AATRN Applied Topology Seminar – 11/06/2025

Detection of representation orbits of compact Lie groups from point clouds

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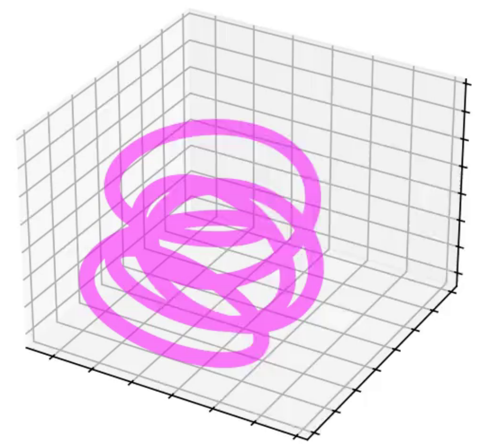
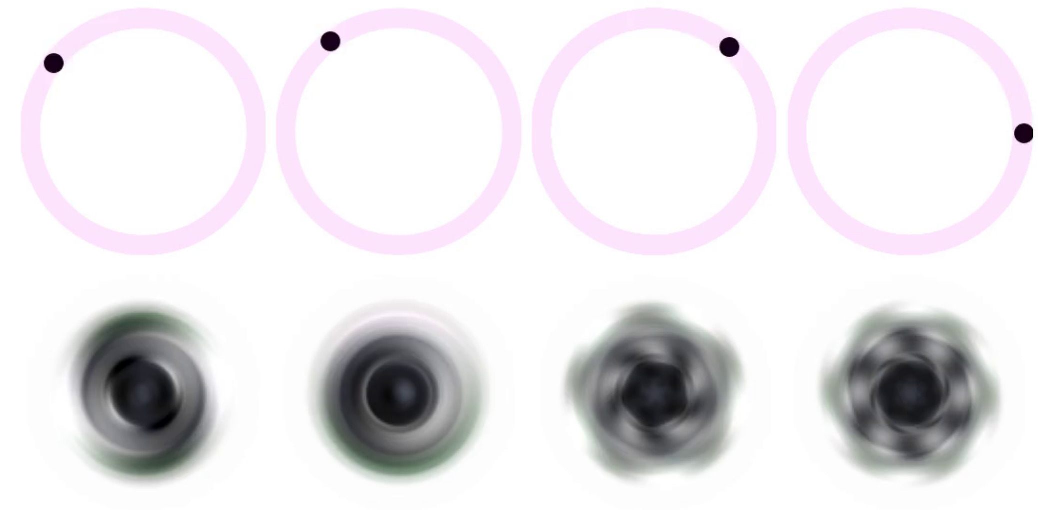
Rotations of $m \times m$ RGB image

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



Projection in eigenplanes



Eigenvalues of the point cloud's covariance matrix:

$$311.2, \quad 311.2, \quad 221.3, \quad 221.3, \quad 82.3, \quad 82.3, \quad 79.4, \quad 79.4, \quad \ldots$$

In these eigenplanes, the orbit is close to

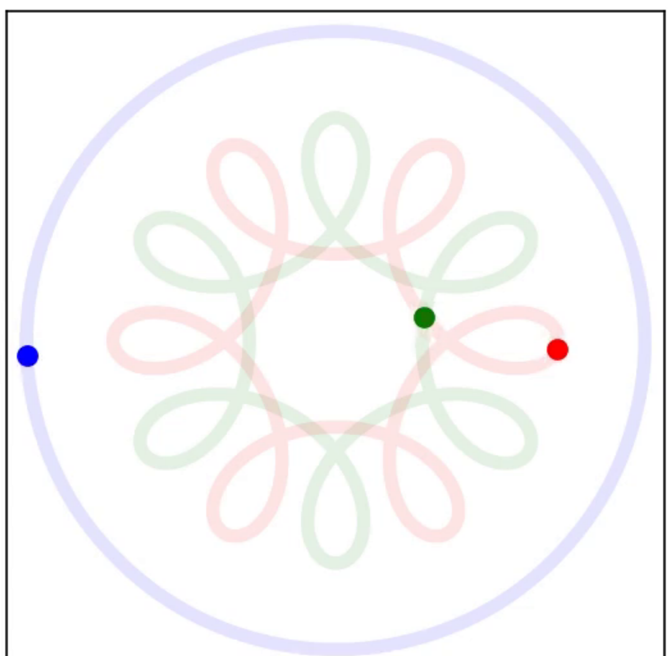
$$\theta \longmapsto \begin{pmatrix} \mu_1 \cos\omega_1\theta \\ \mu_1 \sin\omega_1\theta \\ \mu_2 \cos\omega_2\theta \\ \mu_2 \sin\omega_2\theta \\ \vdots \\ \mu_k \cos\omega_k\theta \\ \mu_k \sin\omega_k\theta \end{pmatrix} = \begin{pmatrix} \cos\omega_1\theta & -\sin\omega_1\theta & & & & & \\ \sin\omega_1\theta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

In 1975, Roger Broucke found several periodic orbits.

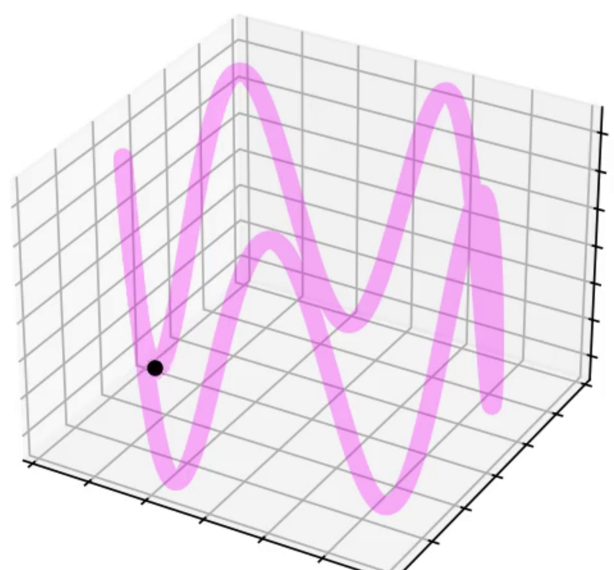
Let $x_1(t)$, $x_2(t)$, $x_3(t)$ be the three bodies, and define $z(t) = (x_1(t), x_2(t), x_3(t)) \in \mathbb{R}^6$.

<u>Orbit `A3`</u>

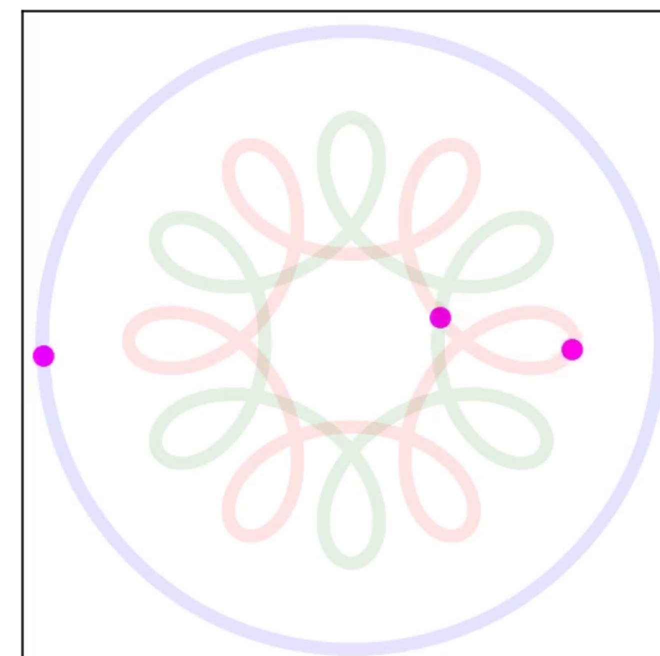
Trajectory of x_1, x_2, x_3 (found by integration)



Trajectory of z



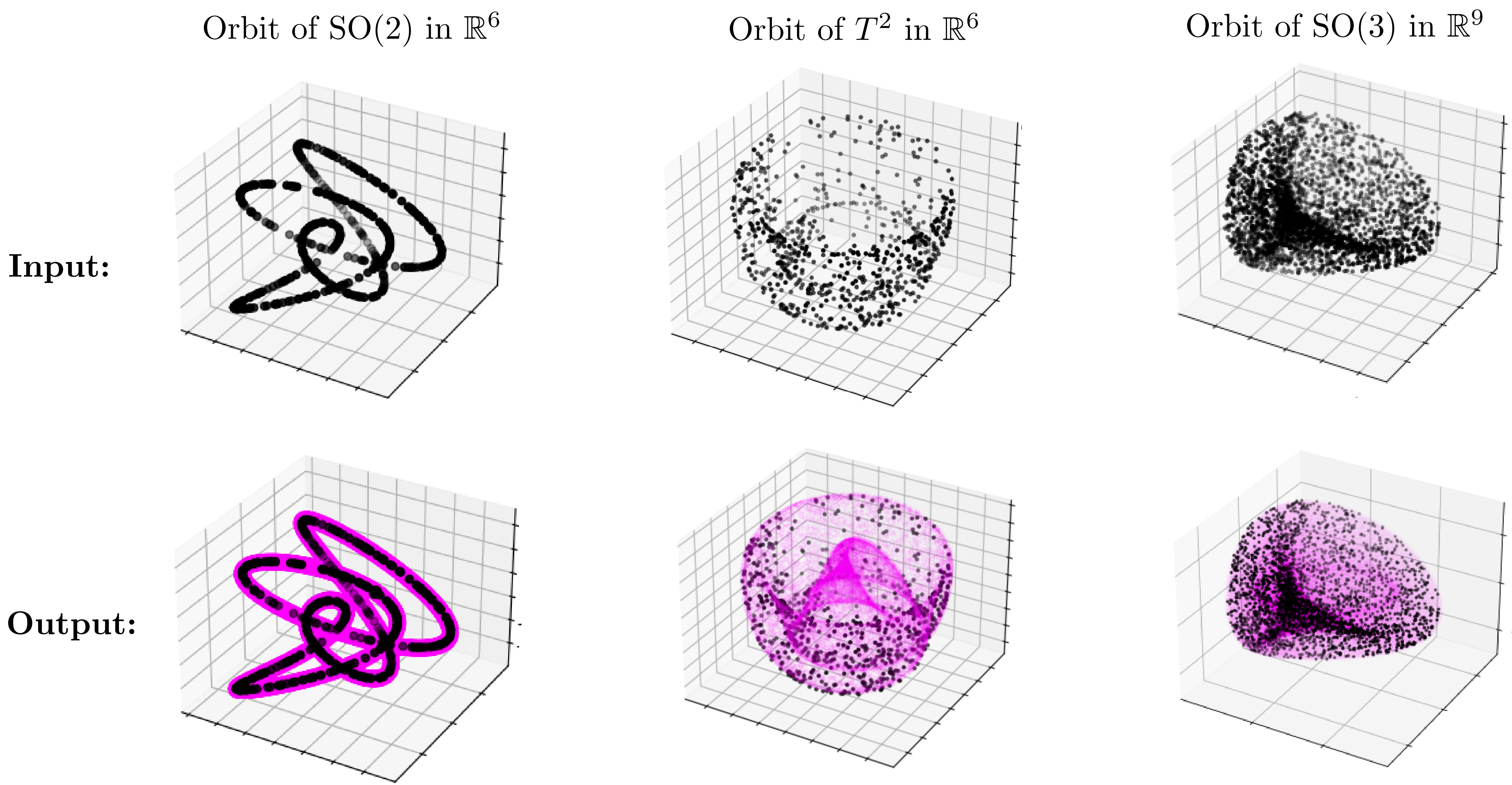
Reconstructed orbit of SO(2)



Formulation of the problem

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

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



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 $\phi\colon G \to \mathrm{GL}_n(\mathbb{R})$.

- If G is a matrix group, the natural embedding $G \to \mathrm{GL}_n(\mathbb{R})$ 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 $\phi\colon G \to \mathrm{GL}_n(\mathbb{R})$ is **irreducible** (irrep) if no non-trivial subspace $V \subset \mathbb{R}^n$ is stabilized.

