

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

DETECTION OF REPRESENTATION ORBITS OF COMPACT LIE GROUPS FROM POINT CLOUDS

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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 possesses 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:

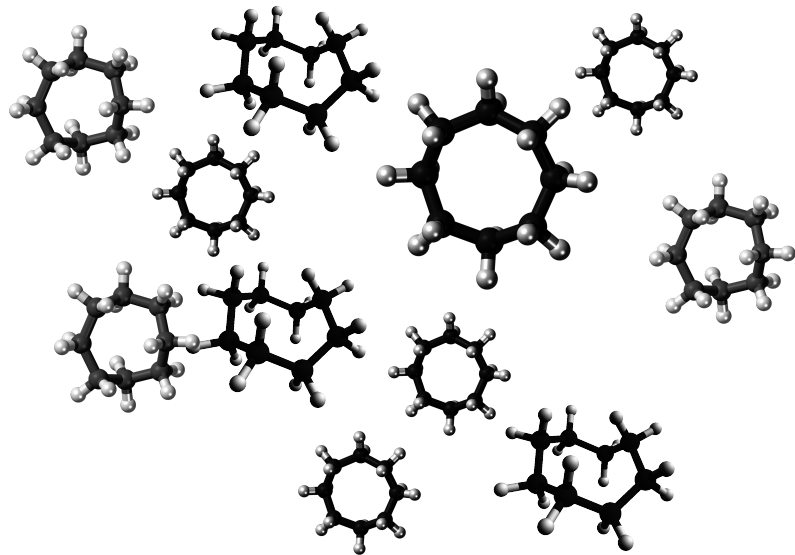
Description of the hydrogen atom through $SO(4)$ -symmetry on top of the Schrödinger equation.

1939, Myers–Steenrod theorem:

The isometry group of a Riemannian manifold is a Lie group.

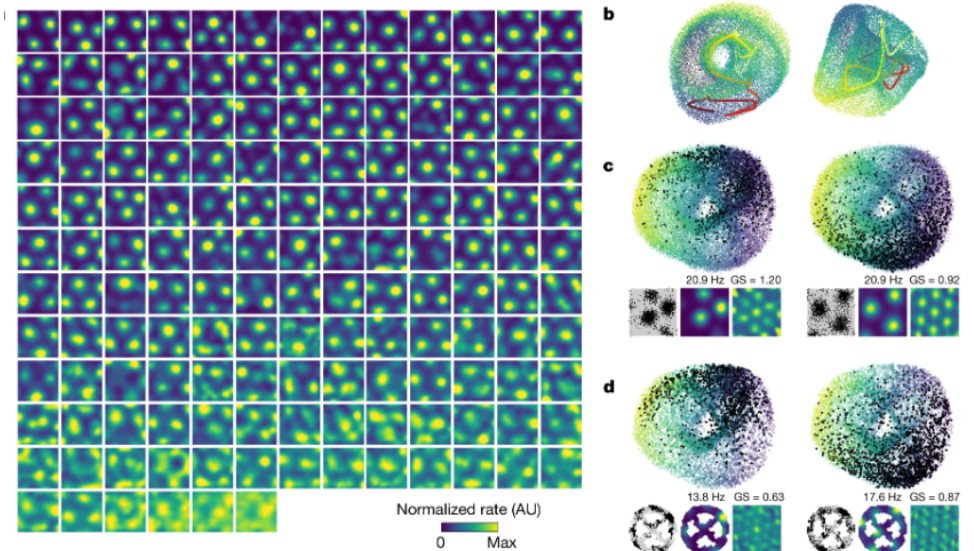
(1) Certain real-life experiments exhibit symmetric objects.

