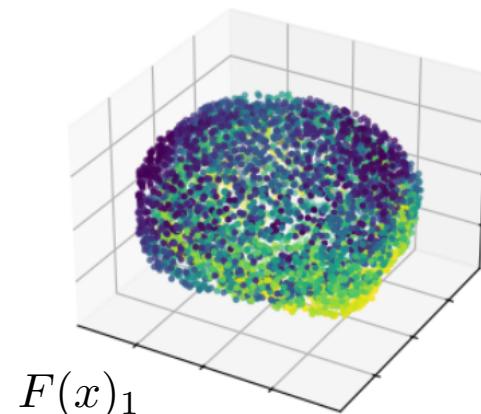
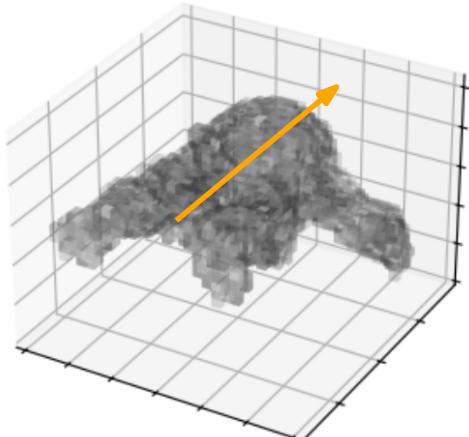
- the minimization problems are computed exactly,
- $\mathfrak{sym}(\mathcal{O})$  is spanned by matrices whose spectra come from primitive vectors of coordinates at most  $\omega_{\max}$ ,
- The candidate Lie group is  $\simeq \text{Sym}(\mathcal{O})$ .



- (1) Take a  $m \times m \times m$  image.
- (2) Generate several rotations to get a point cloud  $X \subset \mathbb{R}^{m \times m \times m}$ .
- (3) Project  $X$  in  $\mathbb{R}^n$  via PCA.

**Problem:** given  $x \in X$ , estimate the unit vector  $F(x) \in \mathbb{R}^3$  that points toward the armadillo's head.

We define train/test sets of 90%/10%.



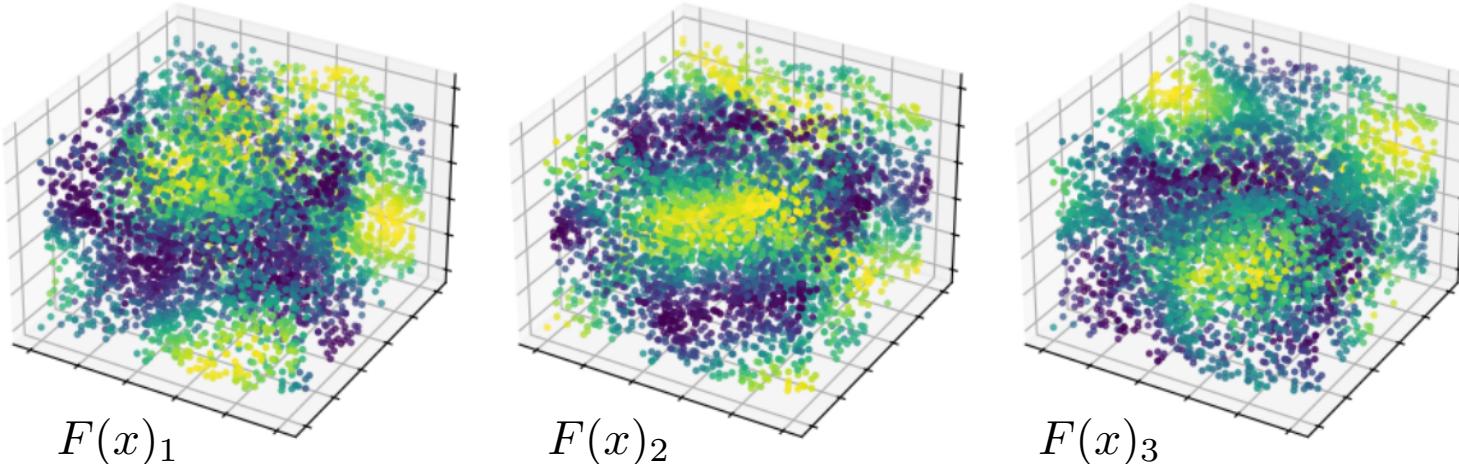
**Conventional solution:** Train a SVM.

**Orthogonal coordinates:** Our algorithm detect a  $\text{SO}(3)$ -orbit in  $\mathbb{R}^8$  that is close to  $X$ :  $d_H(X, \mathcal{O}) \simeq 0.1909$ .

$$\begin{array}{ccc} \text{SO}(3) & \xrightarrow{\phi} & \text{GL}_n(\mathbb{R}) \\ \exp \uparrow & & \uparrow \exp \\ \mathfrak{so}(3) & \xrightarrow{d\phi} & \mathfrak{gl}(n) \end{array}$$

The orbit is  $\mathcal{O} = \{\phi(g) \cdot x_0 \mid g \in G\}$ . Every  $x \in X$  can be pulled back to  $\mathfrak{so}(3)$  via

