XIV Brazilian Workshop on Continuous Optimization - 08/03/2024

DETECTION OF REPRESENTATION ORBITS OF COMPACT LIE GROUPS FROM POINT CLOUDS

Henrique Ennes - DataShape/COATI (Sophia Antipolis)
Raphaël Tinarrage - EMAp/FGV (Rio de Janeiro)

The idea of symmetry in the late XIX century

Bernhard Riemann
1826 - 1866

Sophus Lie
1842 – 1899

Wilhelm Killing
1847 - 1923

Felix Klein
1849 – 1925

Élie Cartan
1869 - 1951

Hermann Weyl
1885 – 1955

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

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

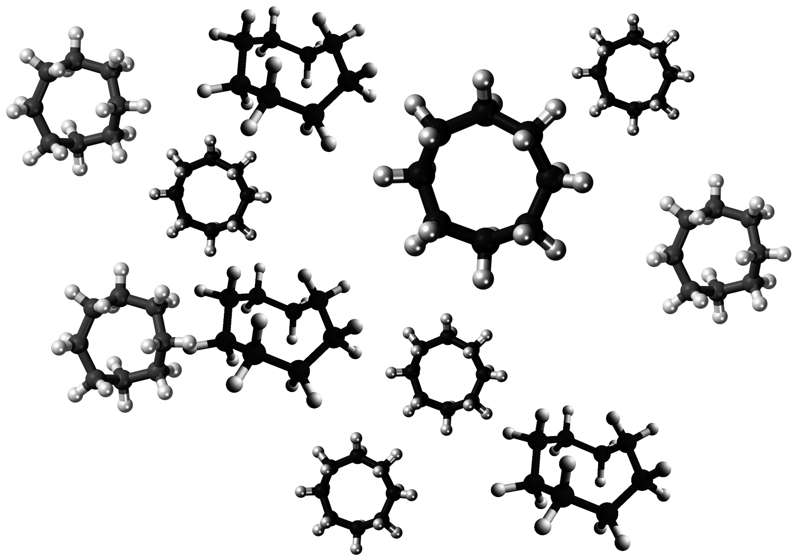
1913, E. Cartan, Theorem of the highest weight:
The irreducible representations of Lie groups are classified by their highest weights.

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

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

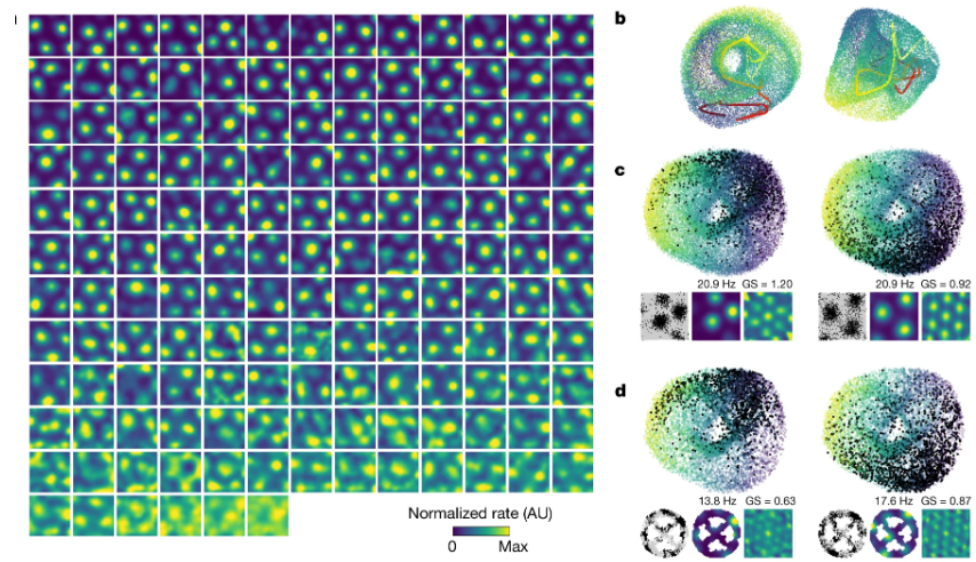
(1) Certain real-life experiments exhibit symmetric objects.

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



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

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

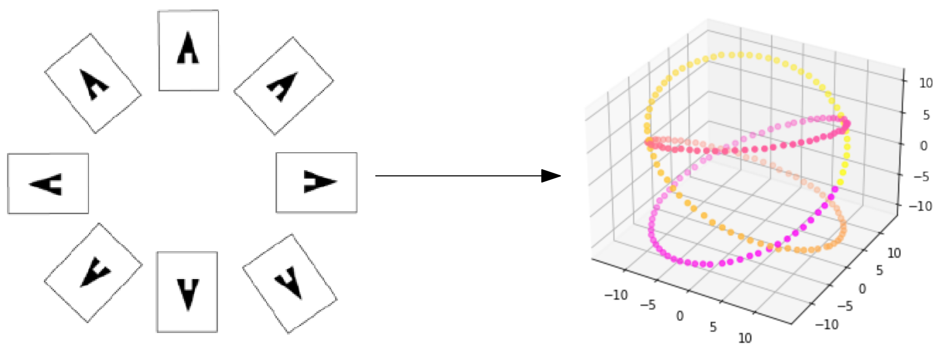


The firing matrix of grid cells in rat brains shows the connecivity of a **torus**.