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



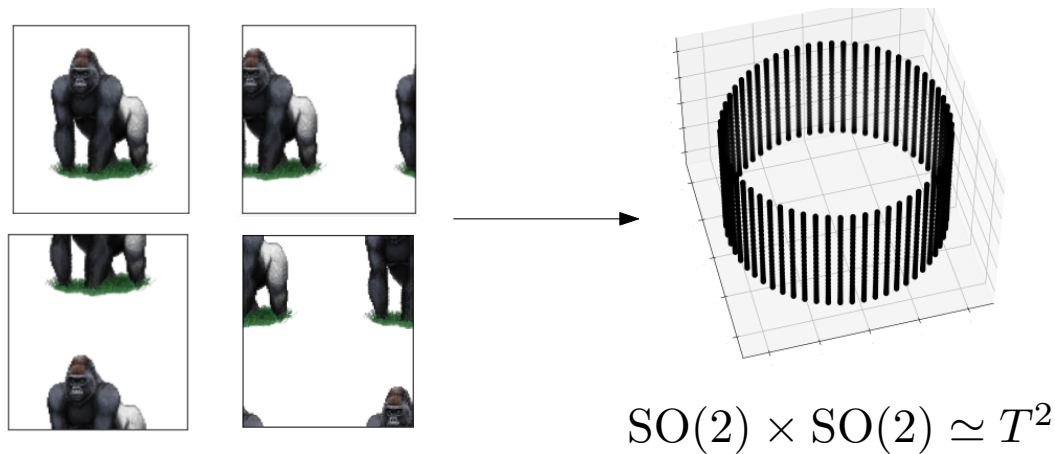
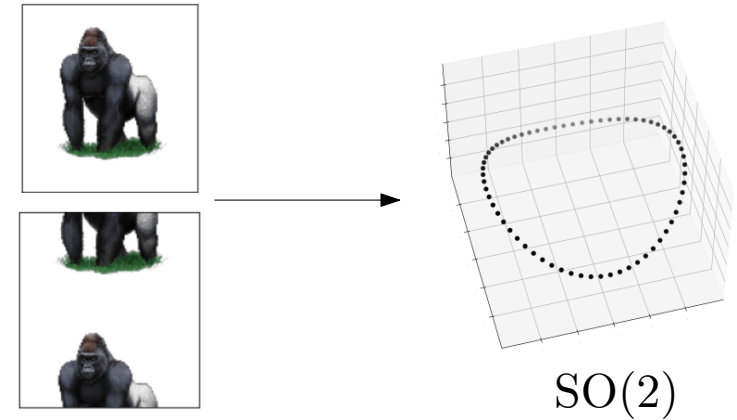
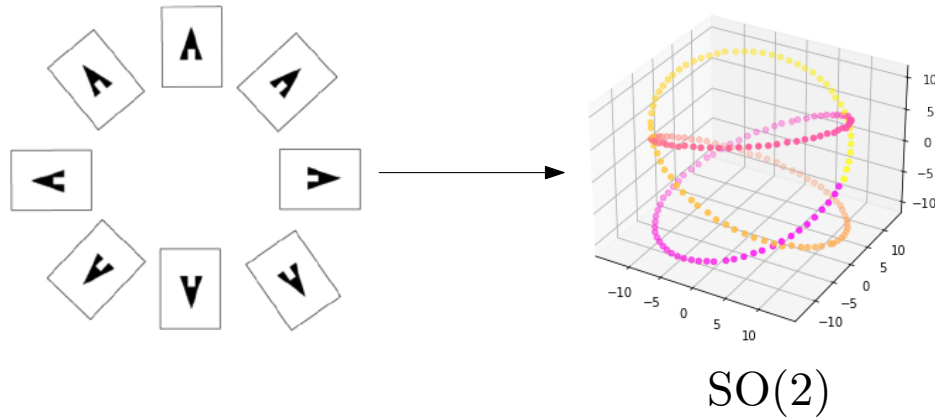
The space of conformation of C_8H_{16} molecules is the union of a **Klein bottle** and a **sphere**.

[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 connectivity of a **torus**.

- (1) Certain real-life experiments exhibit symmetric objects.
- (2) Euclidean transformations are governed by Lie group representations.



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**.

- (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

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}} \qquad \frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}}.$$