$$\min_{c \in \mathfrak{so}(3)} \|x - \phi(\exp(c)) \cdot x_0\|.$$



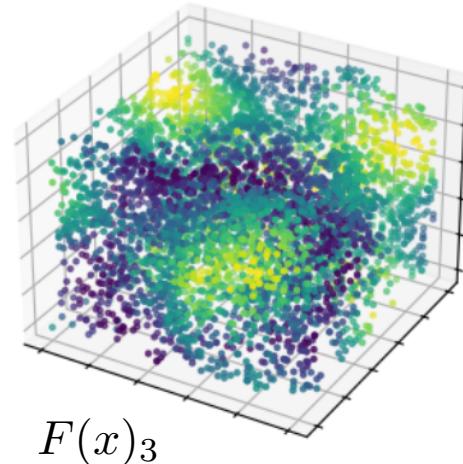
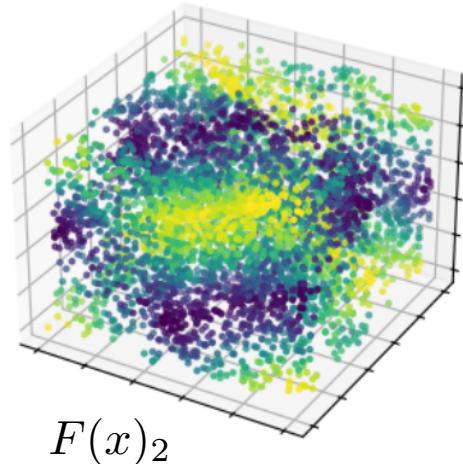
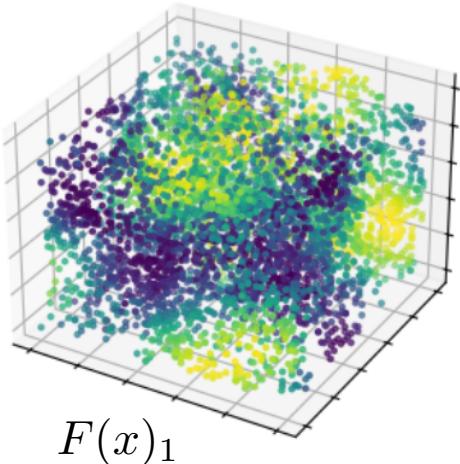
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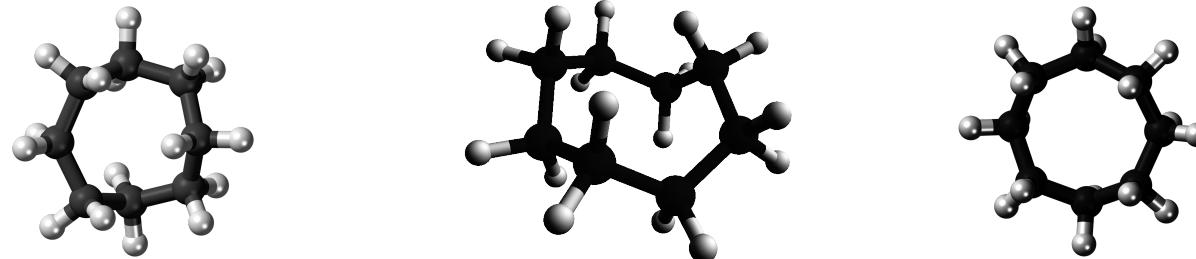
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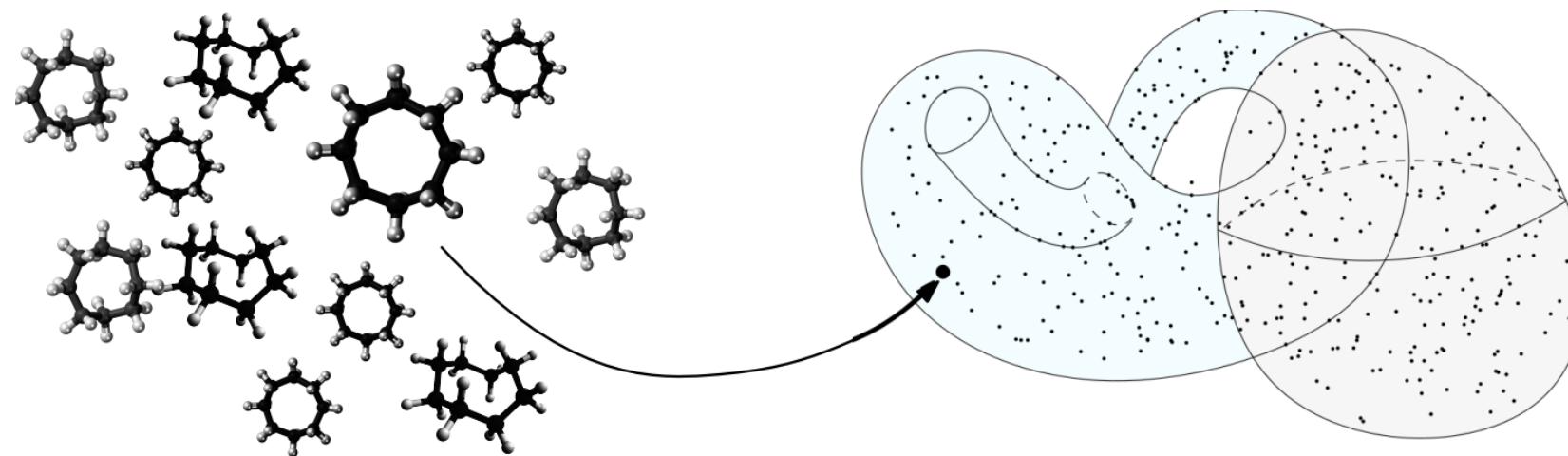


Model	MSE on test data
SVM in dimension 3	0.4003
SVM in dimension 4	0.2496
SVM in dimension 5	0.1295
SVM in dimension 6	0.0380
SVM in dimension 7	0.0148
SVM in dimension 8	0.0119
SVM in dimension 9	0.0114
SVM in dimension 10	0.0122
SVM on orthogonal coordinates	<b>0.0066</b>



A conformer of cyclooctane can be seen as a point in  $\mathbb{R}^{72}$  ( $3 \times 24 = 72$ ).

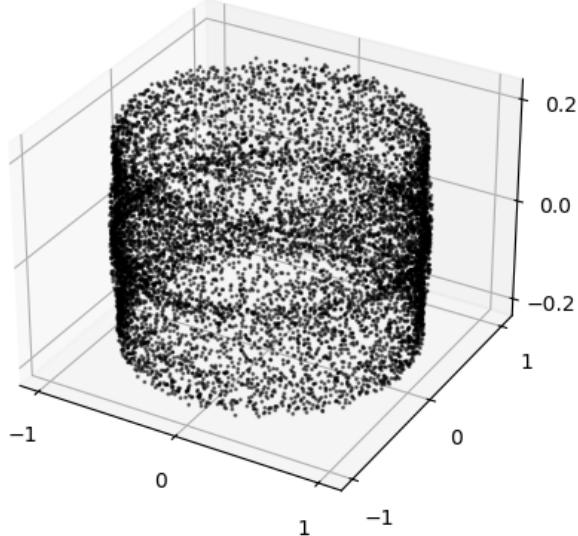
A collection of conformers yield a point cloud  $X \subset \mathbb{R}^{72}$ .



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

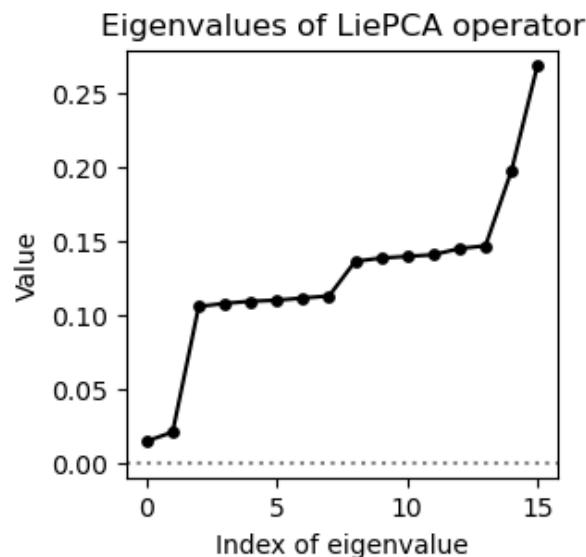
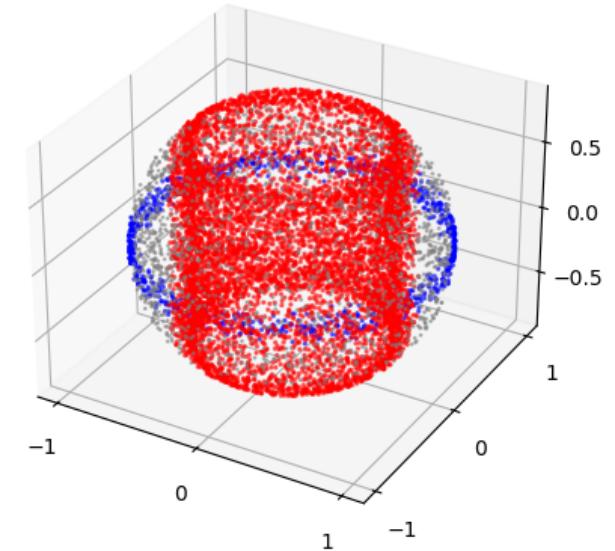
**Idea:** check whether  $X$  lies close to a linear orbit of a Lie group.

**Unaligned conformers:** We generate 10,000 cyclooctane conformers without aligning them.



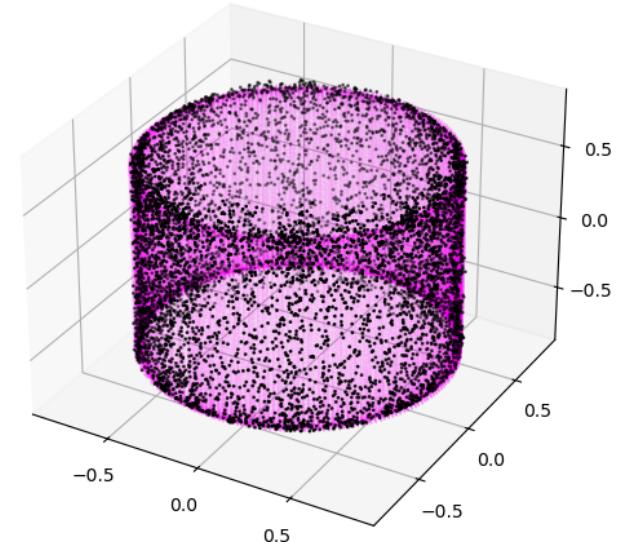
We see a cylinder surrounded by a circle.