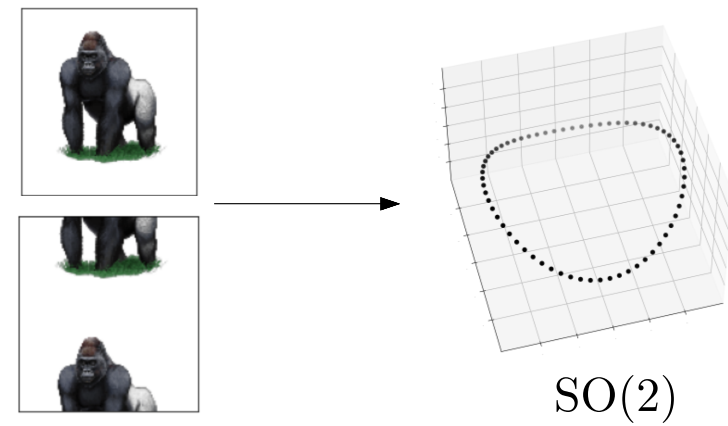
Symmetries in datasets

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

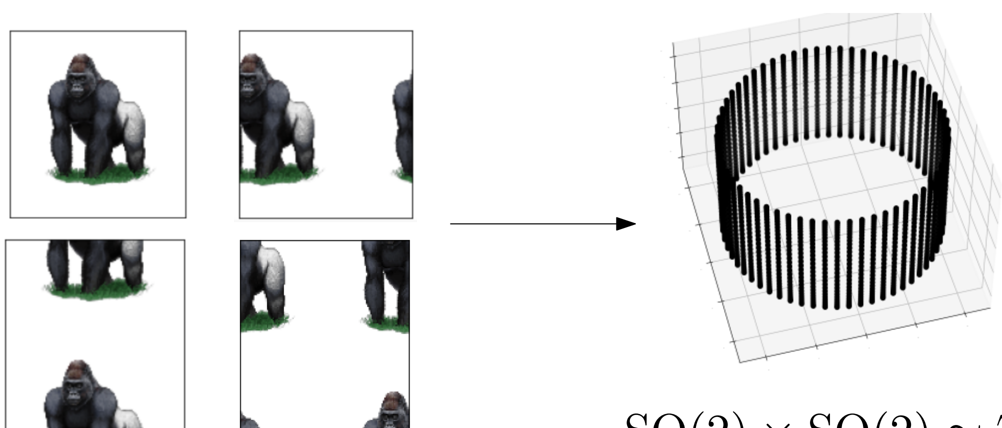
(2) Euclidean transformations are governed by Lie group representations.



$\mathrm{SO}(2)$



$\mathrm{SO}(2)$



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

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

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

Symmetries in datasets

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

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

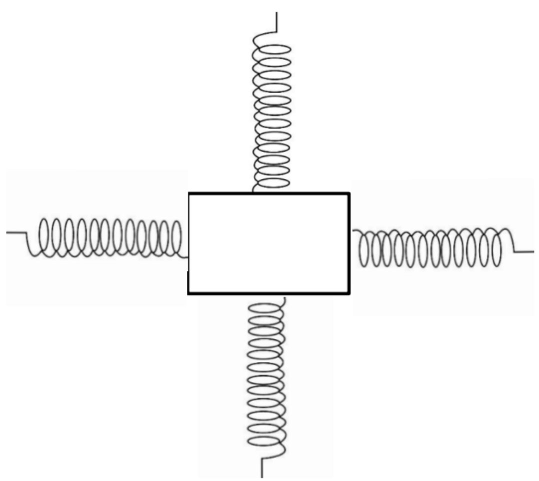
(3) Symmetries in Hamiltonian systems yield conservation laws.

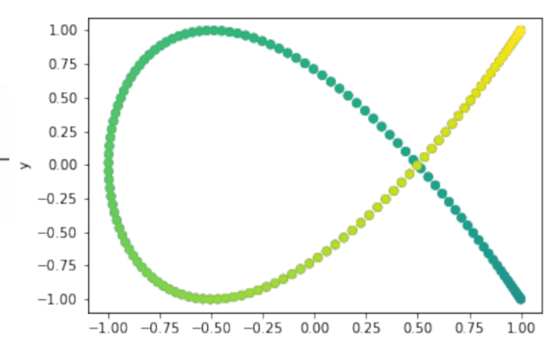
Hamiltonian's systems follow the equations $\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial \mathbf{q}} \qquad \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \frac{\partial H}{\partial \mathbf{p}}.$

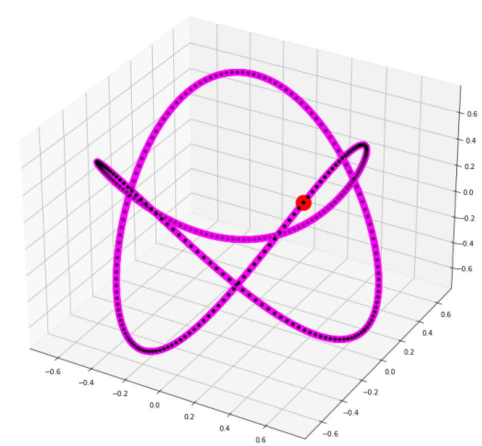
Let ω be the canonical symplectic form in $\mathbb{R}^{2n}$. A *symplectomorphism* is a Lie group representation $L : G \to \mathrm{GL}_{2n}(\mathbb{R})$ on $\mathbb{R}^{2n}$ that preserves the the system's dynamics, i.e. $L(g)^*\omega = \omega \ \forall g \in G$.