Fact: Every representation ϕ is equivalent to a sum of irreps. That is, one has a decomposition $\mathbb{R}^n = V_1 \oplus \cdots \oplus V_k$, irreps $\phi_i\colon G \to V_i$ 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:

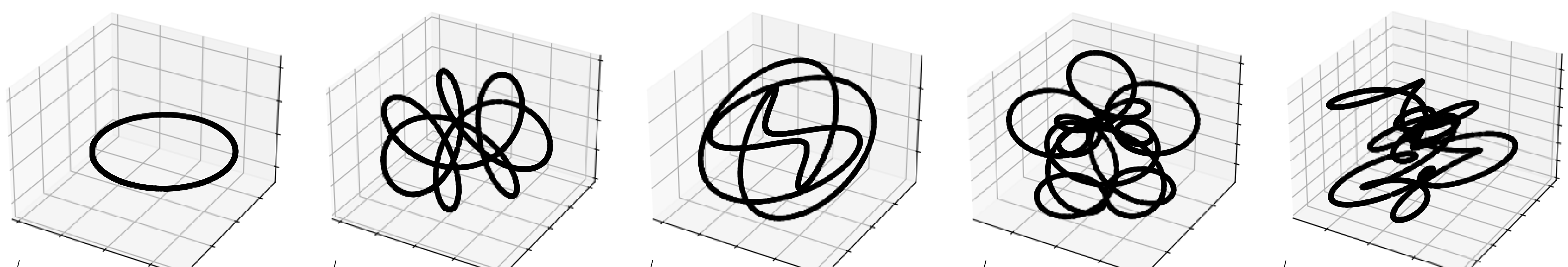
- SO(2) — the $\theta \mapsto R(\omega\theta)$ for $\omega \in \mathbb{Z} \setminus \{0\}$, where $R(\theta) \mapsto \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$.
- T^d — the $(\theta_i)_{i=1}^d \mapsto R(\sum_{i=1}^d \omega_i\theta_i)$ for $(\omega_i)_{i=1}^d \in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

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

Example: Orbits of 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

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



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

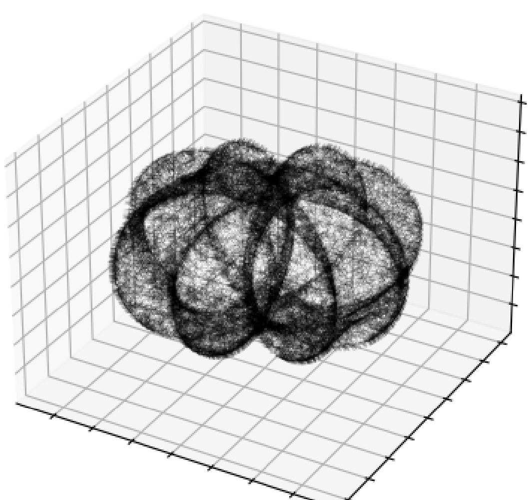
The **orbit** of $x_0 \in \mathbb{R}^n$ under a representation $\phi\colon G \to \mathrm{GL}_n(\mathbb{R})$ is $\mathcal{O} = \{\phi(g)x_0 \mid g \in G\}$.

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

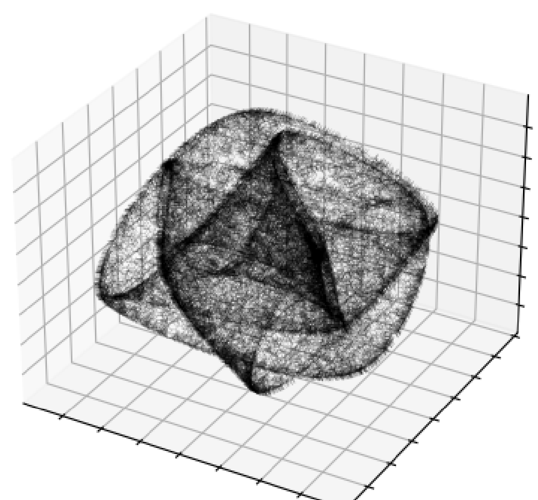
Let us write

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

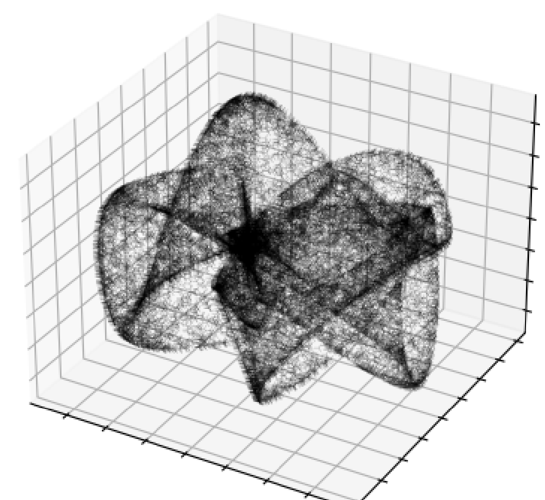
One builds the integer matrix of weights $\begin{pmatrix}\omega_1^{(1)} & \cdots & \omega_k^{(1)}\\ \omega_1^{(2)} & \cdots & \omega_k^{(2)}\end{pmatrix}$.



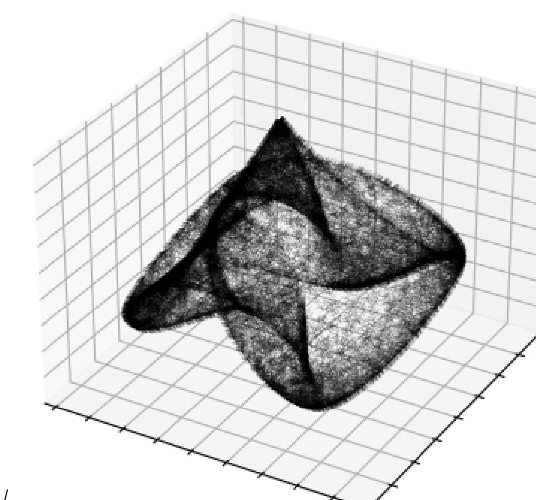
$\phi_{\begin{pmatrix}1&1&3\\1&2&1\end{pmatrix}}$



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



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



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

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

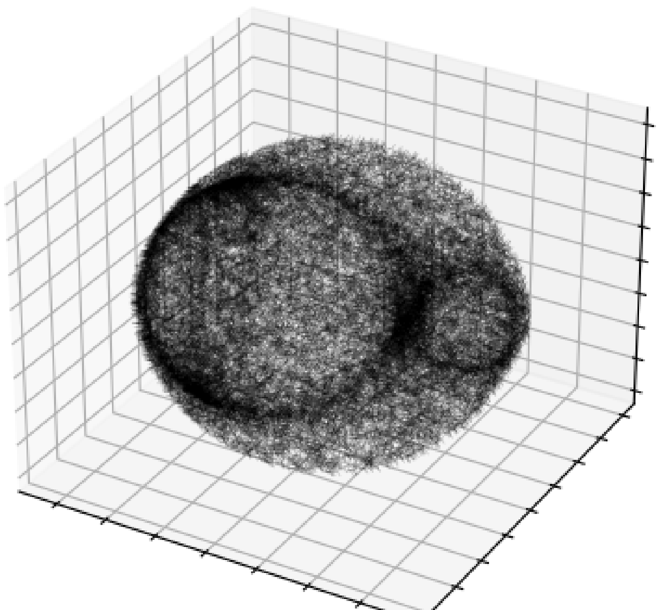
Example: Orbits of SO(3) and SU(2) in $\mathbb{R}^n$.

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

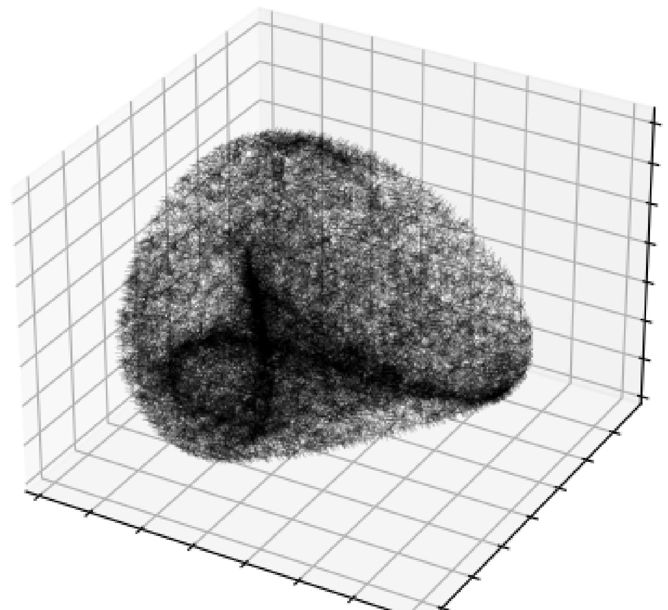
$$n = \omega_1 + \cdots + \omega_k$$

where the ω_i are odd.

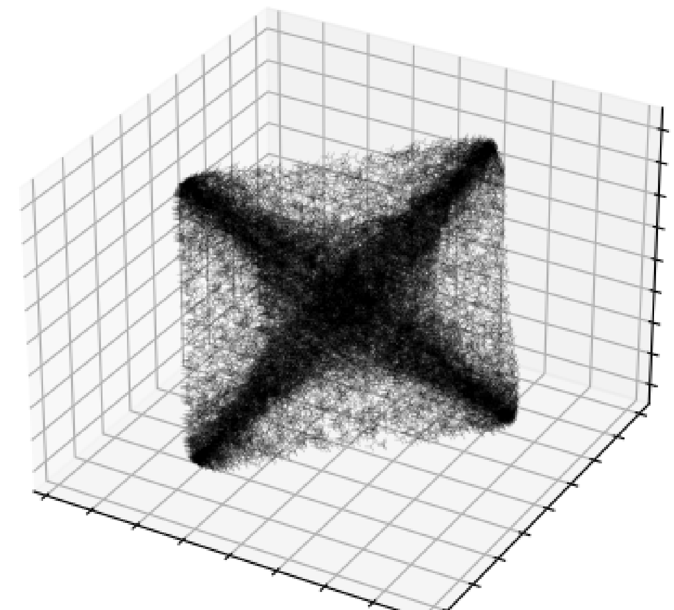
For SU(2), one can also use multiples of 4.



$\phi_{(5)}$ 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 $\phi_1 : G \to \mathrm{GL}_n(\mathbb{R})$, and we want to find ϕ_1.

Identifiability problem: another representation ϕ_2 may generate $\mathcal{O}$.

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

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 (increasing and positive) primitive k-tuples of integers.
- T^d in $\mathbb{R}^{2k}$ are the primitive d-dimensional lattices in $\mathbb{Z}^k$.

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

Derived representation

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

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

- $\mathrm{GL}_n(\mathbb{R})$ $\quad\mathfrak{gl}(n)$ is the set of $n \times n$ matrices.
- $\mathrm{SO}(n)$ $\quad\mathfrak{so}(n)$ 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 2×2 block-diagonal.

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

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

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

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

Fact: Two representations ϕ_1, ϕ_2 are orbit-equivalent iff there exists $A \in \mathrm{GL}_n(\mathbb{R})$ such that

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

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

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

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

$$\begin{tikzcd}
G \arrow[r, "\phi"] & \phi(G) & \subset & \mathrm{Sym}(\mathcal{O}) & \subset & \mathrm{GL}_n(\mathbb{R}) \\
\mathfrak{g} \arrow[u, "\exp"] \arrow[r, "\mathrm{d}\phi"] & \mathrm{d}\phi(\mathfrak{g}) \arrow[u, "\exp"] & \subset & \mathfrak{sym}(\mathcal{O}) \arrow[u, "\exp"] & \subset & \mathfrak{gl}(n) \arrow[u, "\exp"]
\end{tikzcd}$$

Symmetry group:

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

Symmetry algebra:

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

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

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

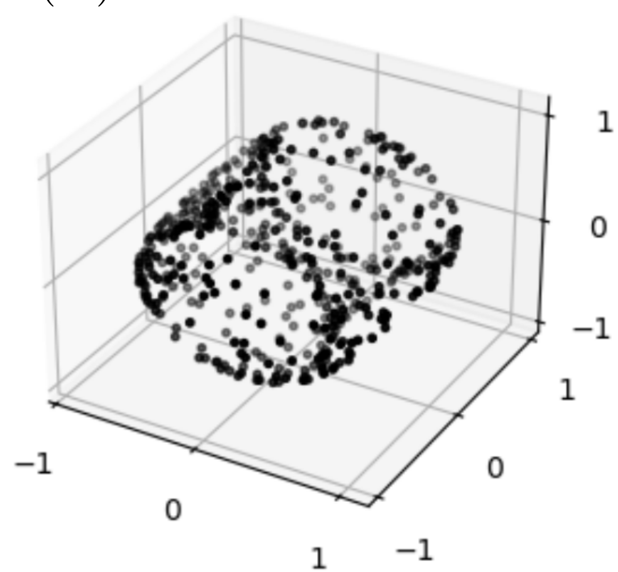
[Cahill, Mixon, Parshall, Lie PCA: Density estimation for symmetric manifolds, 2023]

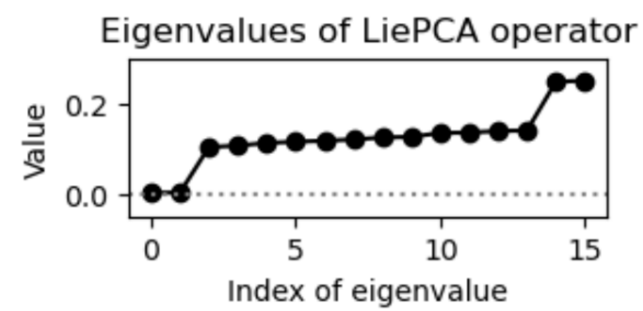
LiePCA operator: Say we observe $X = \{x_1, \dots, x_N\} \subset \mathbb{R}^n$, assumed close to $\mathcal{O}$.