$X$  is projected onto  $\mathbb{R}^4$  and orthonormalized. After discarding 15% of the outliers (gray), two clusters appear. We take the red one.

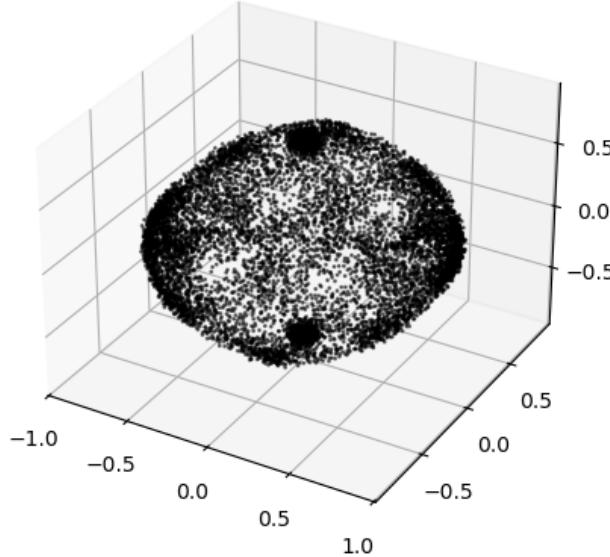


LiePCA has two small eigenvalues, suggesting a symmetry group of dim 2.

We find a  $T^2$ -orbit in  $\mathbb{R}^4$  close  $X$ :  $d_H(X, \mathcal{O}) \simeq 0.2$ .

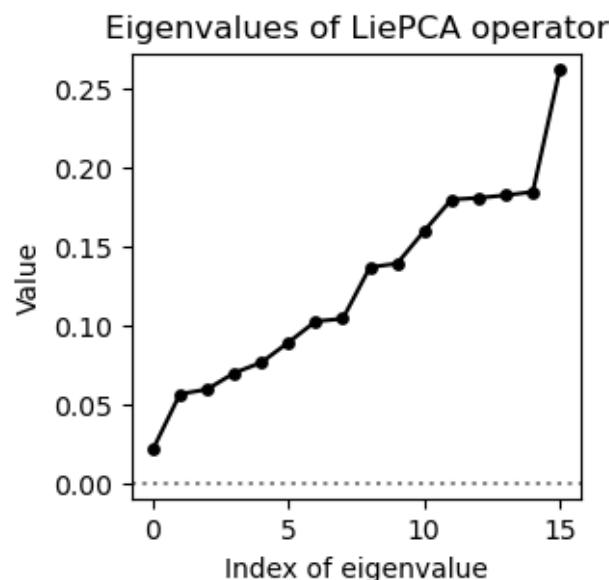


**Aligned conformers:** We now generate 10,000 aligned conformers (`AlignMolConformers` in RDKit).



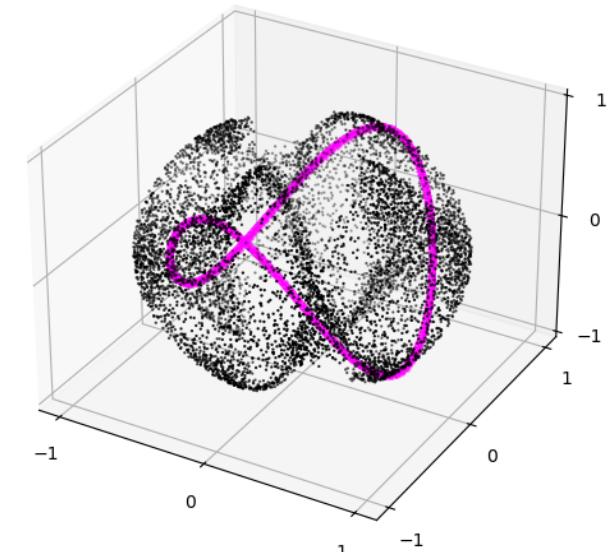
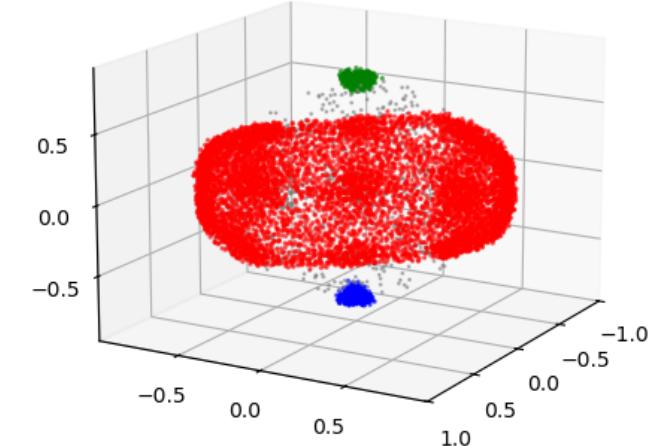
We see three components:  
a surface and two clusters.

After discarding 10% of the outliers (gray),  
the points are grouped into three classes.  
We keep the red class.



LiePCA has one small eigenvalue,  
suggesting a symmetry group of dim 1.

We find a SO(2)-action that stabilizes  $X$ .  
Average distance:  $d_H(\widehat{\mathcal{O}}_x | X) \simeq 0.1$ .



Consider a neural network

$$V = V_1 \xrightarrow{f_1} V_2 \xrightarrow{f_2} V_3 \xrightarrow{f_3} \dots \xrightarrow{f_{p-1}} V_p = W.$$

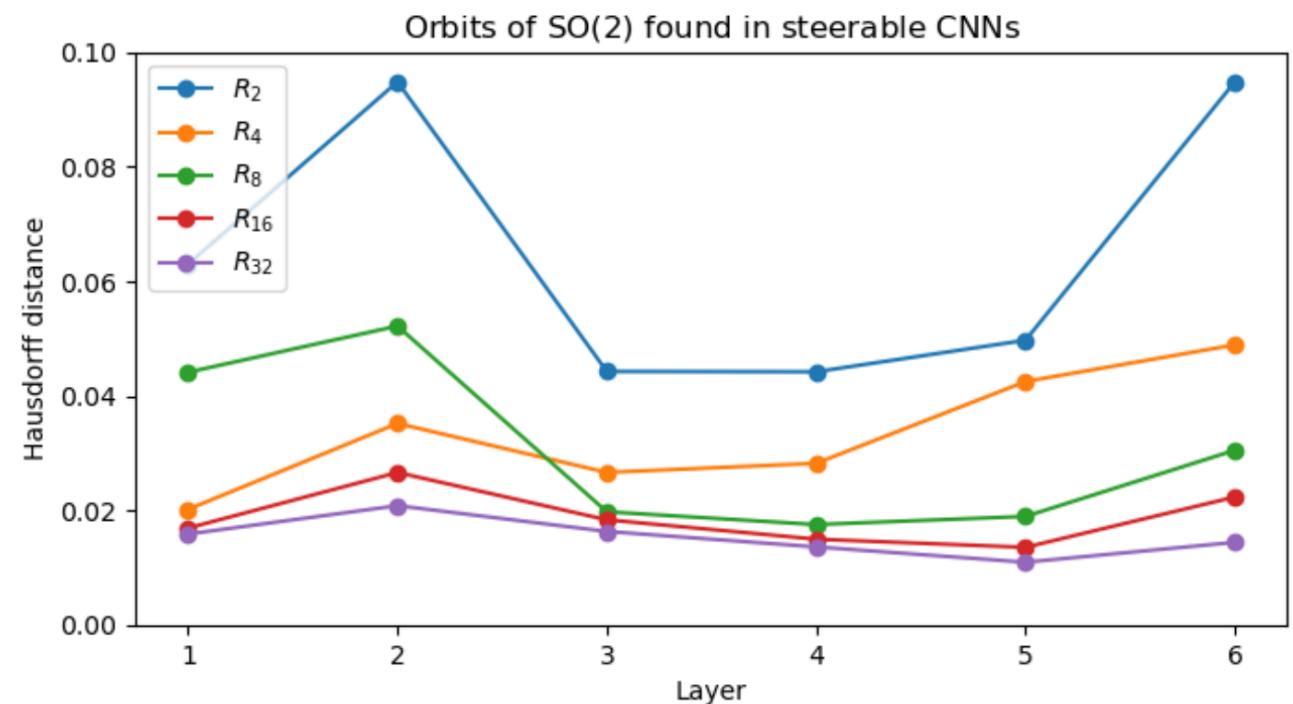
Denote  $\mathcal{F}_i = f_1 \cdots f_i$  and  $\mathcal{F} = \mathcal{F}_{p-1}$ .