Emmy Noether
1882 - 1935

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







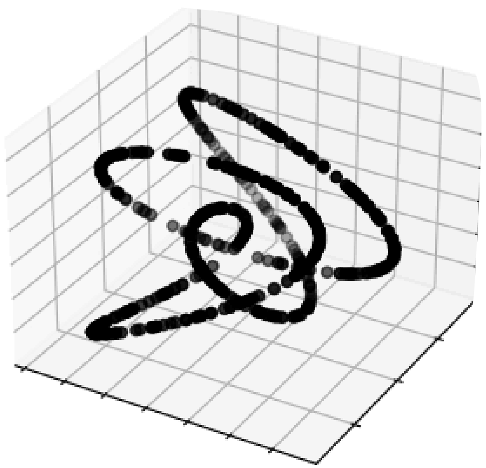
Formulation of our problem

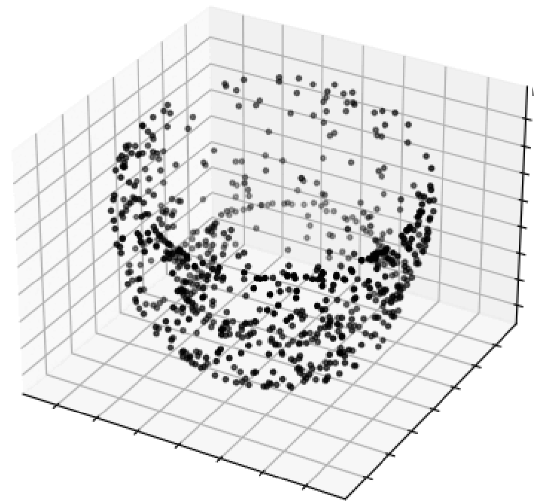
Input: A point cloud $X = \{x_1 \ldots, x_N\} \subset \mathbb{R}^n$.

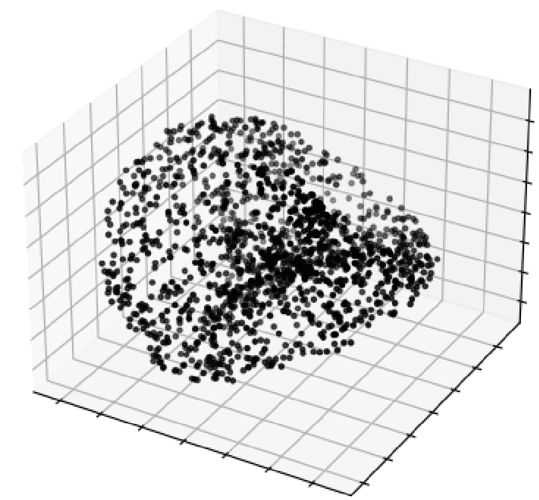
Output: A compact Lie group G, a representation ϕ of it in $\mathbb{R}^n$, and an orbit $\mathcal{O}$ close to X.

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

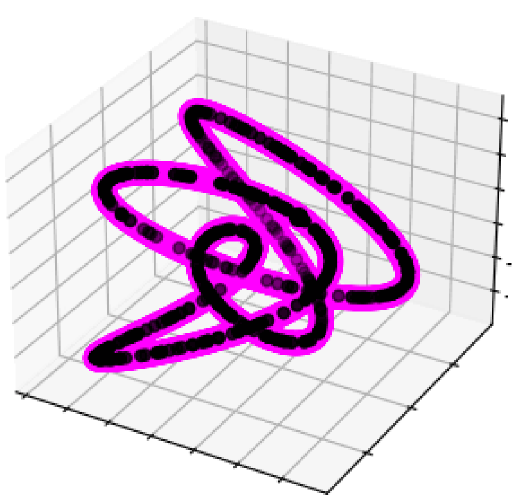
Input:

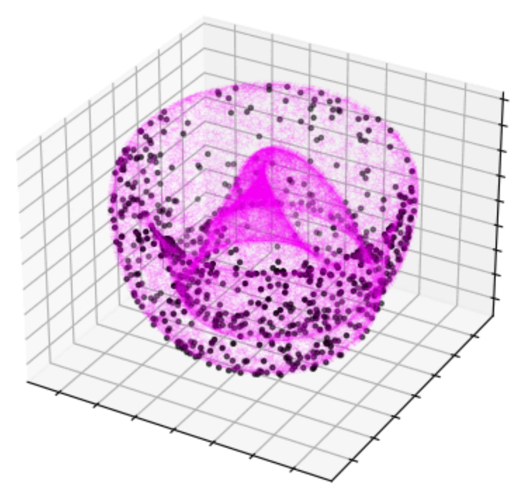


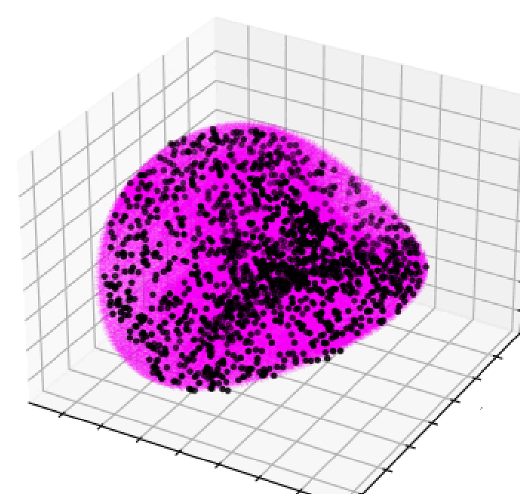




Output:







1. Lie group - Lie algebra correspondence
2. Closest Lie algebra problem
3. Examples

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

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

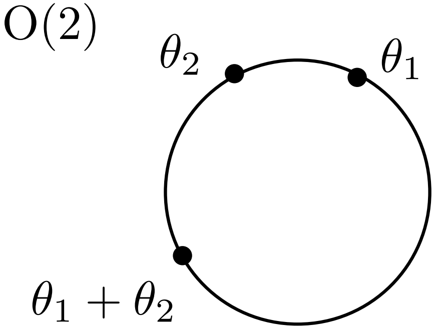
- $\mathrm{O}(n)$ orthogonal group: the set of orthogonal $n \times n$ matrices $(A^\top = A^{-1})$
- $\mathrm{SO}(n)$ special orthogonal group: set of orthogonal $n \times n$ matrices of determinant $+1$
- $\mathrm{Sp}(2n, \mathbb{C})$ symplectic group: the set of complex sympletic $n \times n$ matrices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

Products of Lie groups are Lie groups:

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

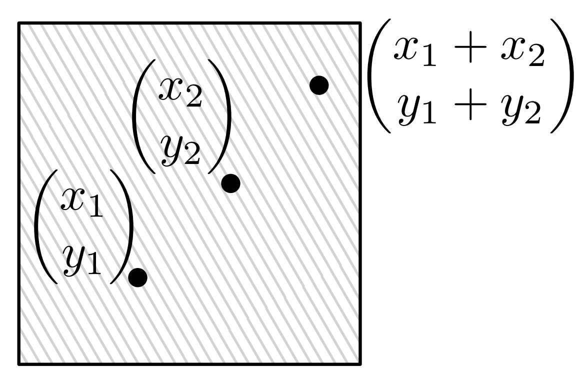
Group structure on $\mathrm{SO}(2)$ (the circle)

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



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

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



Definition: A *representation* of a group G in $\mathbb{R}^n$ is a group morphism $G \to \mathrm{GL}_n(\mathbb{R})$.

In other words, it is an immersion of G in a matrix space, that preserves the algebraic structure.

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

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

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

However, more sophisticated representations exist.

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

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

Definition: A *representation* of a group G in $\mathbb{R}^n$ is a group morphism $G \to \mathrm{GL}_n(\mathbb{R})$.

In other words, it is an immersion of G in a matrix space, that preserves the algebraic structure.

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

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

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

However, more sophisticated representations exist.

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

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

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

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

Definition: A *representation* of a group G in $\mathbb{R}^n$ is a group morphism $G \to \mathrm{GL}_n(\mathbb{R})$.

In other words, it is an immersion of G in a matrix space, that preserves the algebraic structure.

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

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

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

However, more sophisticated representations exist.

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

They are “equal up to a change of coordinates’.

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

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

Definition: A *representation* of a group G in $\mathbb{R}^n$ is a group morphism $G \to \mathrm{GL}_n(\mathbb{R})$.

In other words, it is an immersion of G in a matrix space, that preserves the algebraic structure.

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

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

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

However, more sophisticated representations exist.

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

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

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

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

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

Orbits

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

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

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

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

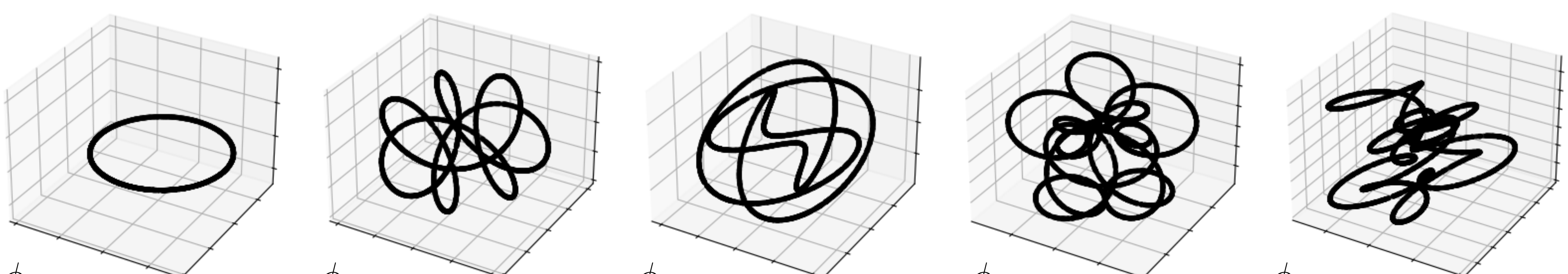
The orbit of $(1,0,1,0)$ under the representation

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

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

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

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



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

Orbits

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

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

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

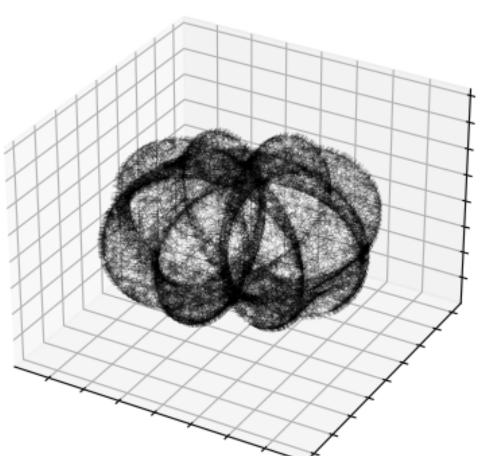
- $T^2 \longrightarrow \mathrm{GL}_6(\mathbb{R})$