Define $\Lambda \colon \mathrm{M}_n(\mathbb{R}) \to \mathrm{M}_n(\mathbb{R})$ as $$\Lambda(A) = \frac{1}{N} \sum_{1 \leq i \leq N} \widehat{\Pi}\big[\mathrm{N}_{x_i} X\big] \cdot A \cdot \Pi\big[\langle x_i \rangle\big]$$

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

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

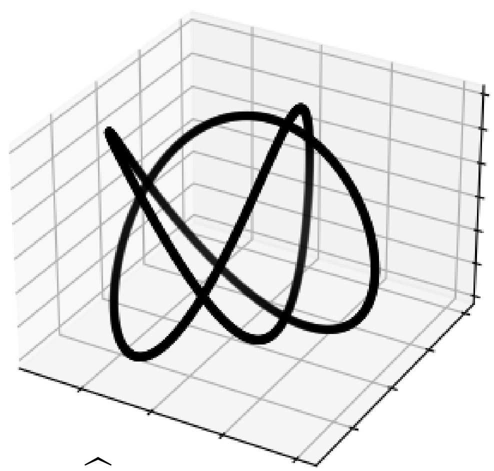




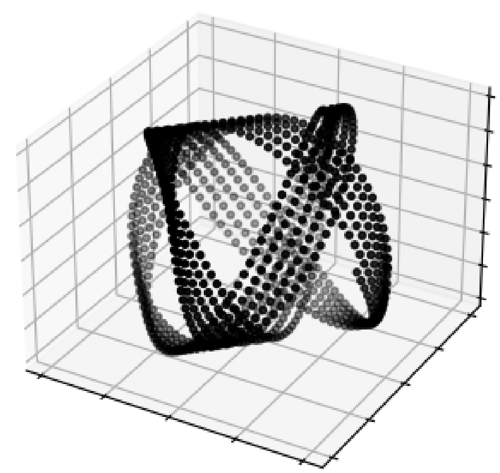
$\boxed{\text{Define } \widehat{\mathfrak{h}} \text{ as the subspace of } \mathfrak{gl}(n) \text{ spanned by the } d \text{ bottom eigenvectors of } \Lambda.}$

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

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

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

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

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

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

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

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

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

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 $\mathbb{R}^n$.

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

Lemma: The optimization problem is equivalent to

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

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

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

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

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$$A \in \mathrm{O}(n)$$

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

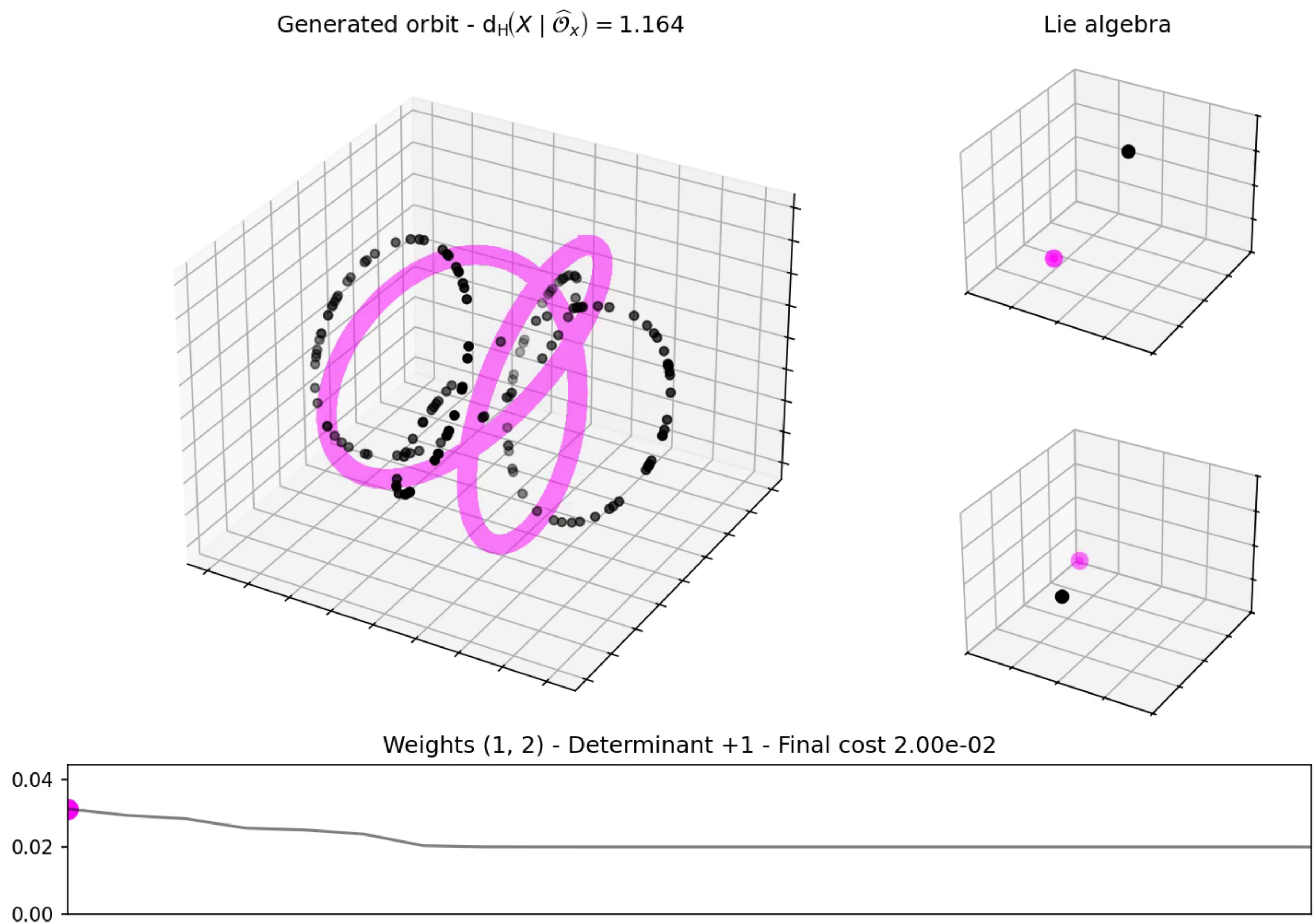
By denoting $B^i = \mathrm{d}\phi_i(\mathfrak{g})$, the element $\mathrm{d}\phi(\mathfrak{g})$ of $\mathfrak{orb}(G,n)$ is associated to $(B^1, \dots, B^p)$.

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

Closest Lie algebra

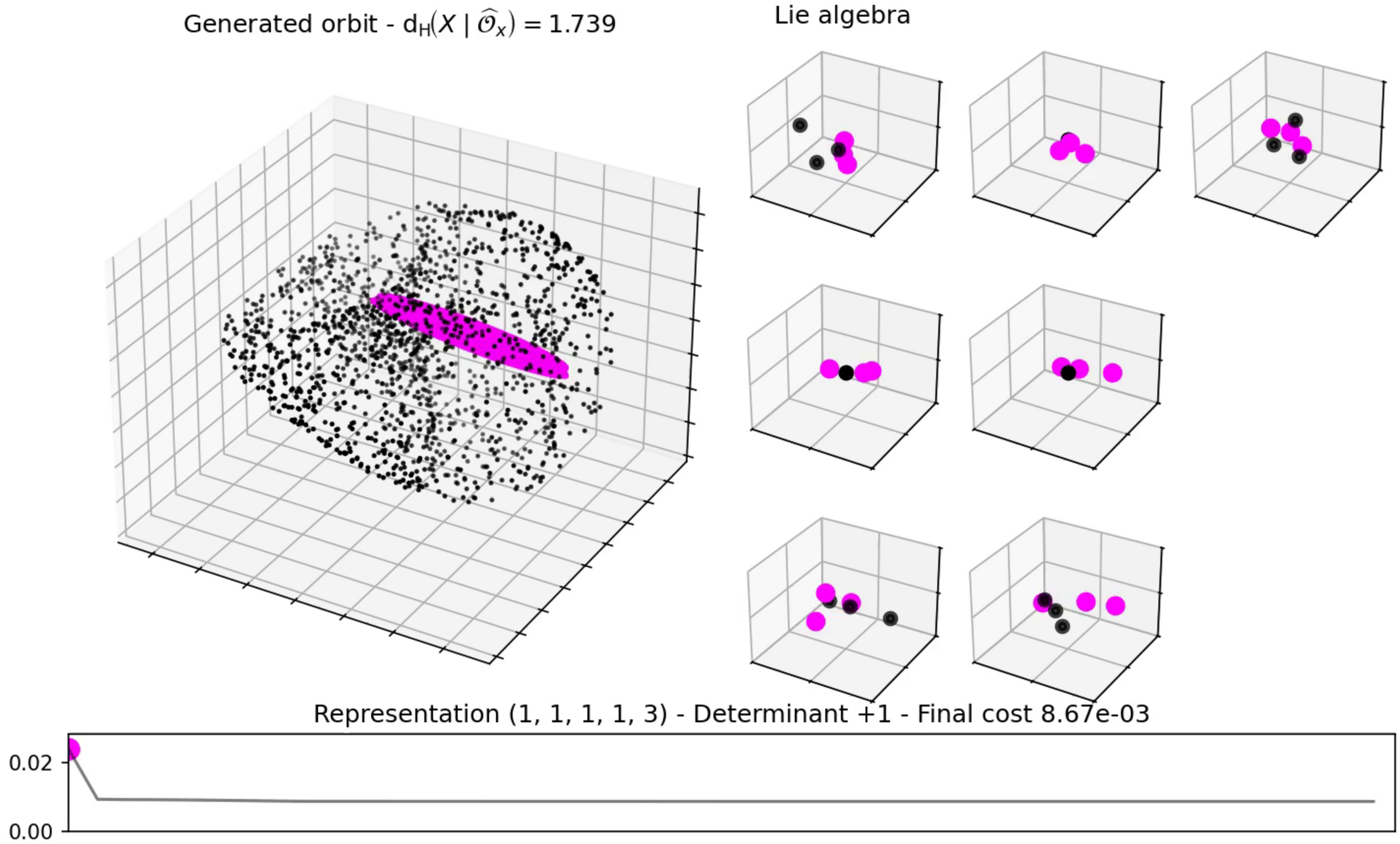
SO(2)-orbit in $\mathbb{R}^4$

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)	$+1 : 0.022$ $-1 : 0.005$



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)	$+1 : 0.005$



Reformulation of the optimization program:

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

reduces to:

- 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 $\mathrm{O}(n)$
- SO(3), SU(2) no reduction found

Fact: If G is compact, for every representation $G \to \mathrm{GL}_n(\mathbb{R})$, 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 μ_G, and define the **covariance matrix**

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

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

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

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

The algorithm

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

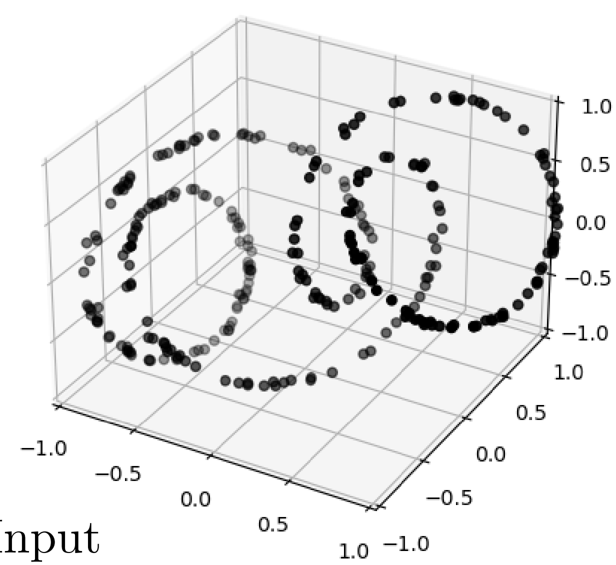
Output: A representation ϕ of G in $\mathbb{R}^n$, and an orbit $\mathcal{O}$ close to X.

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

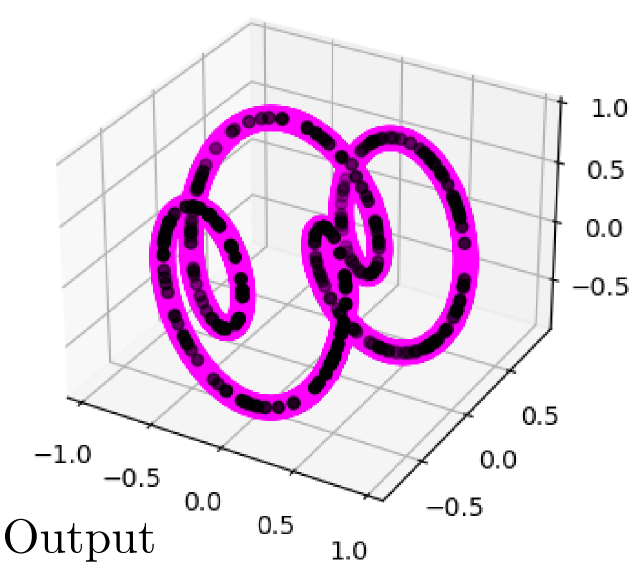
Step 2 (LiePCA): Diagonalize the operator $\Lambda\colon \mathrm{M}_n(\mathbb{R}) \to \mathrm{M}_n(\mathbb{R})$.