Say  $G$  acts linearly on  $V$ , via  $\phi: G \rightarrow \text{GL}(V)$ .

The network is **equivariant** if there exists representations  $\phi_i: G \rightarrow \text{GL}(V_i)$  such that  $\forall x \in V, \forall g \in G$ ,

$$\mathcal{F}_i(\phi(g)x) = \phi_i(g)\mathcal{F}_i(x).$$

**Experiment:** Consider **steerable CNNs** for several rotation groups  $R_n$ . We pick an image, and generate 500 rotations. In each of the layers, we apply our algorithm to find a linear-orbit of  $\text{SO}(2)$ .



LieDetect: Detection of representation orbits of compact Lie groups from point clouds  
Foundations of Computational Mathematics (2025)  
DOI:10.1007/s10208-025-09728-4

<https://github.com/HLovisiEnnes/LieDetect>

**Thanks!**

Detection of **actions** via the induced representation on space of vector fields

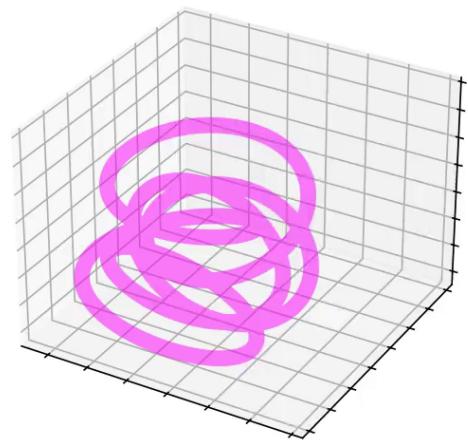
$$\begin{array}{ccc} G & \xrightarrow{\phi} & \text{Diff}(\mathcal{M}) \\ \exp \uparrow & & \uparrow \exp \\ \mathfrak{g} & \xrightarrow{d\phi} & \mathcal{X}(\mathcal{M}) \end{array}$$

**Statistical** guarantees to test the linear-orbit hypothesis.

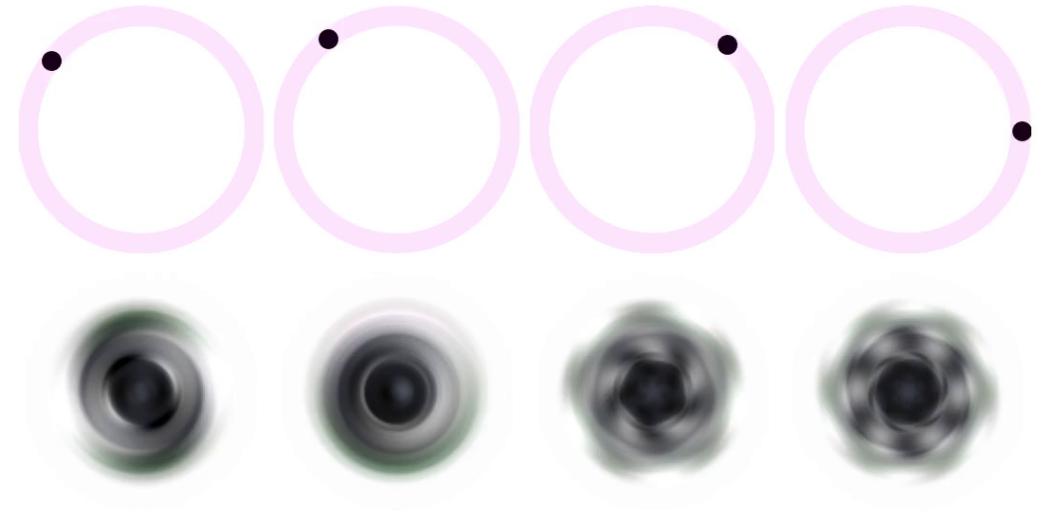
Rotations of  $m \times m$  RGB image



Embedding in  $\mathbb{R}^{m \times m \times 3}$



Projection in eigenplanes



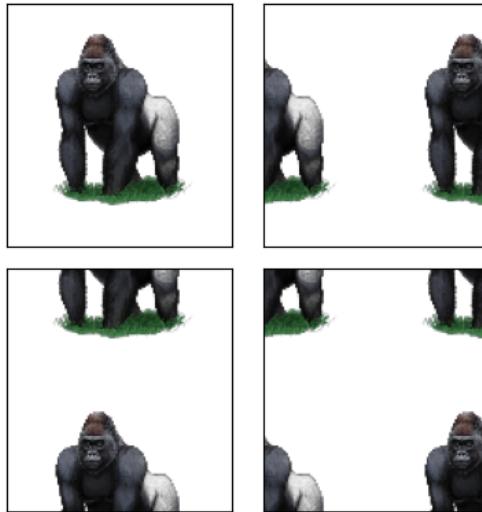
Eigenvalues of the point cloud's covariance matrix:

0.155, 0.155, 0.11, 0.11, 0.041, 0.041, 0.04, 0.04, 0.038, 0.038, 0.026, 0.026, ...

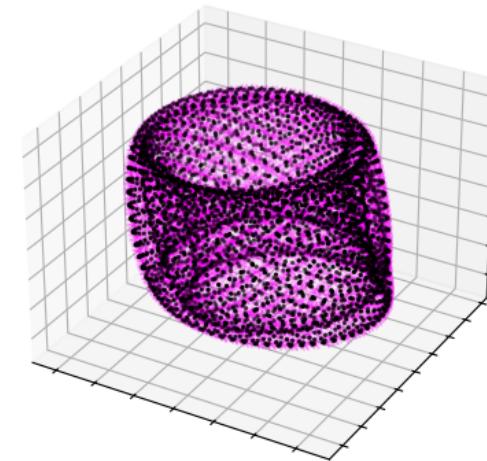
In these eigenplanes, the orbit is close to

$$\theta \mapsto \begin{pmatrix} \mu_1 \cos \omega_1 \theta \\ \mu_1 \sin \omega_1 \theta \\ \mu_2 \cos \omega_2 \theta \\ \mu_2 \sin \omega_2 \theta \\ \vdots \\ \mu_k \cos \omega_k \theta \\ \mu_k \sin \omega_k \theta \end{pmatrix} = \begin{pmatrix} \cos \omega_1 \theta & -\sin \omega_1 \theta \\ \sin \omega_1 \theta & \cos \omega_1 \theta \\ & & \cos \omega_2 \theta & -\sin \omega_2 \theta \\ & & \sin \omega_2 \theta & \cos \omega_2 \theta \\ & & & & \ddots \\ & & & & \cos \omega_k \theta & -\sin \omega_k \theta \\ & & & & \sin \omega_k \theta & \cos \omega_k \theta \end{pmatrix} \begin{pmatrix} \mu_1 \\ 0 \\ \mu_2 \\ 0 \\ \vdots \\ \mu_k \\ 0 \end{pmatrix}$$

Translations of  $m \times m$  RGB image



Embedding in  $\mathbb{R}^{m \times m \times 3}$



Covariance matrix eigenvalues: 0.228, 0.228, 0.142, 0.142, 0.108, 0.108, 0.022, 0.022, ...