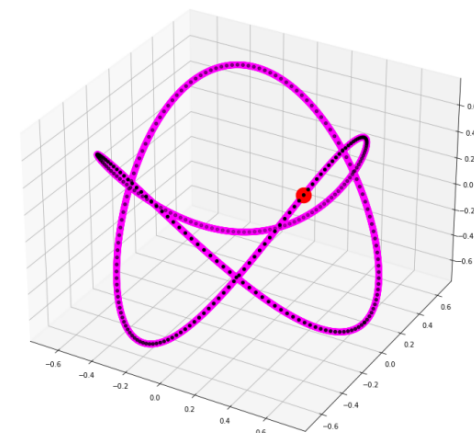
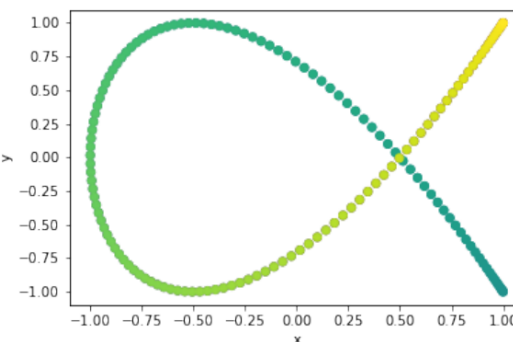
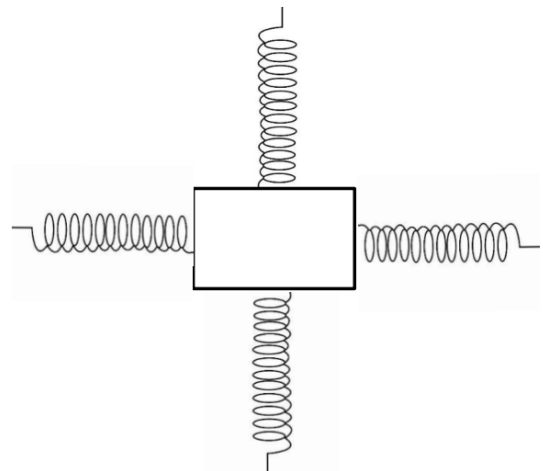
Let ω be the canonical symplectic form in \mathbb{R}^{2n} . A *symplectomorphism* is a Lie group representation $L : G \rightarrow \text{GL}_{2n}(\mathbb{R})$ on \mathbb{R}^{2n} that preserves the the system's dynamics, i.e. $L(g)^*\omega = \omega \ \forall g \in G$.



Emmy Noether
1882 - 1935

Noether's theorem (1915):

If H is invariant under the action of G , then the moment mapping is conserved.



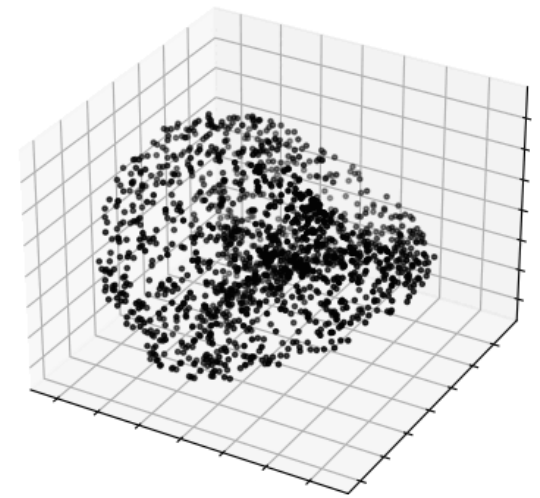
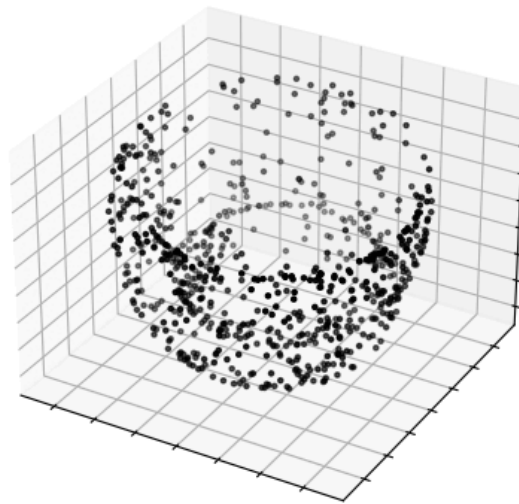
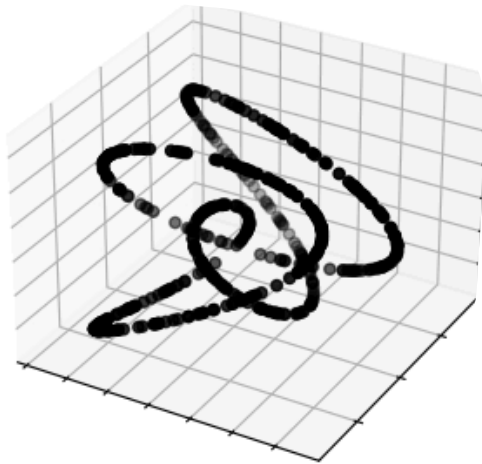
Input: A point cloud $X = \{x_1 \dots, x_N\} \subset \mathbb{R}^n$.