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

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.



Input



Output

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

The algorithm

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

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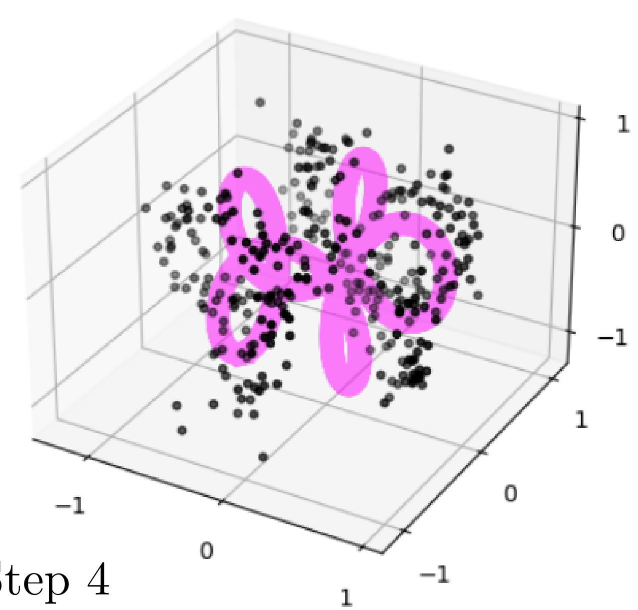
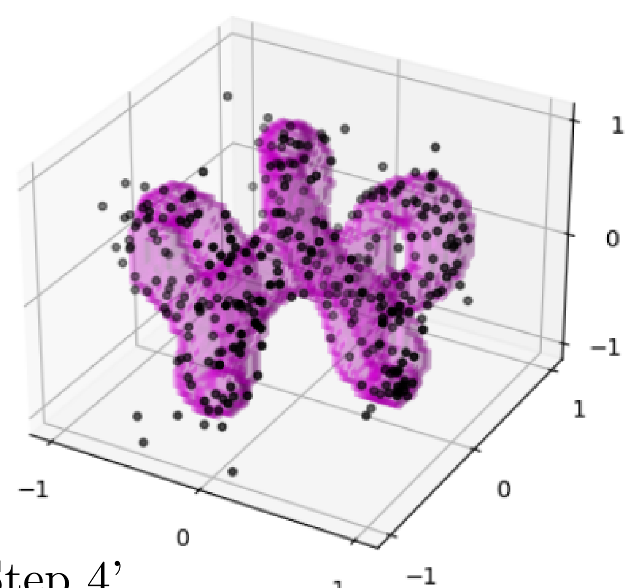
Step 4 (Distance to orbit): Choose a $x \in X$, generate $\widehat{\mathcal{O}}_x = \exp(\widehat{\mathfrak{h}}) \cdot x$ and verify that it is close to X.

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 μ_X.



Step 4



Step 4'

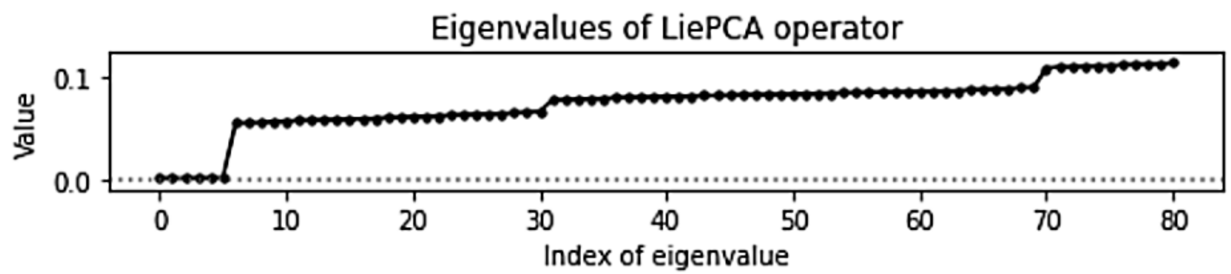
In **Step 4**, we compute the (non-symmetric) Hausdorff distance $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}_x\big)$.

In **Step 4'**, we compute the Wasserstein distance $\mathrm{W}_2\big(\mu_X, \mu_{\widehat{\mathcal{O}}}\big)$.

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

`LiePCA` shows a kernel of dimension 6.

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



We look for an action of SO(3) or SU(2). **Step 3** 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 $(3,5)$: $\mathrm{d_H}\left(X|\widehat{\mathcal{O}}_x\right) \approx 2.658$. However, $\mathrm{d_H}\left(\widehat{\mathcal{O}}_x|X\right) \approx 0.543$.

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

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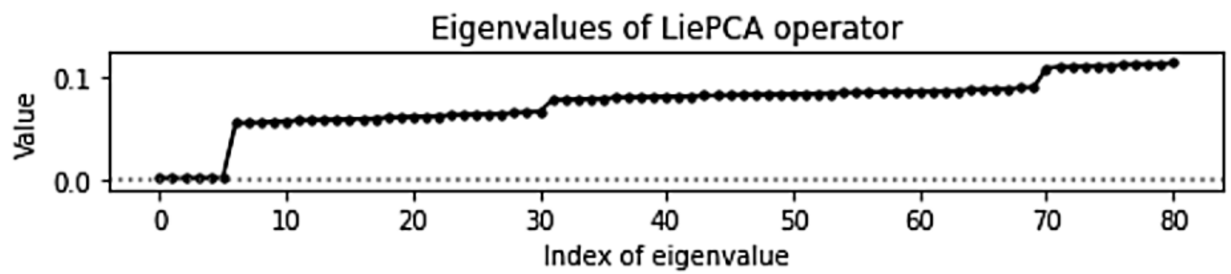

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action $\mathrm{SO}(3) \curvearrowright \mathrm{SO}(3)$ by conjugation (not transitive)

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

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

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

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

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

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

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

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

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

Robustness

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 $\phi\colon G \to \mathbb{R}^n$

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

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

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

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

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

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

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

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

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

$\arg\min \sum_{i=1}^{d} \lVert \Lambda[\mu](A_i) \rVert^2$
with $(A_i)_{i=1}^d \in \mathcal{V}^{\mathrm{Lie}}(G, \mathfrak{so}(n))$

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

Show that $\mathrm{W}_2\big(\mu_{\widehat{\mathcal{O}}_x}, \mu_{\mathcal{O}}\big)$ is small

Theorem: Under technical assumptions (sufficiently small $\mathrm{W}_2\big(\mu_X, \mu_{\mathcal{O}}\big)$), for a certain choice of parameters, the algorithm outputs a representation $\widehat{\phi}$ that is orbit-equivalent to ϕ.

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

$$\mathrm{W}_2\big(\mu_{\widehat{\mathcal{O}}}, \mu_{\mathcal{O}}\big) \leq \text{constant} \cdot \mathrm{W}_2\big(\mu_X, \mu_{\mathcal{O}}\big)^{1/4(l+3)}.$$

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

$$\mathrm{d_H}\big(\widehat{\mathcal{O}}_x, \mathcal{O}\big) \leq \text{constant} \cdot \mathrm{d}(x, \mathcal{O}) + \text{constant} \cdot \mathrm{W}_2\big(\mu_X, \mu_{\mathcal{O}}\big)^{1/4(l+3)}.$$

Theorem: Let G be a compact Lie group of dimension d, $\mathcal{O}$ an orbit of an almost-faithful representation $\phi\colon G \to \mathbb{R}^n$, 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. Let $X \subset \mathbb{R}^n$ be a finite point cloud and μ_X its empirical measure.

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

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

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

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

where

- $\rho = 16l(l+2)6^l \max(\mathrm{vol}(\widetilde{\mathcal{O}}), \mathrm{vol}(\widetilde{\mathcal{O}})^{-1}) / \min(1, \mathrm{reach}(\widetilde{\mathcal{O}}))$,
- $\sigma_{\max}^2$, $\sigma_{\min}^2$ 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 $\upsilon = \left(\frac{\mathbb{V}\left[\|\mu_{\mathcal{O}}\|\right]}{\sigma_{\min}^2}\right)^{1/2}$,
- r is the radius of local PCA (estimation of tangent spaces),
- λ the bottom nonzero eigenvalue of the ideal Lie-PCA operator $\Lambda_{\mathcal{O}}$.

Technical assumptions: Define the quantities

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

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

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

Suppose that ω is small enough, so as to satisfy

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

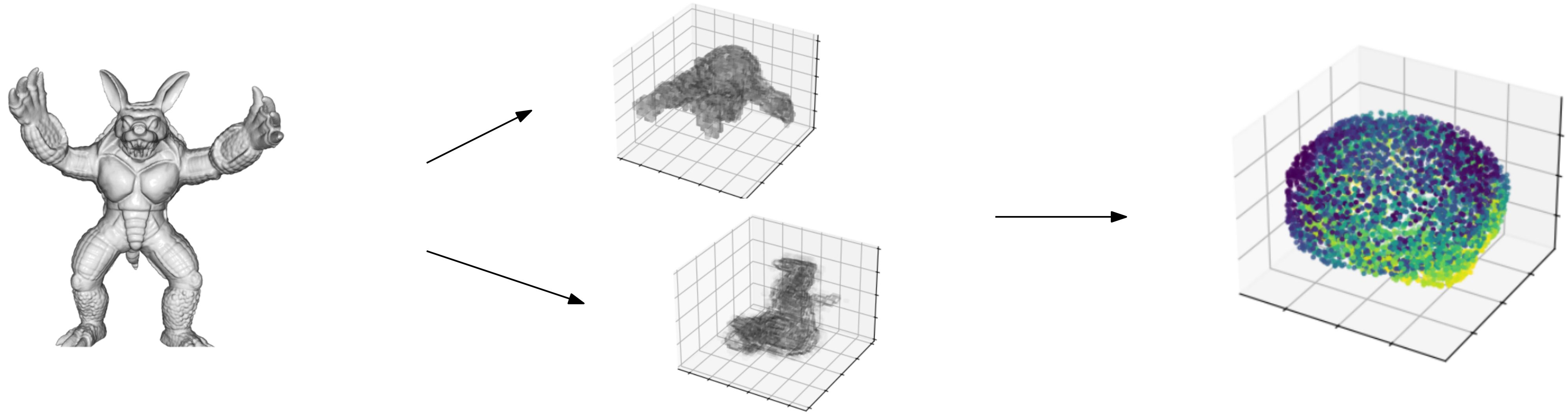
Choose two parameters ϵ and r in the following nonempty sets:

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

Moreover, we suppose that

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

Orientation estimation



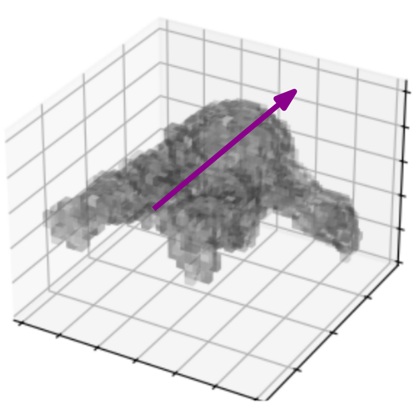
(1) Take a $m \times m \times m$ image.

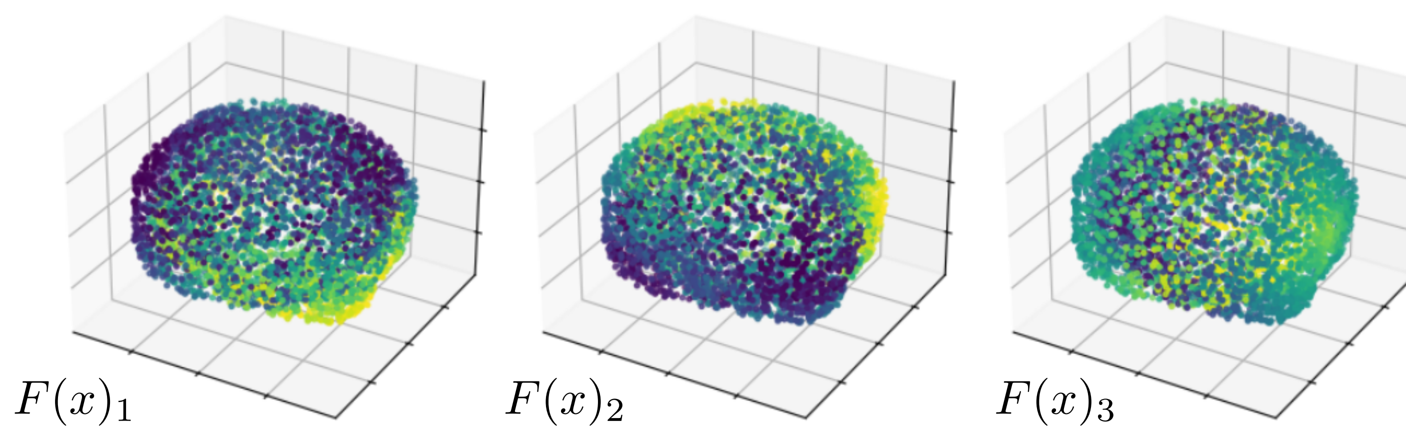
(2) Generate several rotations to get a point cloud $X \subset \mathbb{R}^{m \times m \times m}$.