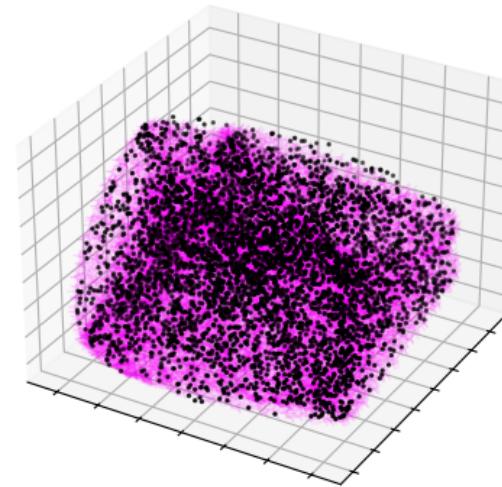
In these eigenplanes, the orbit is close to

$$\theta^{(1)}, \theta^{(2)} \longmapsto \begin{pmatrix} \mu_1 \cos(\omega_1^{(1)}\theta^{(1)} + \omega_1^{(2)}\theta^{(2)}) \\ \mu_1 \sin(\omega_1^{(1)}\theta^{(1)} + \omega_1^{(2)}\theta^{(2)}) \\ \mu_2 \cos(\omega_2^{(1)}\theta^{(1)} + \omega_2^{(2)}\theta^{(2)}) \\ \mu_2 \cos(\omega_2^{(1)}\theta^{(1)} + \omega_2^{(2)}\theta^{(2)}) \\ \vdots \\ \mu_k \cos(\omega_k^{(1)}\theta^{(1)} + \omega_k^{(2)}\theta^{(2)}) \\ \mu_k \cos(\omega_k^{(1)}\theta^{(1)} + \omega_k^{(2)}\theta^{(2)}) \end{pmatrix} = \text{linear action of } T^2 \text{ on } \begin{pmatrix} \mu_1 \\ 0 \\ \mu_2 \\ 0 \\ \vdots \\ \mu_k \\ 0 \end{pmatrix}$$

Rotations of  $m \times m \times m$  greyscale object



Embedding in  $\mathbb{R}^{m \times m \times m}$



Covariance matrix eigenvalues:      0.246,  0.239,  0.234,  0.058,  0.057,  0.056,  0.055,  0.054 ...

In these eigenplanes, the orbit is close to

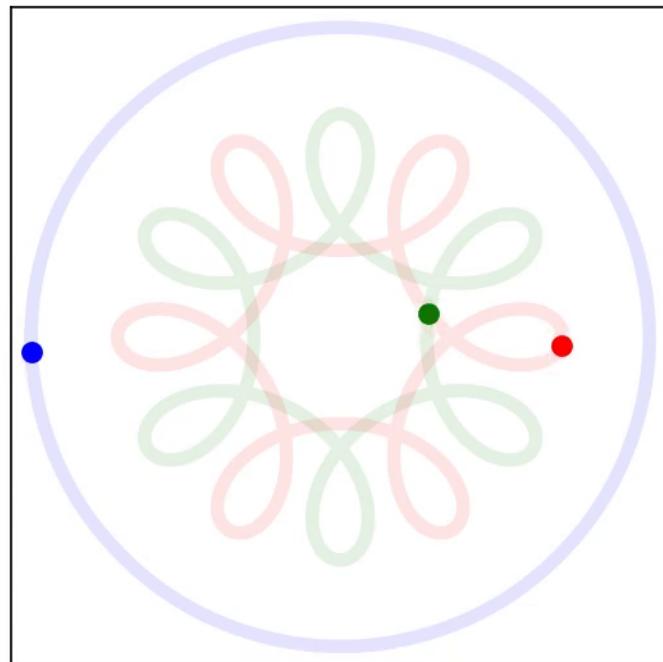
$$\theta^{(1)}, \theta^{(2)}, \theta^{(3)} \longmapsto \text{linear action of } \text{SO}(3) \text{ on } \begin{pmatrix} \mu_1 \\ 0 \\ \vdots \\ \mu_2 \\ 0 \\ \vdots \end{pmatrix}$$

In 1975, Roger Broucke found several periodic orbits.

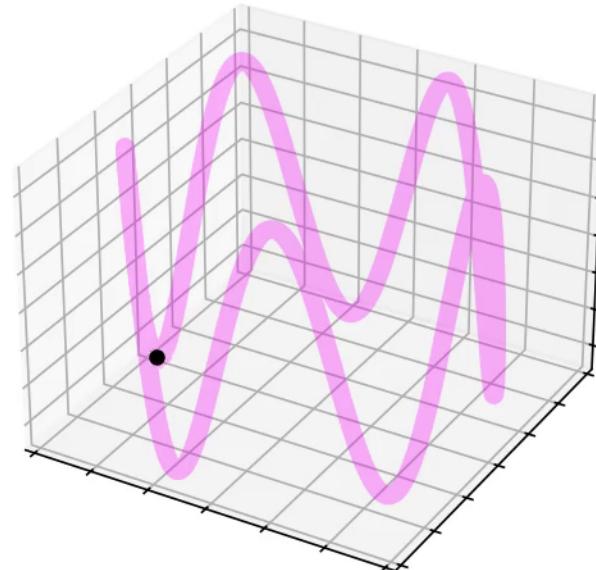
Let  $x_1(t), x_2(t), x_3(t)$  be the three bodies, and define  $z(t) = (x_1(t), x_2(t), x_3(t)) \in \mathbb{R}^6$ .

### Orbit A3

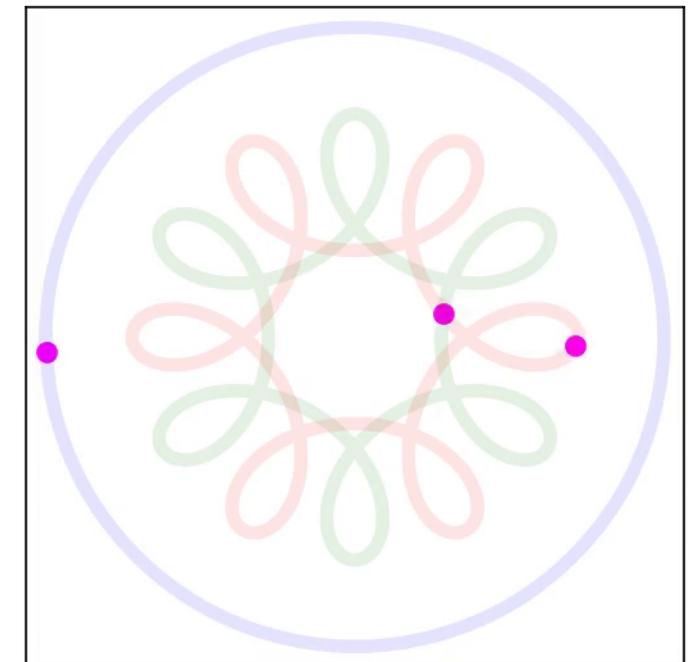
Trajectory of  $x_1, x_2, x_3$   
(found by integration)



Trajectory of  $z$



Reconstructed orbit of  $\text{SO}(2)$

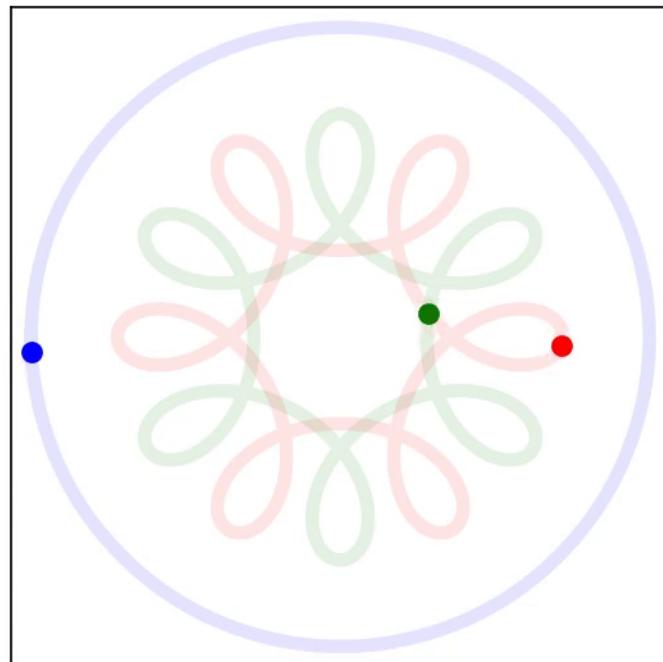


In 1975, Roger Broucke found several periodic orbits.