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

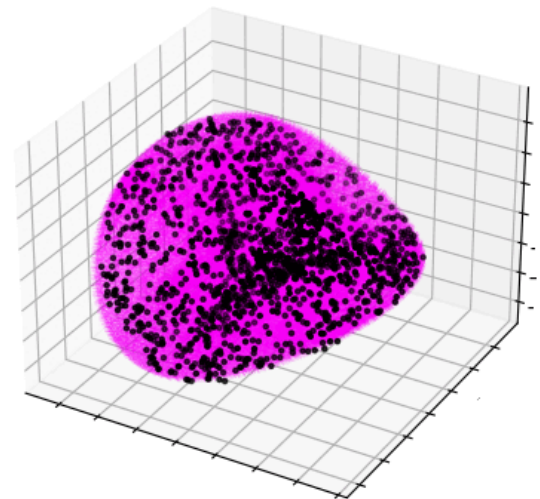
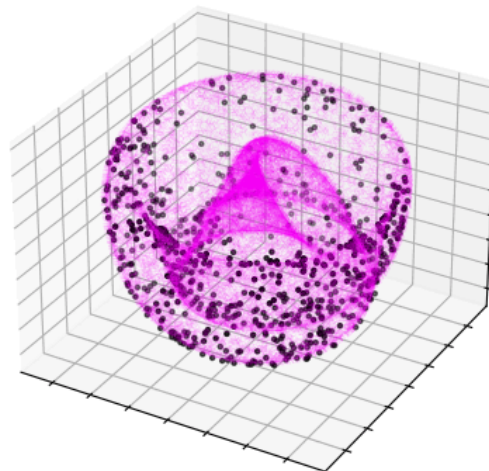
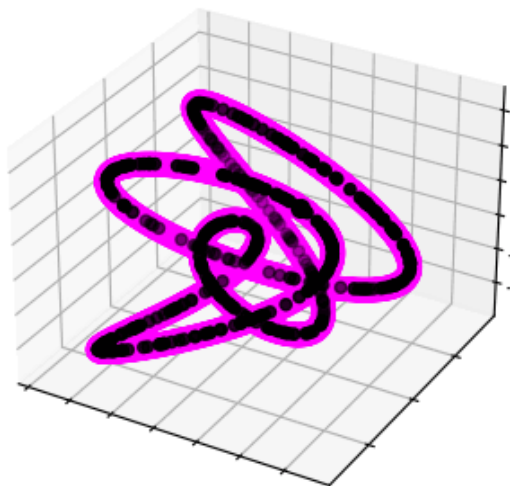
Orbit of $SO(2)$ in \mathbb{R}^6

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

Orbit of $SU(2)$ 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, one has the *matrix groups*

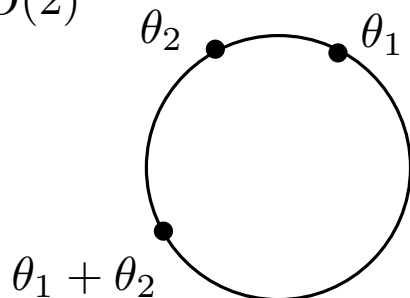
- $O(n)$ orthogonal group: the set of orthogonal $n \times n$ matrices ($A^\top = A^{-1}$)
- $SO(n)$ special orthogonal group: set of orthogonal $n \times n$ matrices of determinant $+1$
- $Sp(2n, \mathbb{C})$ symplectic group: the set of complex symplectic $n \times n$ matrices
- $U(n)$ unitary group: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