(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%.





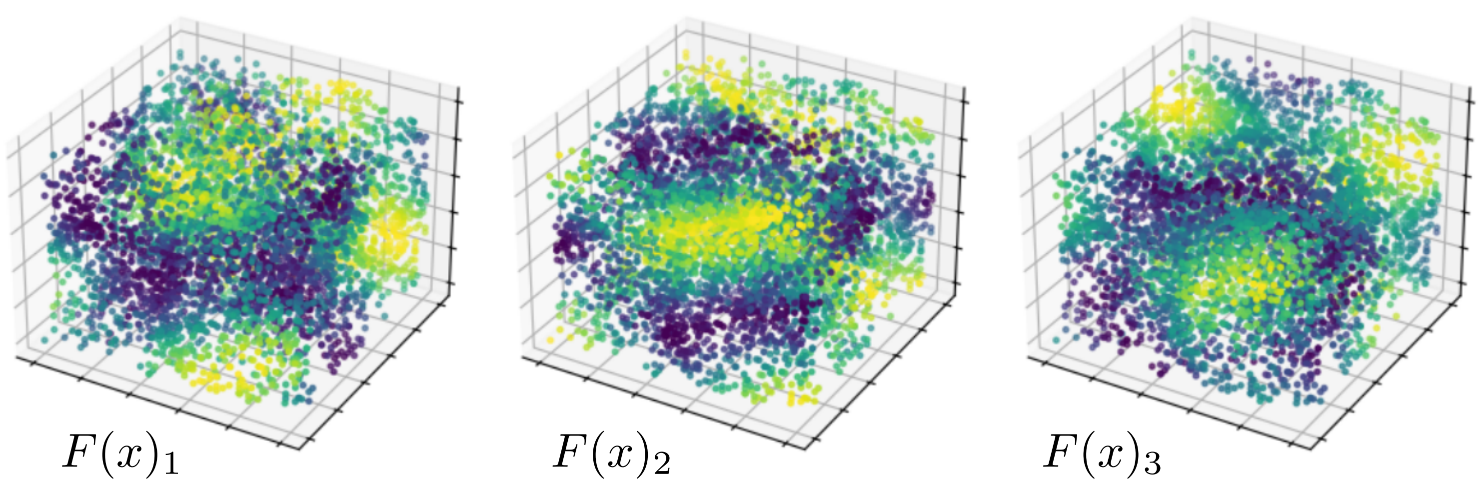
Conventional solution: Train a SVM.

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

$$\begin{tikzcd} \mathrm{SO}(3) \arrow[r, "\phi"] & \mathrm{GL}_n(\mathbb{R}) \\ \mathfrak{so}(3) \arrow[u, "\exp"] \arrow[r, "\mathrm{d}\phi"] & \mathfrak{gl}(n) \arrow[u, "\exp"'] \end{tikzcd}$$

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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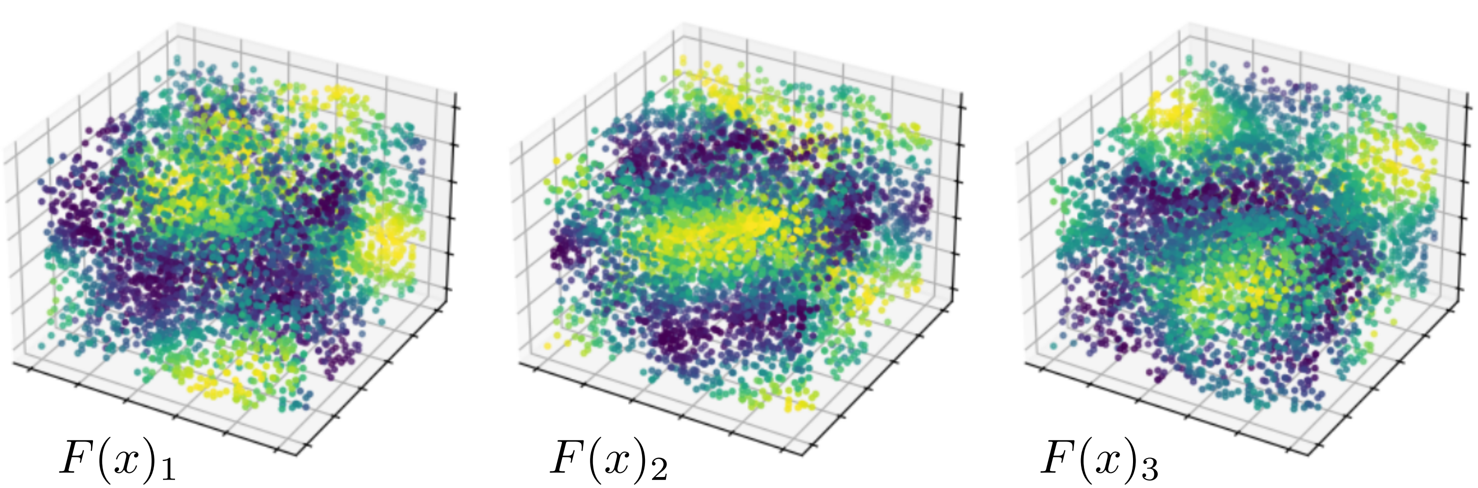
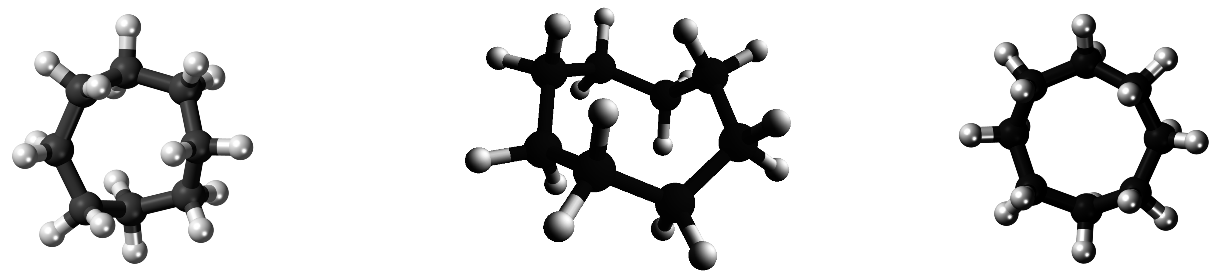
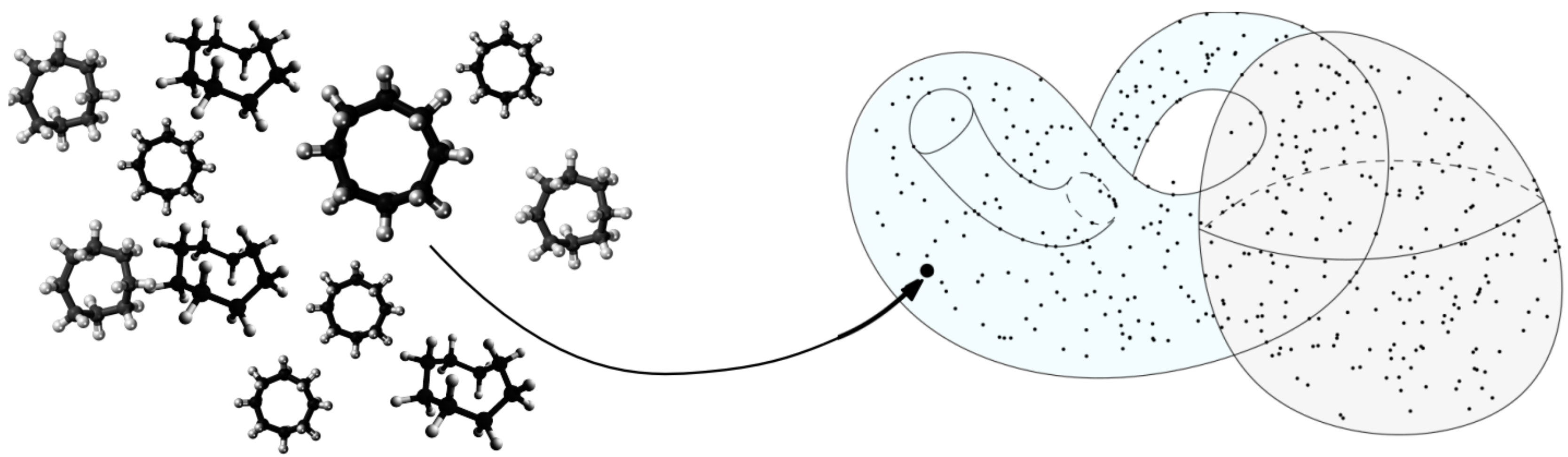


Model	MSE on test data
SVM in dimension 3	0.4003
SVM in dimension 4	0.2496
SVM in dimension 5	0.1295
SVM in dimension 6	0.0380
SVM in dimension 7	0.0148
SVM in dimension 8	0.0119
SVM in dimension 9	0.0114
SVM in dimension 10	0.0122
SVM on orthogonal coordinates	**0.0066**



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 $X \subset \mathbb{R}^{72}$.

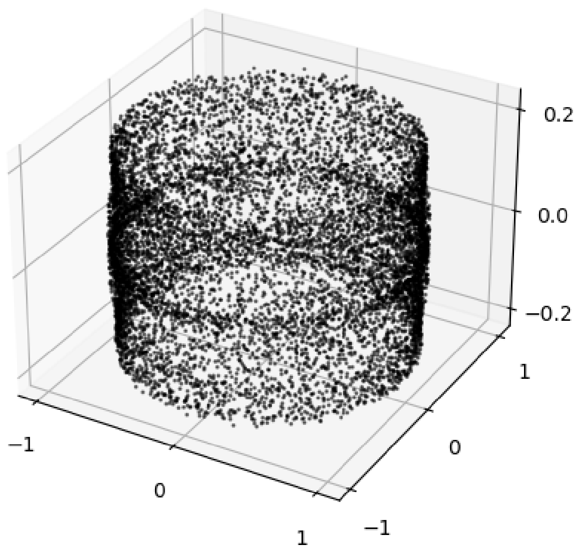


[Martin, Thompson, Coutsias & Watson, Topology of cyclo-octane energy landscape, 2010]

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

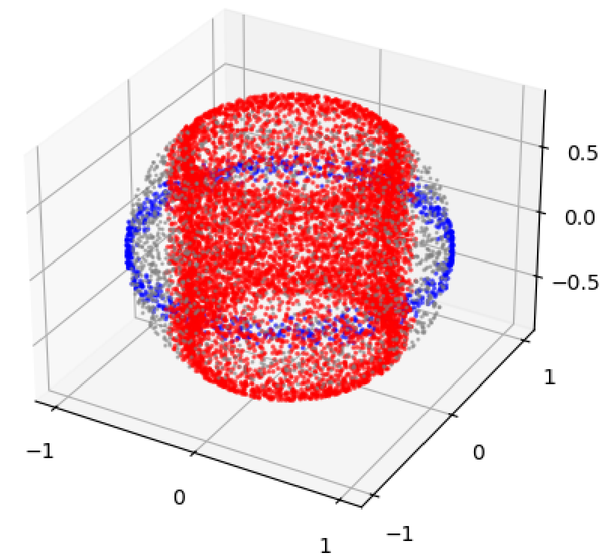
Conformational space of cyclooctane C_8H_{16}

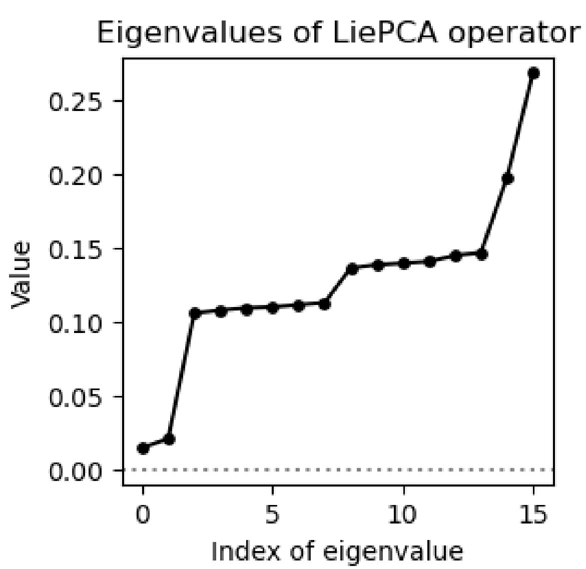
Unaligned confomers: We generate 10,000 cyclooctane confomers without aligning them.