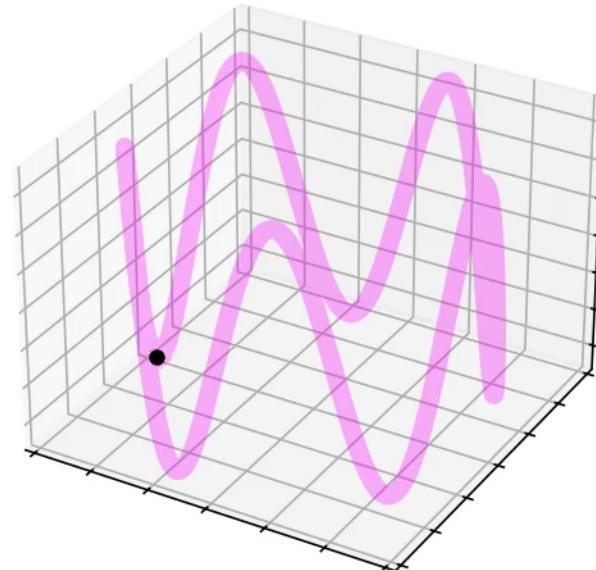
Let  $x_1(t), x_2(t), x_3(t)$  be the three bodies, and define  $z(t) = (x_1(t), x_2(t), x_3(t)) \in \mathbb{R}^6$ .

### Orbit R2

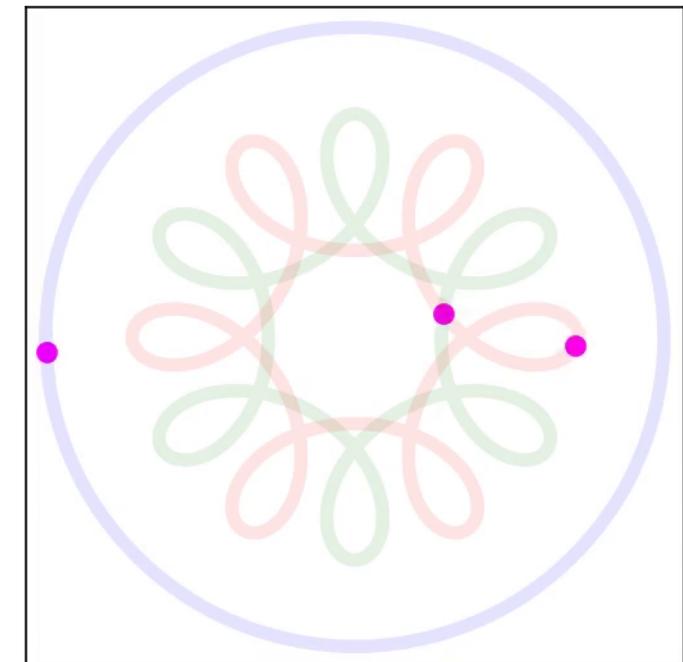
Trajectory of  $x_1, x_2, x_3$   
(found by integration)



Trajectory of  $z$



Reconstructed orbit of  $\text{SO}(2)$



Let  $G = \mathrm{SO}(2)$ , whose dimension is  $d = 1$ . The output  $\hat{h}$  of LiePCA is a skew symmetric  $n \times n$  matrix  $A$ .

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 frequency  $\omega_{\max} \in \mathbb{N}$ .

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

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

This is equivalent to

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

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

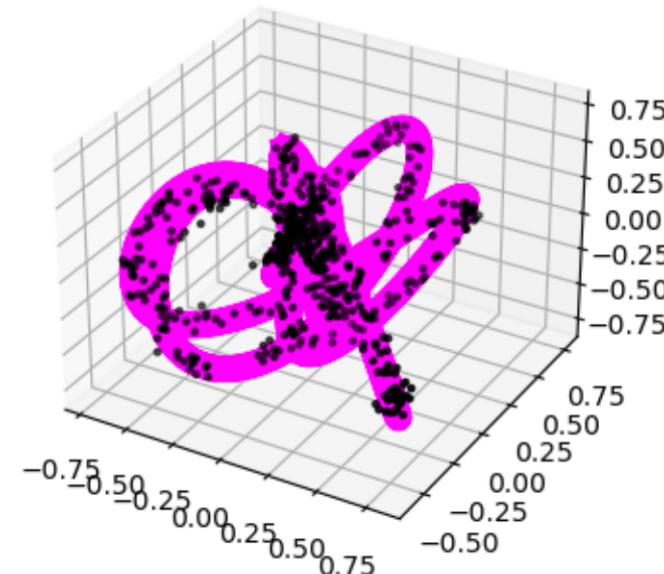
**Example:** We consider a representation of  $\text{SO}(2)$  in  $\mathbb{R}^{10}$  with frequencies  $(2, 4, 5, 7, 8)$  and sample 600 points on one of its orbits, that we corrupt with a Gaussian additive noise of deviation  $\sigma = 0.03$ .

We perform the minimization over all representations of  $\text{SO}(2)$  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	<b>0.028</b>	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.

The Hausdorff distance between the point cloud and the estimated orbit is  $d_H(X \mid \hat{\mathcal{O}}) \approx 0.231$ .



Let  $G = T^d$  the torus of dim  $d$ . The output of LiePCA is a  $d$ -tuple  $(A_1, \dots, A_d)$  of skew symmetric 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  $(\omega_i^j)_{1 \leq i \leq n/2}^{1 \leq j \leq d}$  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

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

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

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

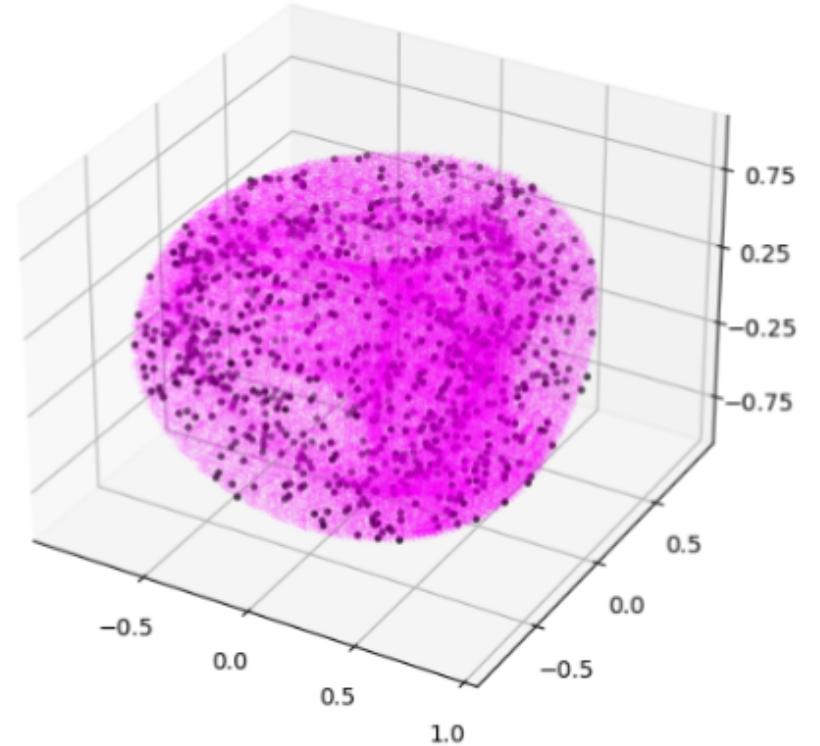
Example: Let  $X$  be a uniform 750-sample of an orbit of the representation  $\phi_{\left(\begin{smallmatrix} 1 & 1 & 2 \\ 1 & 2 & 1 \end{smallmatrix}\right)}$  of the torus  $T^2$  in  $\mathbb{R}^6$ .