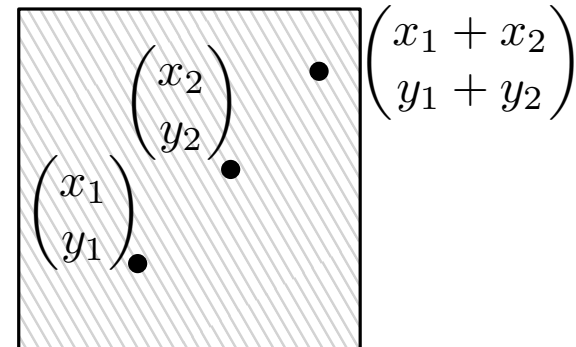
Group structure on $SO(2)$
(the circle)

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



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

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



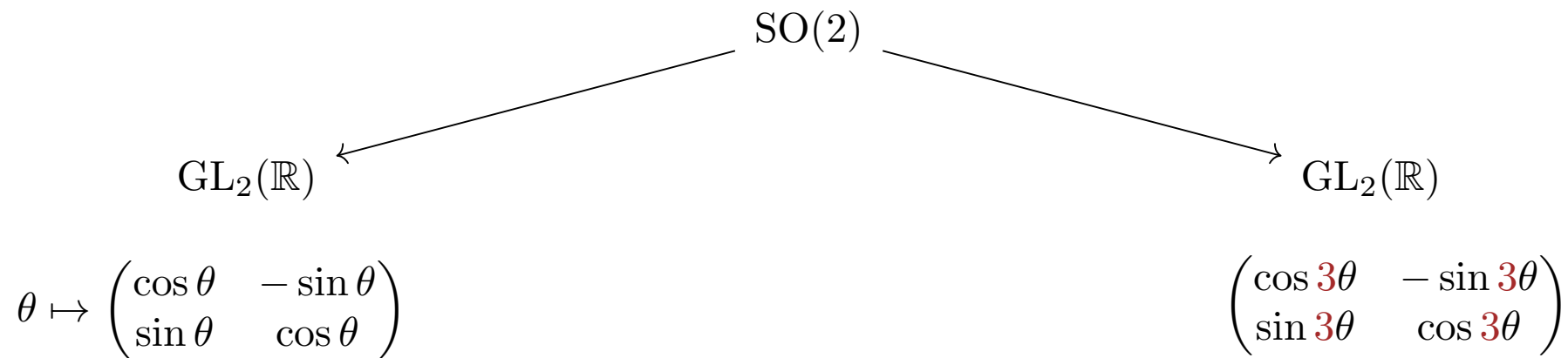
Definition: A representation of a group G in \mathbb{R}^n is a smooth group morphism $G \rightarrow \text{GL}_n(\mathbb{R})$ (the $n \times n$ invertible matrices).

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

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

$$\begin{array}{l} \text{O}(n) \hookrightarrow \text{GL}_n(\mathbb{R}) \\ \text{SO}(n) \hookrightarrow \text{GL}_n(\mathbb{R}) \end{array} \qquad \begin{array}{l} \text{Sp}(2n, \mathbb{C}) \hookrightarrow \text{GL}_n(\mathbb{C}) \hookrightarrow \text{GL}_{2n}(\mathbb{R}) \\ \text{U}(n) \hookrightarrow \text{GL}_n(\mathbb{C}) \hookrightarrow \text{GL}_{2n}(\mathbb{R}) \\ \text{SU}(n) \hookrightarrow \text{GL}_n(\mathbb{C}) \hookrightarrow \text{GL}_{2n}(\mathbb{R}) \end{array}$$

However, more sophisticated representations exist.