Projected in dimension 3, we see a cylinder surrounded by a circle.

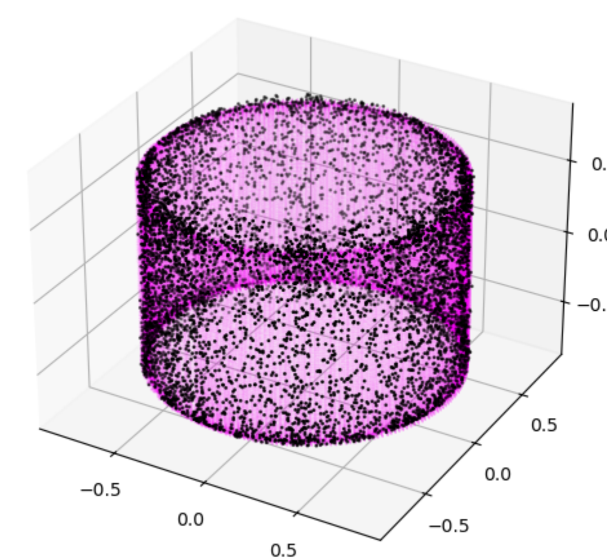
X is projected onto $\mathbb{R}^4$ and orthonormalized. After discarding 15% of the outliers (gray), two clusters appear. We take the red one.





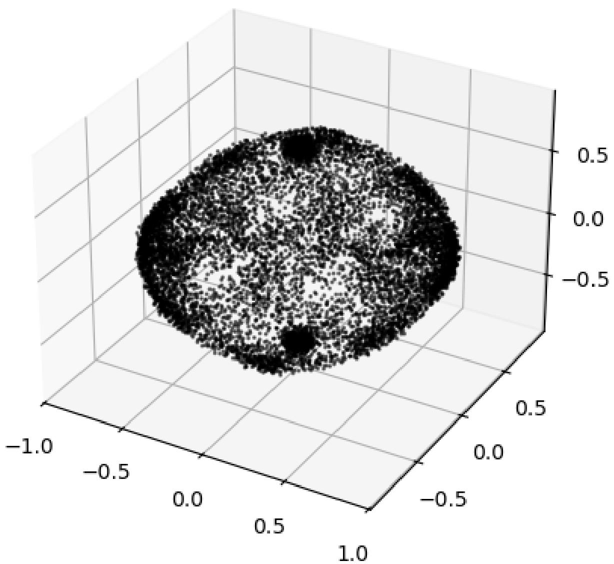
`LiePCA` has two small eigenvalues, suggesting a symmetry group of dim 2.

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



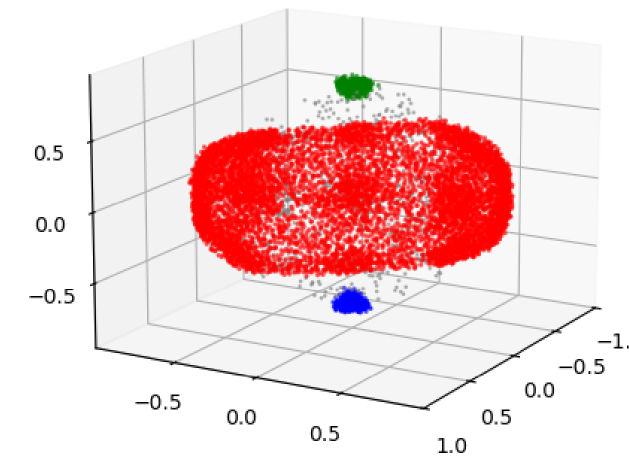
Conformational space of cyclooctane C_8H_{16}

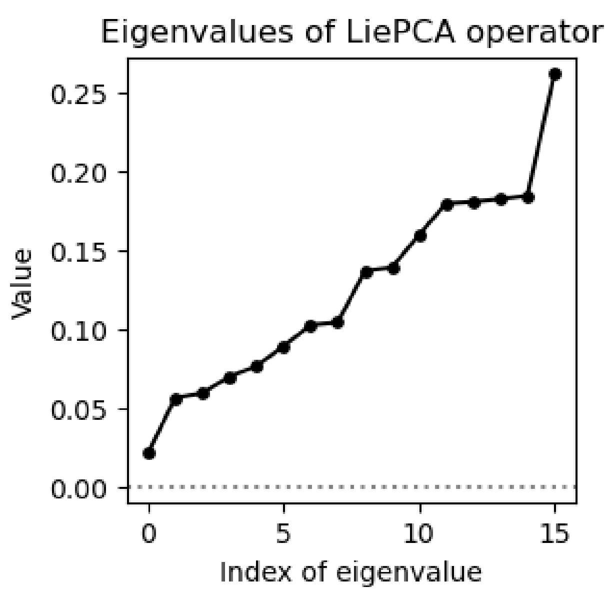
Aligned confomers: We now generate 10,000 aligned confomers (`AlignMolConformers` in `RDKit`).



We see three components:
a surface and two clusters.

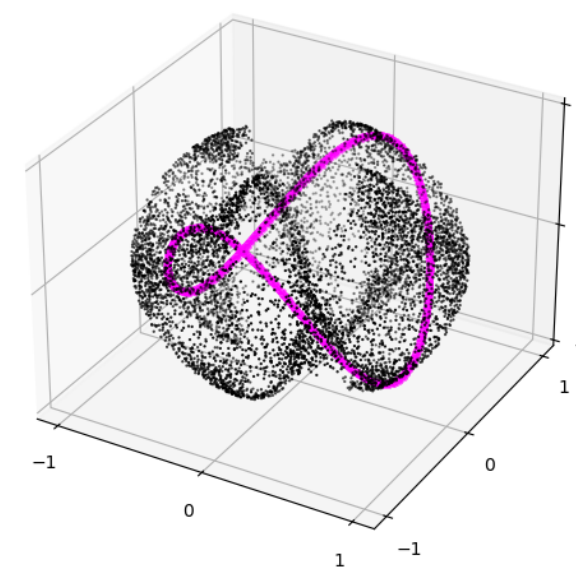
After discarding 10% of the outliers (gray),
the points are grouped into three classes.
We keep the red class.





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

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



Consider a neural network $$V = V_1 \xrightarrow{f_1} V_2 \xrightarrow{f_2} V_3 \xrightarrow{f_3} \cdots \xrightarrow{f_{p-1}} V_p = W.$$

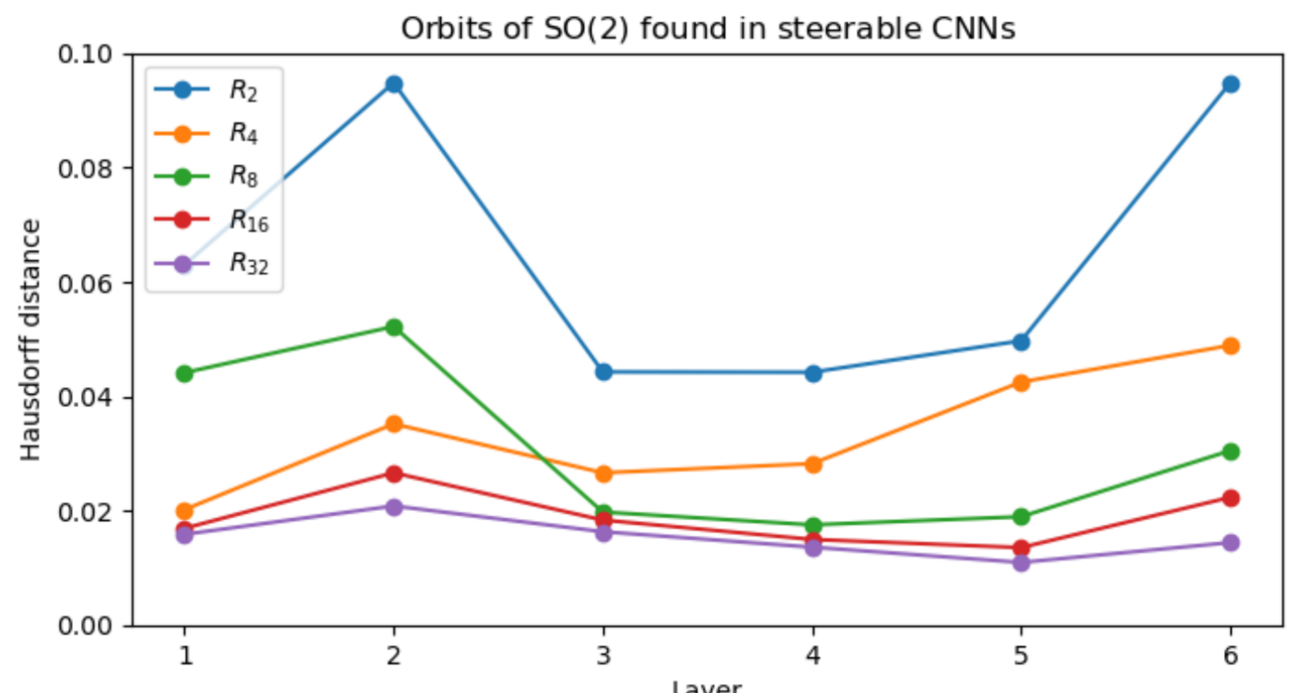
Denote $\mathcal{F}_i = f_1 \cdots f_i$ and $\mathcal{F} = \mathcal{F}_{p-1}$.

Say G acts linearly on V, via $\phi\colon G \to \mathrm{GL}(V)$.

The network is **equivariant** if there exists representations $\phi_i\colon G \to \mathrm{GL}(V_i)$ 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 SO(2).



`https://arxiv.org/abs/2309.03086`

`https://github.com/HLovisiEnnes/LieDetect`

Thanks!

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

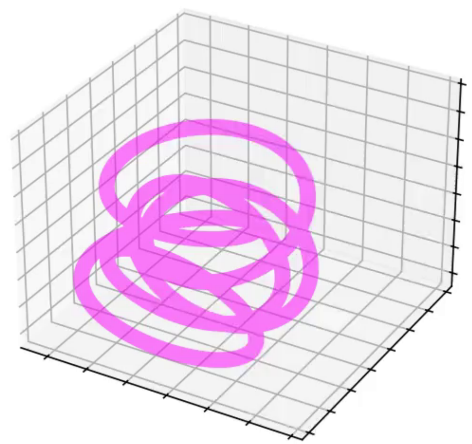
$$\begin{tikzcd} G \arrow[r, "\phi"] & \mathrm{Diff}(\mathcal{M}) \\ \mathfrak{g} \arrow[u, "\exp"] \arrow[r, "\mathrm{d}\phi"] & \mathscr{X}(\mathcal{M}) \arrow[u, "\exp"'] \end{tikzcd}$$

Statistical guarantees to test the linear-orbit hypothesis.

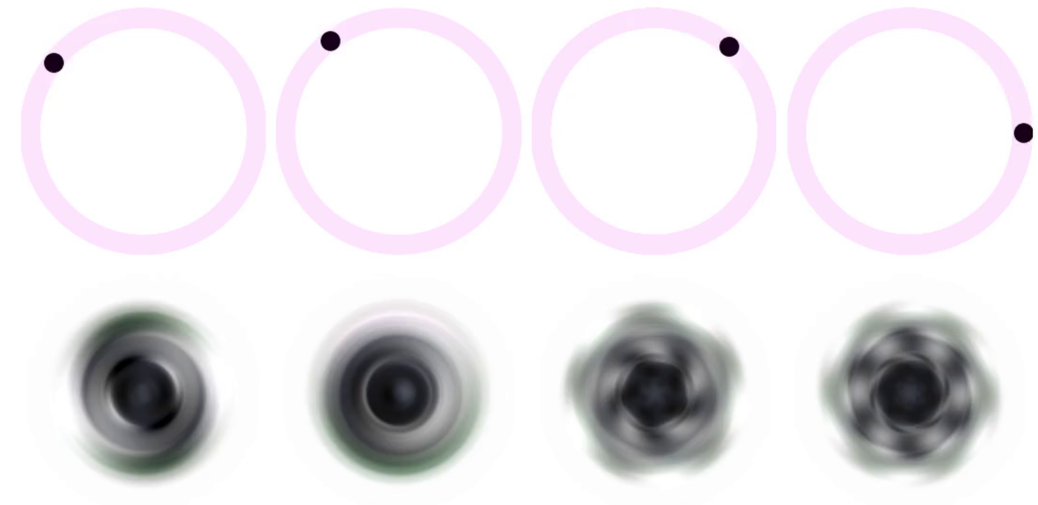
Additional experiments: Pixel permutations

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:

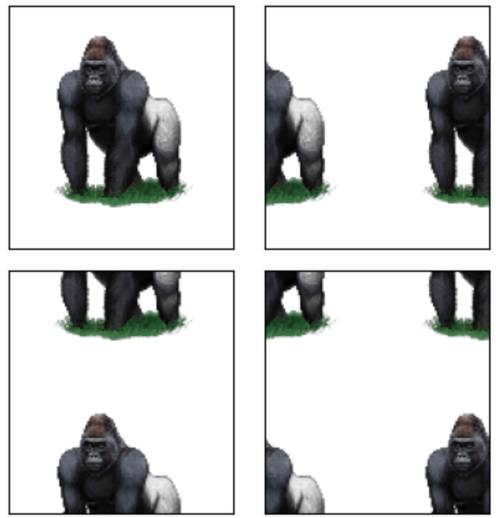
$$0.155,\quad 0.155,\quad 0.11,\quad 0.11,\quad 0.041,\quad 0.041,\quad 0.04,\quad 0.04,\quad 0.038,\quad 0.038,\quad 0.026,\quad 0.026,\quad \ldots$$

In these eigenplanes, the orbit is close to

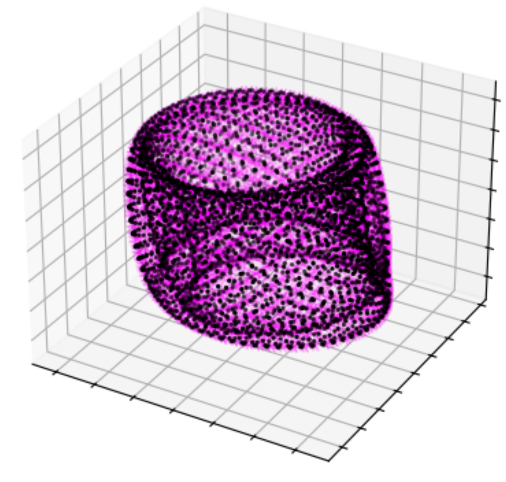
$$\theta \longmapsto \begin{pmatrix} \mu_1 \cos\omega_1\theta \\ \mu_1 \sin\omega_1\theta \\ \mu_2 \cos\omega_2\theta \\ \mu_2 \sin\omega_2\theta \\ \vdots \\ \mu_k \cos\omega_k\theta \\ \mu_k \sin\omega_k\theta \end{pmatrix} = \begin{pmatrix} \cos\omega_1\theta & -\sin\omega_1\theta & & & & & \\ \sin\omega_1\theta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

Additional experiments: Pixel permutations

Translations of $m \times m$ RGB image



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



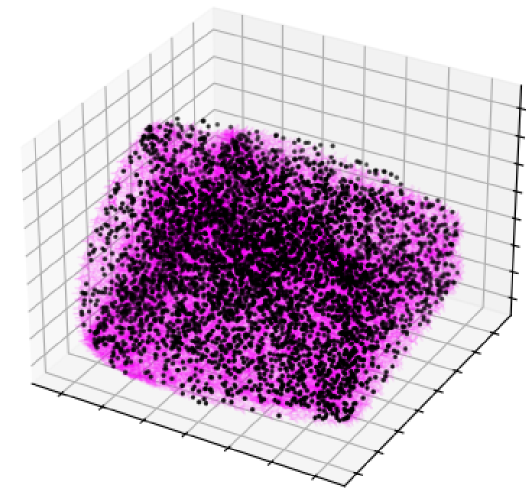
Covariance matrix eigenvalues: 0.228, 0.228, 0.142, 0.142, 0.108, 0.108, 0.022, 0.022, ...

In these eigenplanes, the orbit is close to

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

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

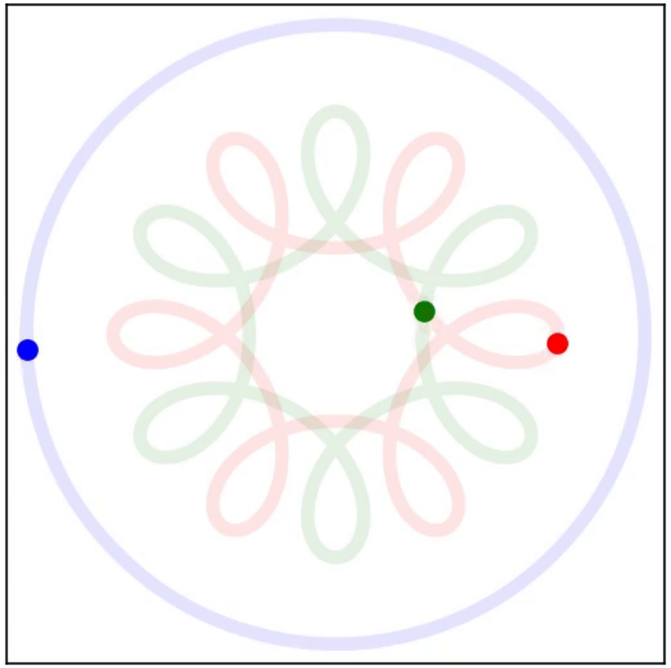
$$\theta^{(1)}, \theta^{(2)}, \theta^{(3)} \longmapsto \text{ linear action of } \mathrm{SO}(3) \text{ on } \begin{pmatrix} \mu_1 \\ 0 \\ \vdots \\ \mu_2 \\ 0 \\ \vdots \end{pmatrix}$$

In 1975, Roger Broucke found several periodic orbits.

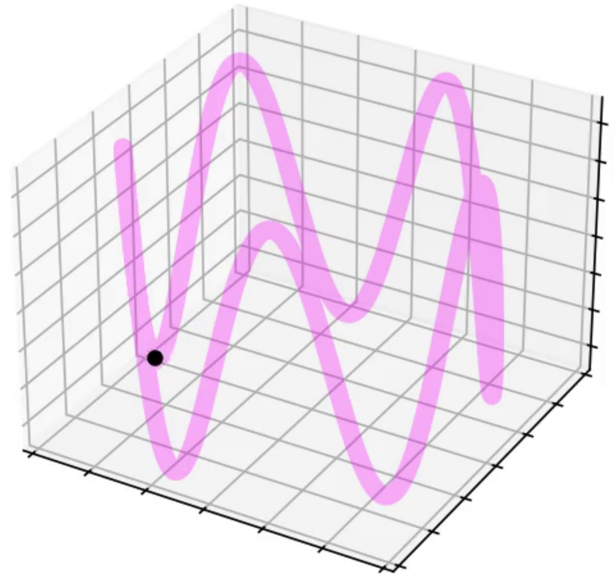
Let $x_1(t)$, $x_2(t)$, $x_3(t)$ be the three bodies, and define $z(t) = (x_1(t), x_2(t), x_3(t)) \in \mathbb{R}^6$.

<u>Orbit `A3`</u>

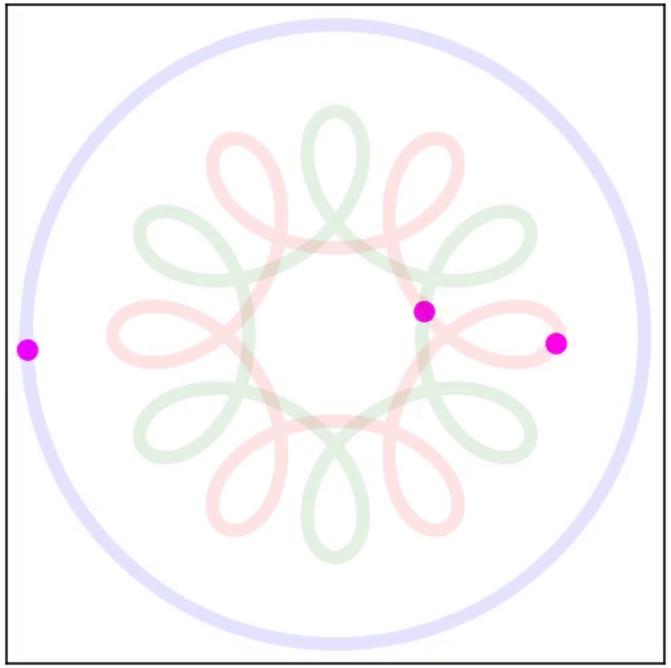
Trajectory of x_1, x_2, x_3
(found by integration)



Trajectory of z



Reconstructed orbit of SO(2)

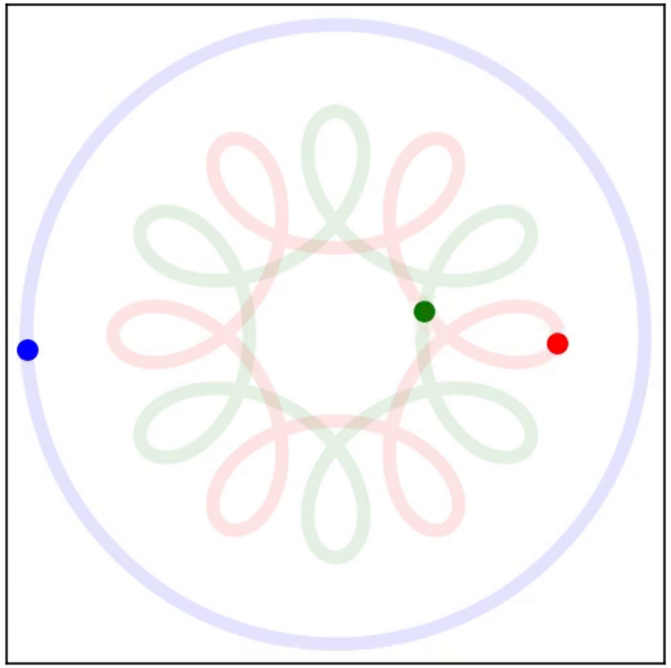


In 1975, Roger Broucke found several periodic orbits.

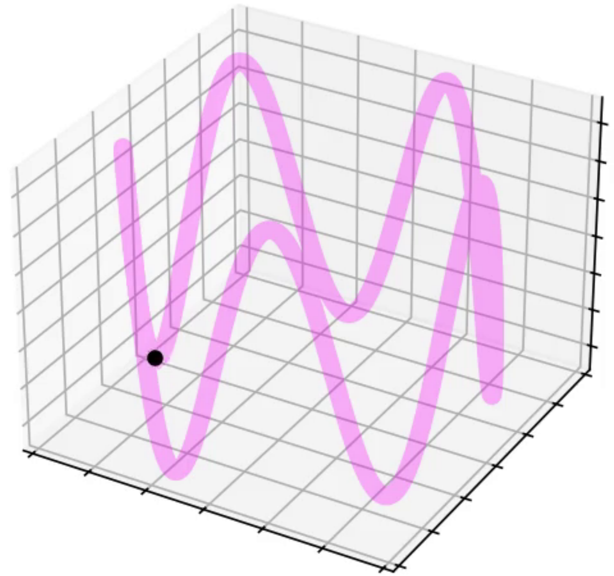
Let $x_1(t)$, $x_2(t)$, $x_3(t)$ be the three bodies, and define $z(t) = (x_1(t), x_2(t), x_3(t)) \in \mathbb{R}^6$.

Orbit `R2`

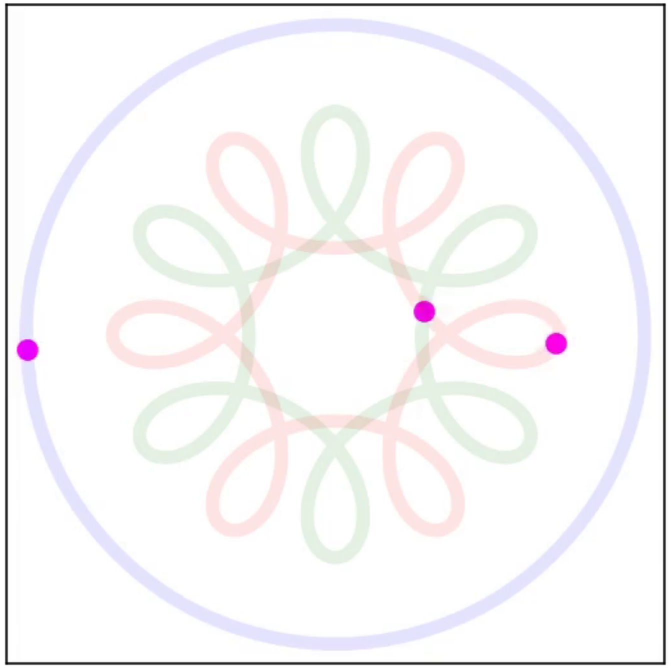
Trajectory of x_1, x_2, x_3
(found by integration)



Trajectory of z



Reconstructed orbit of SO(2)



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

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

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

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

The corresponding pushforward Lie algebra is spanned by the matrix

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

In this context, the minimization problem reads

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

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**.