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

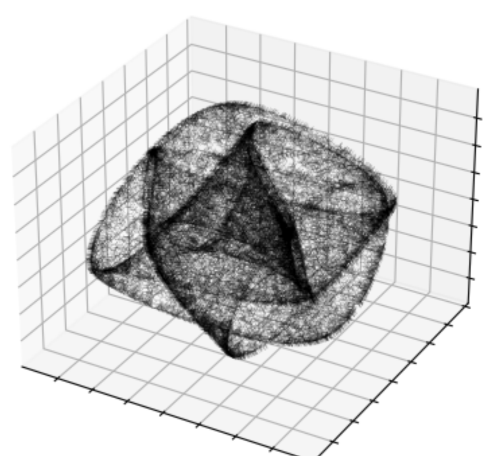
$$\mu \longmapsto \begin{pmatrix} \cos\mu & -\sin\mu & 0 & 0 & 0 & 0 \\ \sin\mu & \cos\mu & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos 2\mu & -\sin 2\mu & 0 & 0 \\ 0 & 0 & \sin 2\mu & \cos 2\mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos\mu & -\sin\mu \\ 0 & 0 & 0 & 0 & \sin\mu & \cos\mu \end{pmatrix}$$

is

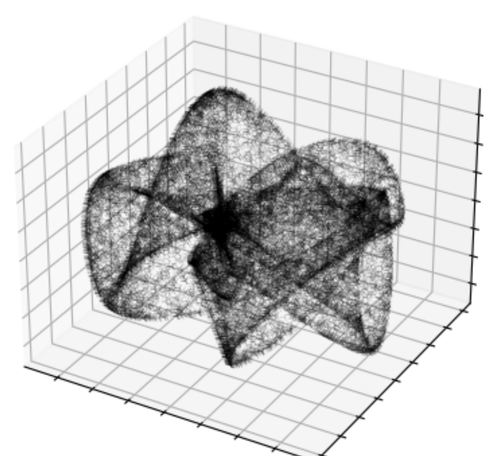
$$\mathcal{O} = \left\{ \begin{pmatrix} \cos\theta + \cos\mu \\ \sin\theta + \sin\mu \\ \cos\theta + \cos 2\mu \\ \sin\theta + \sin 2\mu \\ \cos 3\theta + \cos\mu \\ \sin 3\theta + \sin\mu \end{pmatrix} \;\middle|\; (\theta, \mu) \in \mathbb{R}^2 \right\}$$



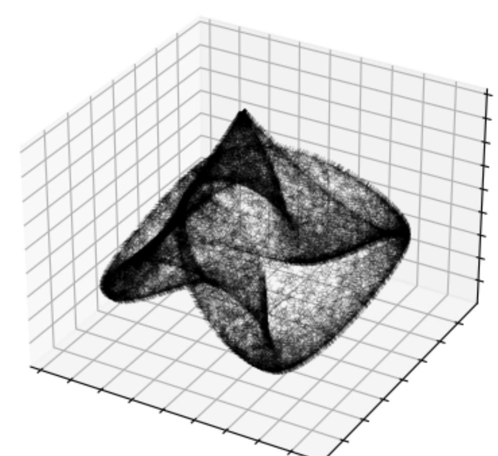
$\phi_{\begin{pmatrix}1&1&3\\1&2&1\end{pmatrix}}$



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



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



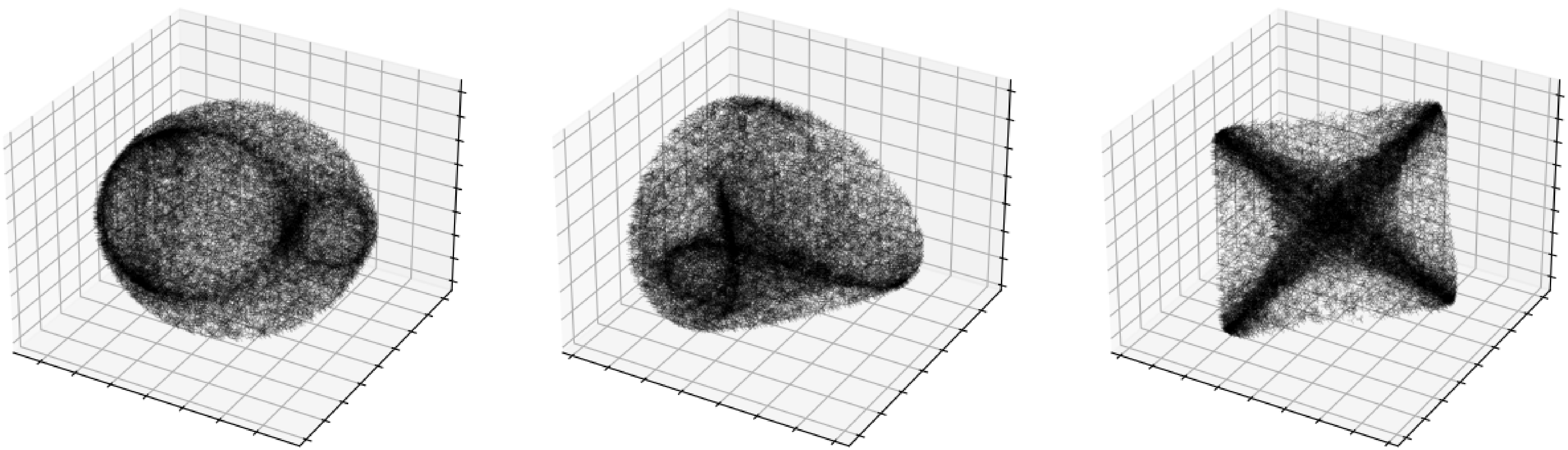
$\phi_{\begin{pmatrix}2&-2&0&2\\1&1&-1&2\end{pmatrix}}$