We apply the algorithm with  $G = T^2$  restrict to representations 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	<b>0.036</b>	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

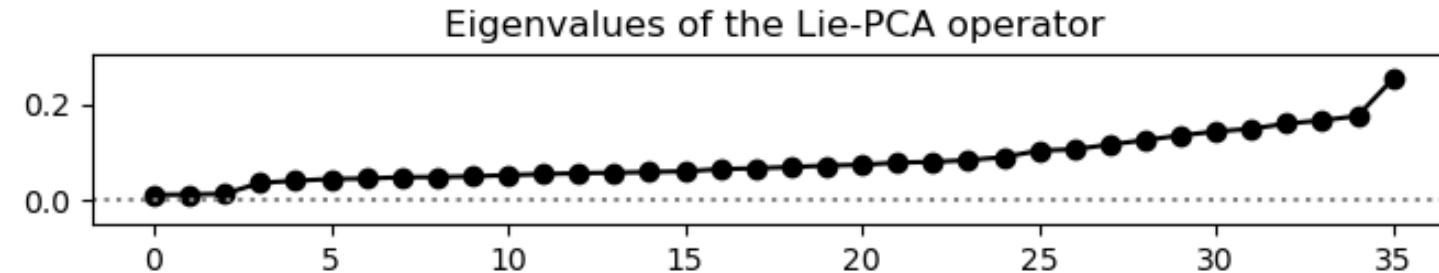
The algorithm's output is  $\left(\begin{smallmatrix} 0 & 1 & 1 \\ 2 & -2 & 1 \end{smallmatrix}\right)$ . It is equivalent to  $\phi_{\left(\begin{smallmatrix} 1 & 1 & 2 \\ 1 & 2 & 1 \end{smallmatrix}\right)}$ .

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



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

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



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

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

Representation of $T^3$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
Cost	<b>0.014</b>

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

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

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

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

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

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

If  $\phi$  is orthogonal, then by Schur's lemma, the  $C_i$  are homotheties:

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

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,  $\Pi[\langle \mathcal{O} \rangle]$  the projection on its span, and  $\sigma_{\max}^2, \sigma_{\min}^2$  the top and bottom nonzero eigenvalues of  $\Sigma[\mu_{\mathcal{O}}]$ .

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

If  $W_2(\mu_{\mathcal{O}}, \nu)$  is small enough, we have the following bound between the pushforward measures after Step 1:

$$\begin{aligned} W_2\left(\sqrt{\Sigma[\mu_{\mathcal{O}}]^{+}}\Pi[\langle \mathcal{O} \rangle]\mu_{\mathcal{O}}, \sqrt{\Sigma[\nu]^{+}}\Pi_{\Sigma[\nu]}^{>\epsilon}\nu\right) \\ \leq 8(n+1)^{3/2}\left(\frac{\sigma_{\max}^3}{\sigma_{\min}^3}\right)\left(\frac{W_2(\mu_{\mathcal{O}}, \nu)}{\sigma_{\min}}\right)^{1/2}\left(\left(\frac{\mathbb{V}[\|\mu_{\mathcal{O}}\|]}{\sigma_{\min}^2}\right)^{1/2} + \frac{W_2(\mu_{\mathcal{O}}, \nu)}{\sigma_{\min}}\right)^{1/2}. \end{aligned}$$

**Proof:** Consequence of Davis-Kahan theorem, together with

$$\|\Sigma[\mu_{\mathcal{O}}]^{-1/2} - \Sigma[\nu]^{-1/2}\|_{\text{op}} \leq \frac{\sqrt{2}}{\sigma_{\min}^2} \cdot \left(2\mathbb{V}[\|\mu_{\mathcal{O}}\|]^{1/2} + W_2(\mu_{\mathcal{O}}, \nu)\right)^{1/2} \cdot W_2(\mu_{\mathcal{O}}, \nu)^{1/2}.$$

LiePCA operator: Say we observe  $X = \{x_1, \dots, x_N\} \subset \mathbb{R}^n$ , assumed close to  $\mathcal{O}$ .

$$\text{Define } \Lambda: M_n(\mathbb{R}) \rightarrow M_n(\mathbb{R}) \text{ as} \quad \Lambda(A) = \frac{1}{N} \sum_{1 \leq i \leq N} \widehat{\Pi}[N_{x_i} X] \cdot A \cdot \Pi[\langle x_i \rangle]$$

where

- $\widehat{\Pi}[N_{x_i} X]$  are estimations of projection matrices onto the normal spaces  $N_{x_i} \mathcal{O}$ ,
- $\Pi[\langle x_i \rangle]$  are projection matrices on the lines  $\langle x_i \rangle$ .

Explanation: On the one hand,  $\mathfrak{sym}(\mathcal{O}) = \{A \in M_n(\mathbb{R}) \mid \forall x \in \mathcal{O}, Ax \in T_x \mathcal{O}\}$ . Thus,

$$\mathfrak{sym}(\mathcal{O}) = \bigcap_{x \in \mathcal{O}} S_x \mathcal{O} \quad \text{where} \quad S_x \mathcal{O} = \{A \in M_n(\mathbb{R}) \mid Ax \in T_x \mathcal{O}\}.$$

On the other hand, considering only  $X$ , one has

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

Last, the authors showed that  $\Pi[(S_{x_i} \mathcal{O})^\perp](A) = \Pi[N_{x_i} \mathcal{O}] \cdot A \cdot \Pi[\langle x_i \rangle]$ .

**Ideal Lie-PCA:** Suppose that  $\mathcal{O}$  is an orbit of the representation  $\phi: G \rightarrow M_n(\mathbb{R})$ , and  $\mu_{\mathcal{O}}$  its uniform measure. We define

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

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

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

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

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

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.,  $\sigma_{\max}^2/\sigma_{\min}^2 = 1$ .

**Stability:** Comparing

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

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

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

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  $\mu$  is a measure on  $\mathbb{R}^n$ , we define its *local covariance matrix* centered at  $x$  at scale  $r$  as

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

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

$$\left\| \frac{1}{l+2} \Pi[T_x \mathcal{M}] - \frac{1}{r^2} \Sigma_y^r[\nu] \right\|_F \leq$$

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

**Lemma:** If the parameters are chosen correctly, this is

$$\lesssim r + \|x - y\| + \left( \frac{W_2(\mu, \nu)}{r^{l+1}} \right)^{\frac{1}{2}}.$$

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

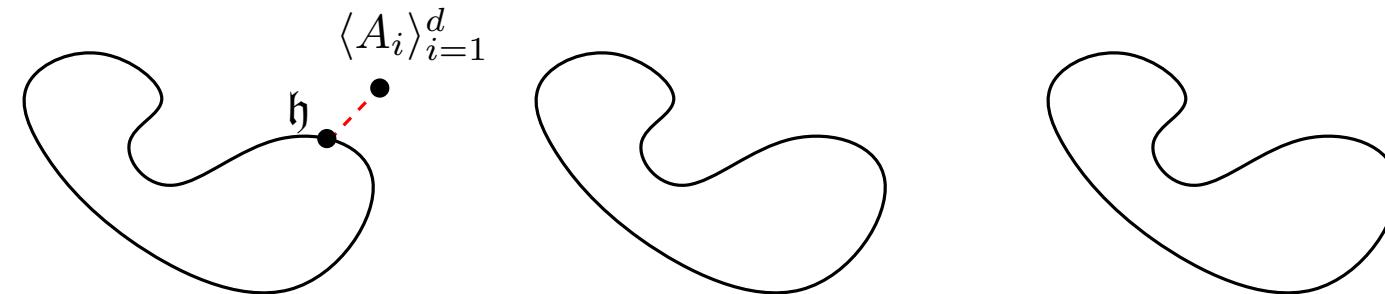
$$\|\Lambda_{\mathcal{O}} - \Lambda\|_{\text{op}} \leq \sqrt{2}\rho \left( r + 4 \left( \frac{W_2(\mu_{\mathcal{O}}, \mu_X)}{r^{l+1}} \right)^{1/2} \right).$$

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

$$\min \sum_{i=1}^d \|\Lambda(A_i)\|^2 \quad \text{s.t.} \quad \langle A_1, \dots, A_d \rangle \in \mathcal{G}^{\text{Lie}}(G, \mathfrak{gl}(n)).$$

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

The set  $\mathcal{G}(G, \mathfrak{so}(n))$  has many connected components, one for each *orbit-equivalence* class of representations. We want to make sure that the minimizer belongs to the correct connected component.