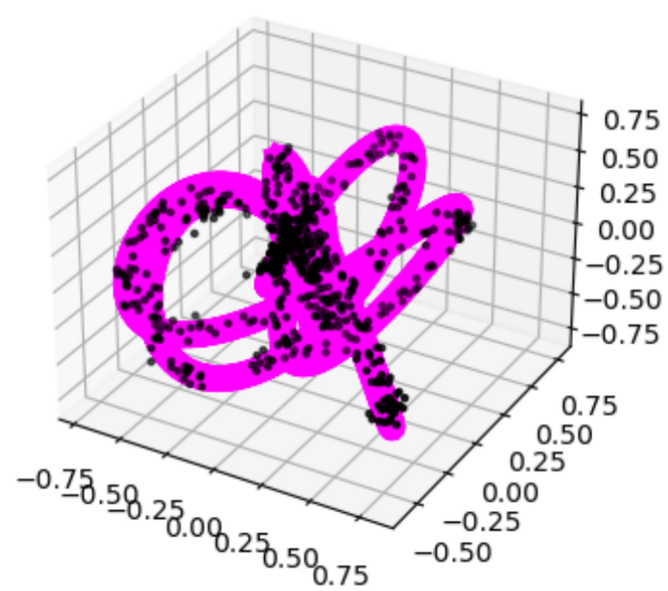
Example: We consider a representation of SO(2) in $\mathbb{R}^{10}$ with frequencies $(2,4,5,7,8)$ and sample 600 points on one of its orbits, that we corrupt with a Gaussian additive noise of deviation $\sigma = 0.03$.

We perform the minimization over all representations of 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	**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.

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



Let $G = T^d$ the torus of dim d. The output of `LiePCA` is a d-tuple $(A_1, \ldots, A_d)$ of skew symmetric matrices.

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

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

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

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

In this context, the minimization problem reads

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

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

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

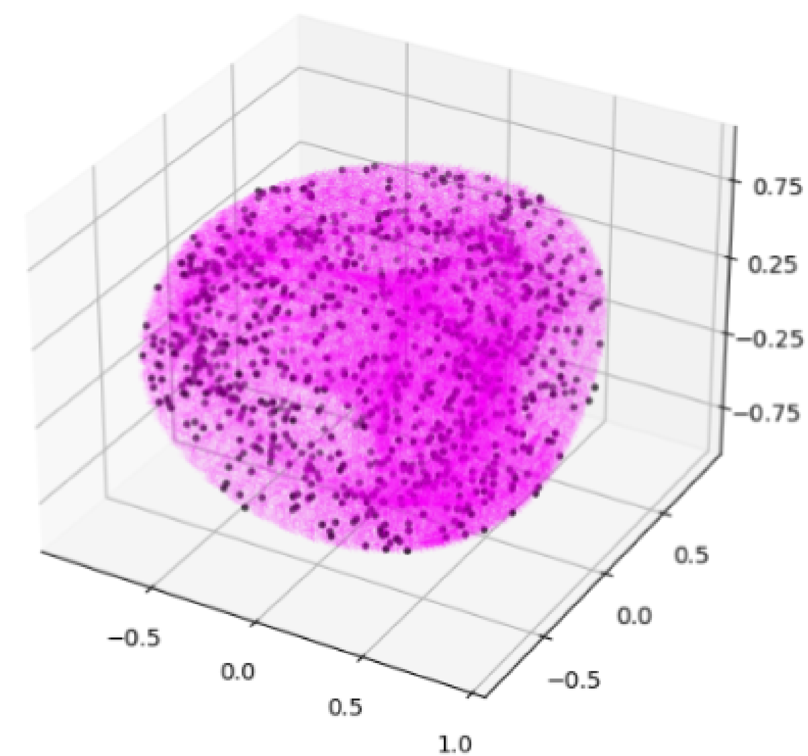
Example: Let X be a uniform 750-sample of an orbit of the representation $\phi_{\left(\begin{smallmatrix}1 & 1 & 2\\ 1 & 2 & 1\end{smallmatrix}\right)}$ of the torus T^2 in $\mathbb{R}^6$.

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	**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

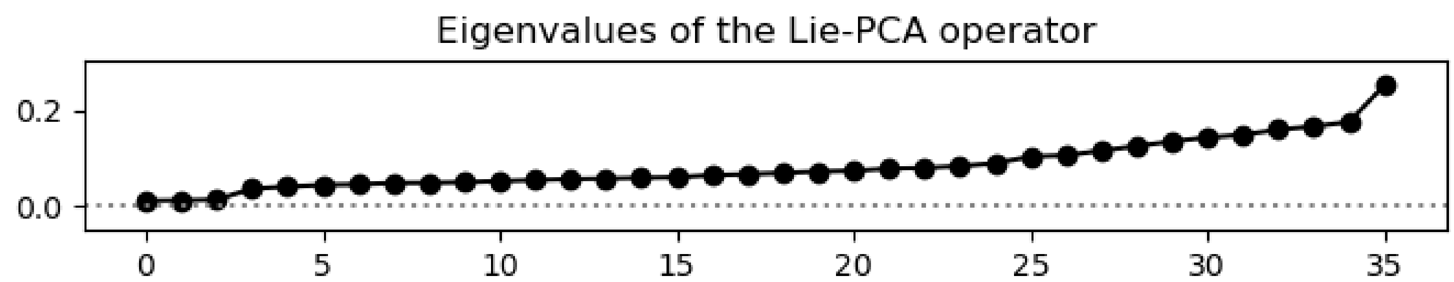
The algorithm's output is $\left(\begin{smallmatrix}0 & 1 & 1\\ 2 & -2 & 1\end{smallmatrix}\right)$. It is equivalent to $\phi_{\left(\begin{smallmatrix}1 & 1 & 2\\ 1 & 2 & 1\end{smallmatrix}\right)}$.

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



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 $\mathrm{SU}(2)$ in $\mathbb{R}^6$.



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

Representation of 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	**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 $\mathrm{d_H}\big(X|\widehat{\mathcal{O}}\big) \approx 0.751$.

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, 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

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

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

Define $\Lambda \colon \mathrm{M}_n(\mathbb{R}) \to \mathrm{M}_n(\mathbb{R})$ as $$\Lambda(A) = \frac{1}{N} \sum_{1 \leq i \leq N} \widehat{\Pi}\big[\mathrm{N}_{x_i} X\big] \cdot A \cdot \Pi\big[\langle x_i \rangle\big]$$

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

Explanation: On the one hand, $\mathfrak{sym}(\mathcal{O}) = \big\{ A \in \mathrm{M}_n(\mathbb{R}) \mid \forall x \in \mathcal{O}, Ax \in \mathrm{T}_x\mathcal{O} \big\}$. Thus,

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

On the other hand, considering only X, one has

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

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

Ideal Lie-PCA: Suppose that $\mathcal{O}$ is an orbit of the representation $\phi\colon G \to \mathrm{M}_n(\mathbb{R})$, and $\mu_{\mathcal{O}}$ its uniform measure. 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., $\sigma_{\max}^2/\sigma_{\min}^2 = 1$.

Stability: Comparing

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

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

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

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

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

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

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

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

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

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

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:

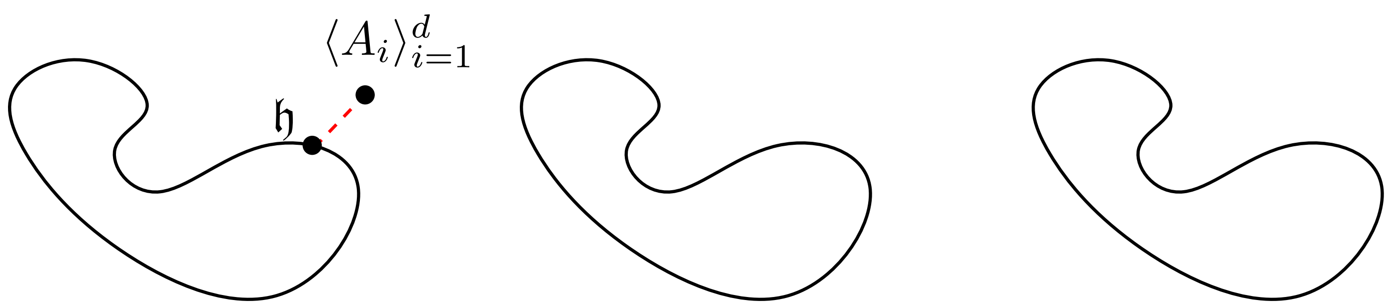
$$\|\Lambda_{\mathcal{O}} - \Lambda\|_{\mathrm{op}} \leq \sqrt{2}\rho\left(r + 4\left(\frac{\mathrm{W}_2(\mu_{\mathcal{O}},\mu_X)}{r^{l+1}}\right)^{1/2}\right).$$

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

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

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.

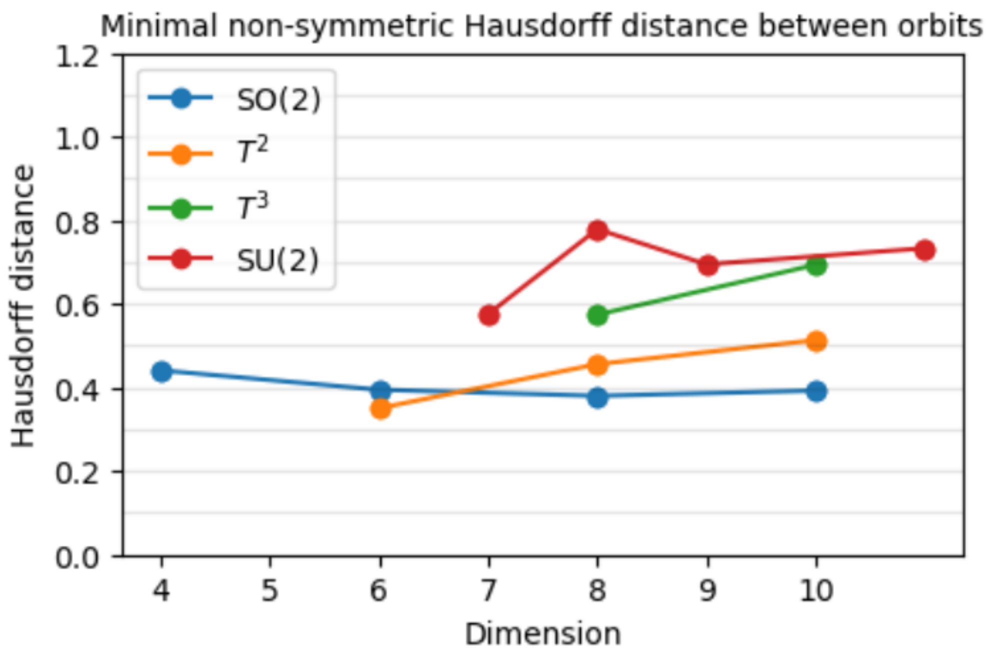


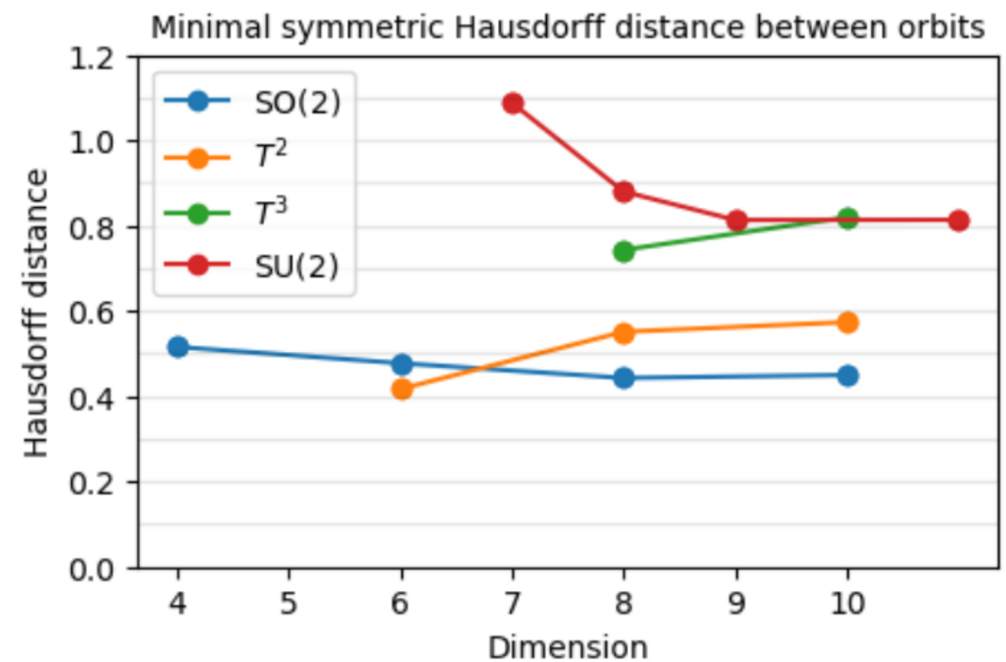
The distance from $\langle A_i \rangle_{i=1}^d$ to $\mathfrak{h}$ must be lower than the *reach* of $\mathcal{G}(G, \mathfrak{so}(n))$. In this context, it is called *rigidity*:

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

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 $\mathrm{d_H}\big(\widehat{\mathcal{O}}_x^1 | \widehat{\mathcal{O}}_x^2\big)$ between two orbits of a same initial point x for two non-orbit equivalent representations ϕ_1, ϕ_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 $\mathrm{d_H}\big(\widehat{\mathcal{O}}_x^1, \widehat{\mathcal{O}}_x^2\big)$. 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 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 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) 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) SU(2)