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

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

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

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



$\psi_{(5)}$ in $\mathbb{R}^5$ $\psi_{(3,4)}$ in $\mathbb{R}^7$ $\psi_{(8)}$ in $\mathbb{R}^8$

Lie algebras I/III: the exponential map

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

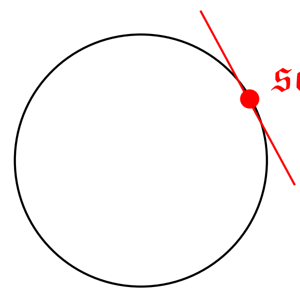
There exists an **exponential map**, denoted $\exp\colon \mathfrak{g} \to G$. It is smooth. When G is connected and compact, it is surjective.

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

Lie algebras allow to study representations from an infinitesimal viewpoint.

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

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

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

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

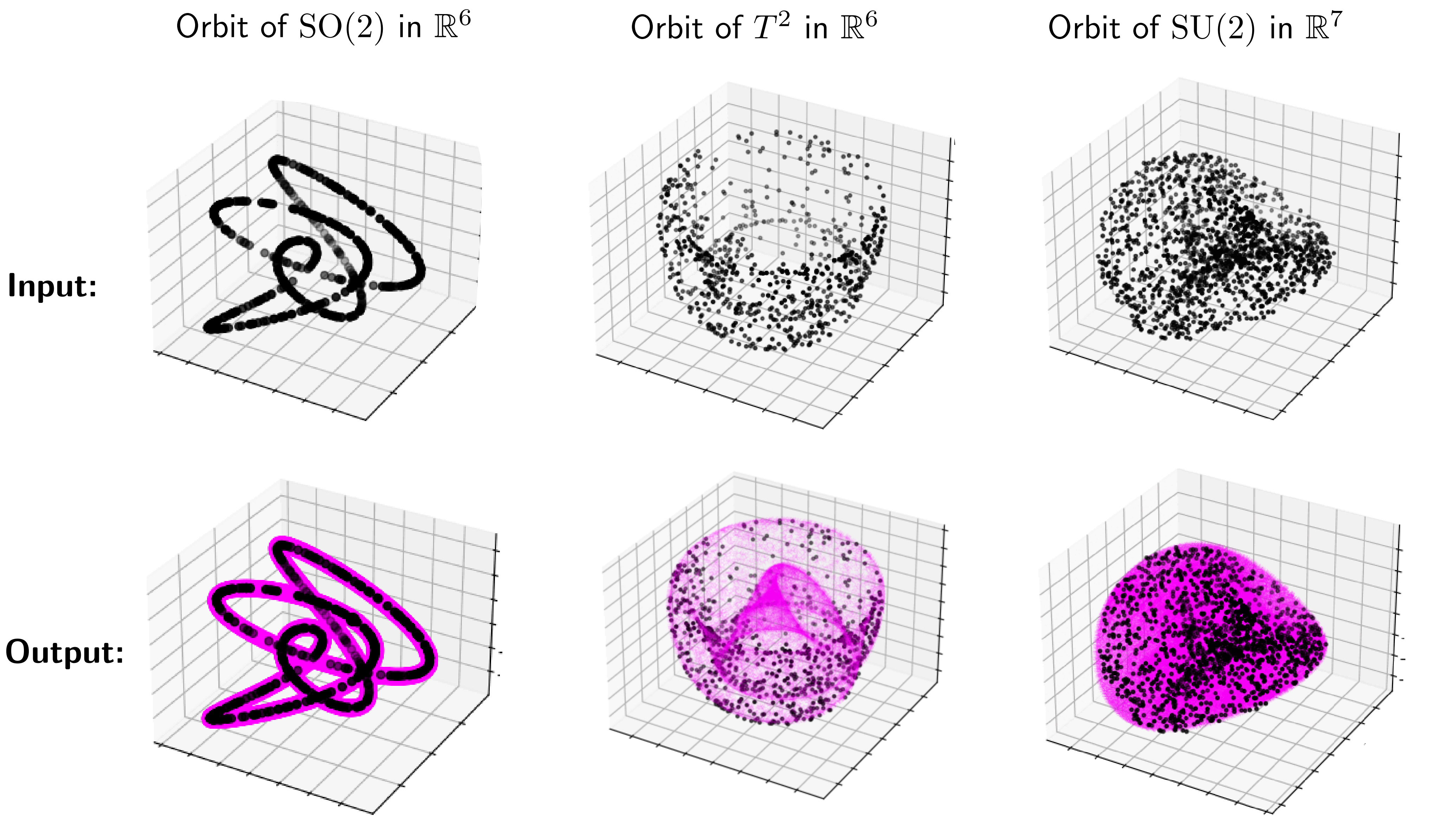
The image $\mathrm{d}\phi(\mathfrak{g}) \subset \mathfrak{so}(n)$ is called the **push-forward Lie algebra**. It will play a key role in our problem.

1. Lie group - Lie algebra correspondence
2. Closest Lie algebra problem
3. Examples

Formulation of our problem - infinitesimal viewpoint

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

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



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

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

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

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

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

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

Definition of orbit: $\mathcal{O} = \left\{\phi(g)x_0 \mid g \in G\right\}$

From the Lie algebra: $\mathcal{O} = \left\{ \exp(h)x_0 \mid h \in \mathrm{d}\phi(\mathfrak{g})\right\}$

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

Lie-PCA is a recently developed algorithm allowing to estimate $\mathrm{d}\phi(\mathfrak{g})$ from X.