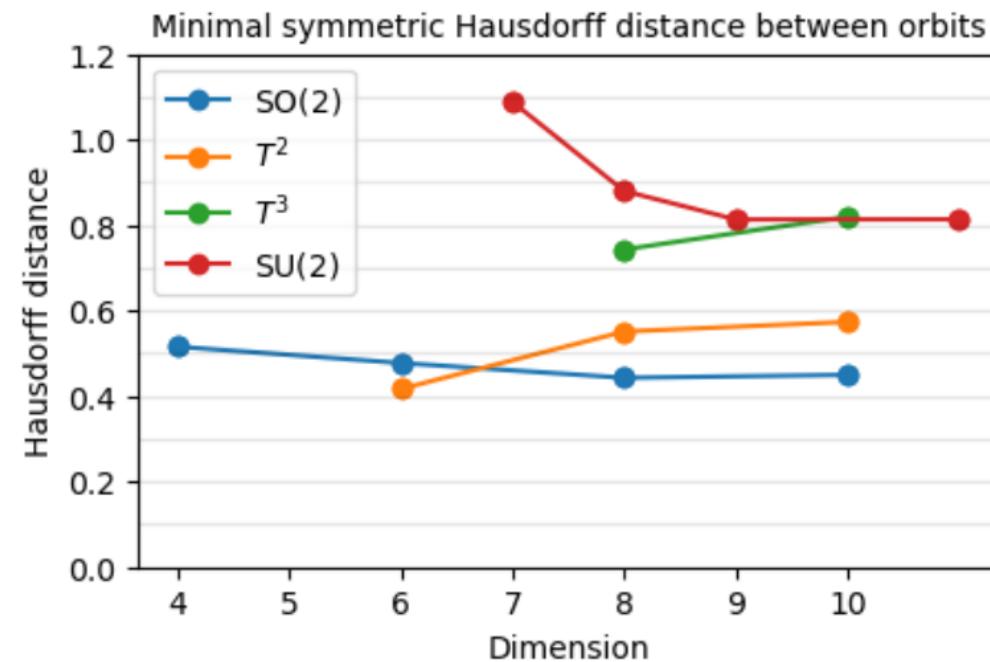
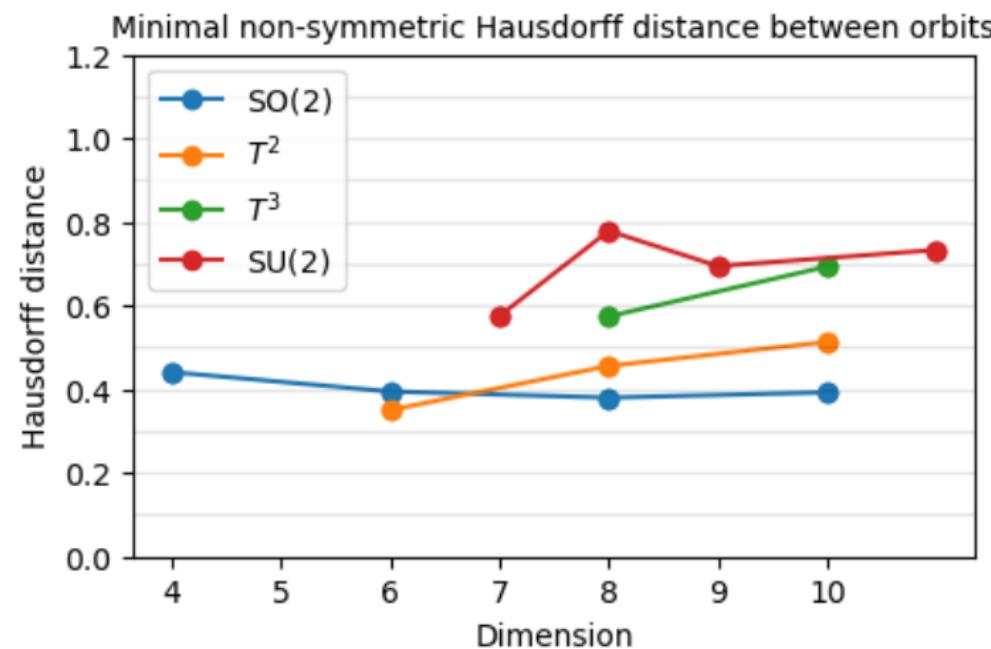


The distance from  $\langle A_i \rangle_{i=1}^d$  to  $\mathfrak{h}$  must be lower than the *reach* of  $\mathcal{G}(G, \mathfrak{so}(n))$ . In this context, it is called *rigidity*:

$$\Gamma(G, n) = \inf \|\Pi[\mathfrak{h}] \Pi[\mathfrak{s}^\perp]\|^2 \quad \text{s.t.} \quad \mathfrak{h} \in \mathcal{G}^{\text{Lie}}(G, \mathfrak{gl}(n)), \mathfrak{s} \in \mathcal{G}^{\text{Lie}}(H, \mathfrak{gl}(n)), s \not\simeq \mathfrak{h}.$$

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

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



**Left:** empirical estimation of the minimal non-symmetric Hausdorff distance  $d_H(\widehat{\mathcal{O}}_x^1 | \widehat{\mathcal{O}}_x^2)$  between two orbits of a same initial point  $x$  for two non-orbit equivalent representations  $\phi_1, \phi_2$  of a compact Lie group  $G$  in  $\mathbb{R}^n$ . The minimal value is approximately 0.35.

**Right:** same for the symmetric Hausdorff distance  $d_H(\widehat{\mathcal{O}}_x^1, \widehat{\mathcal{O}}_x^2)$ . The minimal value is 0.42.

Running time (in seconds or minutes) and success rate (percentage) of full execution of `LieDetect`, as a function of the input group, and the dimension of the ambient Euclidean space. The input of the algorithm is a point cloud sampled from the uniform measure on an orbit chosen randomly.

For the Abelian groups  $\text{SO}(2)$ ,  $T^2$ , and  $T^3$ , the representations are considered up to a maximal frequency, 100 runs of the algorithm are performed, and the results are averaged. For  $\text{SU}(2)$ , 10 runs have been performed.

Dimension	4	6	8	10
Running time	0.04s	0.05s	0.08s	0.14s
Success	100.0%	100.0%	100.0%	100.0%

(a)  $\text{SO}(2)$ 

Dimension	6	8	10
Running time	0.24s	0.63s	4.03s
Success	82.0%	100.0%	98.0%

(b)  $T^2$ 

Dimension	8	10
Running time	1.44s	5.98s
Success	100.0%	100.0%

(c)  $T^3$ 

Dimension	4	5	7	8	9	10
Running time	0.6s	5.04s	4min 21s	13min 7s	16min 9s	10min 53s
Success	100.0%	100.0%	90.0%	100.0%	100.0%	100.0%

(d)  $\text{SU}(2)$