The output, denoted $\widehat{\mathfrak{g}}$, is a d-dimensional linear subspace of $\mathfrak{so}(n)$.
It is spanned by the matrices $\widehat{\mathfrak{g}}_1, \ldots, \widehat{\mathfrak{g}}_d$.

Proposition: Under assumptions, $\widehat{\mathfrak{g}}$ is close to the "groundtruth" Lie algebra.

Definition of Lie-PCA

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

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

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

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

Definition of Lie-PCA

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

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

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

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

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

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

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

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

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

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

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

Closest Lie algebra I/II: Space of algebras

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

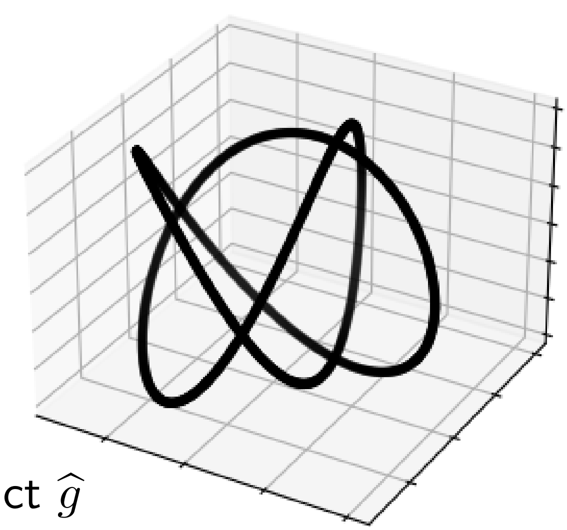
$$\begin{tikzcd} G \arrow[r, "\phi"] & \mathrm{SO}(n) \\ \mathfrak{g} \arrow[u, "\exp"] \arrow[r, "\mathrm{d}\phi"] & \mathfrak{so}(n) \arrow[u, "\exp"'] \end{tikzcd}$$

Definition of orbit: $\mathcal{O} = \{\phi(g)x_0 \mid g \in G\}$

From the Lie algebra: $\mathcal{O} = \{\exp(h)x_0 \mid h \in \mathrm{d}\phi(\mathfrak{g})\}$

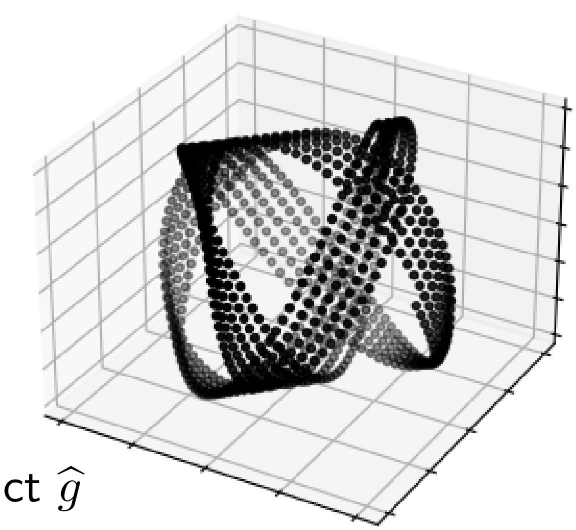
Via Lie-PCA, we get $\widehat{\mathfrak{g}}$, a d-dimensional linear subspace of $\mathfrak{so}(n)$. It is an estimation of $\mathrm{d}\phi(\mathfrak{g})$.

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



exact $\widehat{g}$

exponentiating a non-Lie algebra may yield large errors



inexact $\widehat{g}$

Closest Lie algebra I/II: Space of algebras

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

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

Stiefel variety of Lie algebras

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

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

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

Grassmannian variety of Lie algebras

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

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

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

Written explicitely in matrix form, this reads:

Stiefel variety of Lie algebras

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

Grassmannian variety of Lie algebras

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

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

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

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

Stiefel variety of pushforward Lie algebras of G

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

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

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

Grassmannian variety of pushforward Lie algebras of G

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

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

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

Stiefel variety of pushforward Lie algebras of G

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

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

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

Lemma: For any orthogonal representation $\phi\colon G \to \mathrm{GL}_n(\mathbb{R})$, and any orthonormal basis $(A_1, \ldots, A_d)$ of its pushforward Lie algebra $\mathrm{d}\phi(\mathfrak{g})$, there exists an integer $p \geq 1$, a p-tuple $(B^1, \ldots, B^p) \in \mathfrak{orb}(G, n)$ and two matrices $O \in \mathrm{O}(n)$ and $P \in \mathrm{O}(d)$ such that, for all $i \in [1 \ldots d]$,

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

In particular, the subspace $\mathrm{d}\phi(\mathfrak{g})$ is spanned by the matrices

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

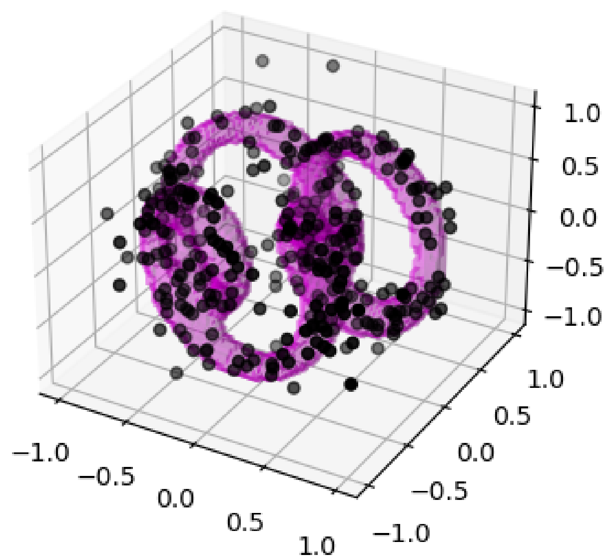
Corollary: The problem $\min\{\|\mathrm{proj}[\widehat{g}] - P\| \mid P \in \mathcal{G}(G, \mathfrak{so}(n))\}$ is equivalent to

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

Remark: This program naturally splits into N minimization problems over $\mathrm{O}(n)$, where N is the cardinal of $\mathfrak{orb}(G, n)$.

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

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



Robustness

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

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

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

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

where

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

Technical assumptions: Define the quantities

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

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

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

Suppose that ω is small enough, so as to satisfy

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

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

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

Moreover, we suppose that

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

1. Lie group - Lie algebra correspondence
2. Closest Lie algebra problem
3. Examples

Let $G = \mathrm{SO}(2)$, whose dimension is $d = 1$.
In this case, the output $\widehat{g}$ of Lie-PCA is a skew symmetric $n \times n$ matrix. Let us denote it A.

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

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

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

The corresponding pushforward Lie algebra is spanned by the matrix

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

In this context, the minimization problem reads

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

This is equivalent to

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

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

Closest Lie algebra - Case of $\mathrm{SO}(2)$

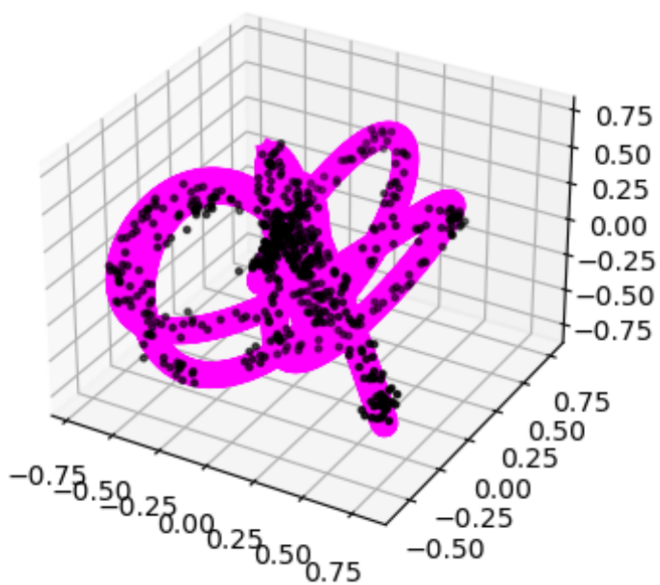
Example: We consider a representation of $\mathrm{SO}(2)$ in $\mathbb{R}^{10}$ with frequencies $(2,4,5,7,8)$ and sample 600 points on one of its orbits, that we corrupt with a Gaussian additive noise of deviation $\sigma = 0.03$.

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

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

The correct representation is found.

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



Closest Lie algebra - Case of T^d

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

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

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

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

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

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

Closest Lie algebra - Case of T^d

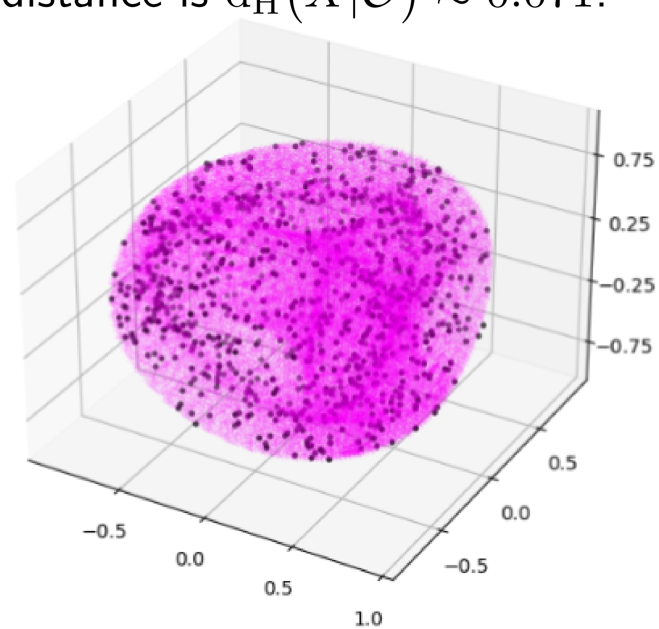
Example: Let X be a uniform 750-sample of an orbit of the representation $\phi_{\left(\begin{smallmatrix}1&1&2\\1&2&1\end{smallmatrix}\right)}$ of the torus T^2 in $\mathbb{R}^6$.

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

<u>Representation $(3,5)$:</u> we get the (non-symmetric) Hausdorff distance $\mathrm{d_H}\left(X|\widehat{\mathcal{O}}\right) \approx 2.658$.
In comparison, $\mathrm{d_H}\left(\widehat{\mathcal{O}}|X\right) \approx 0.543$.
This indicates that the representation is not transitive on X.

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

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

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

Conclusion

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

Limitations:

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

Next goals:

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

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

- Group Equivariant Convolutional Networks