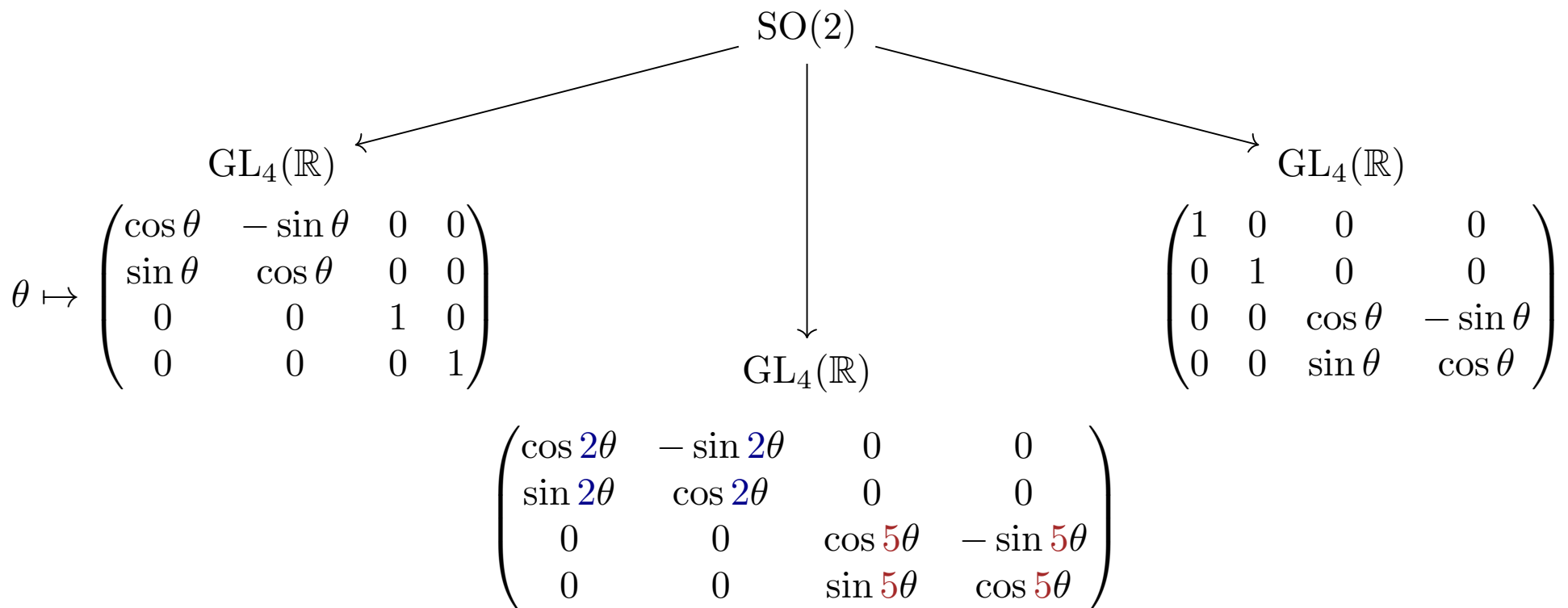
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However, more sophisticated representations exist.

Definition: Two representations $\phi_1, \phi_2: G \rightarrow \mathrm{GL}_n(\mathbb{R})$ are *equivalent* if there exists $A \in \mathrm{GL}_n(\mathbb{R})$ such that $\phi_2 = A\phi_1A^{-1}$.

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 $(\omega_1, \dots, \omega_n) \in \mathbb{Z}^n$ is associated a representation $\phi_{(\omega_1, \dots, \omega_n)}: \mathrm{SO}(2) \rightarrow \mathrm{GL}_{2n}(\mathbb{R})$.

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

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Proposition: Representations of 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*.

Definition: Let $G \rightarrow GL_n(\mathbb{R})$ 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 $SO(2)$ are “circles”. For instance, the orbit of $(1, 0)$ under the representation

- $SO(2) \rightarrow GL_2(\mathbb{R})$

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

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

- $SO(2) \rightarrow GL_4(\mathbb{R})$

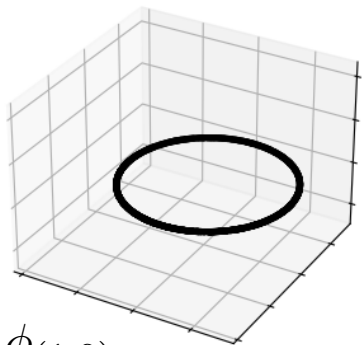
$$\theta \mapsto \begin{pmatrix} \cos \theta & -\sin \theta & 0 & 0 \\ \sin \theta & \cos \theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

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

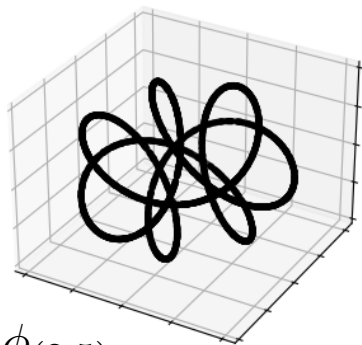
- $SO(2) \rightarrow GL_4(\mathbb{R})$

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

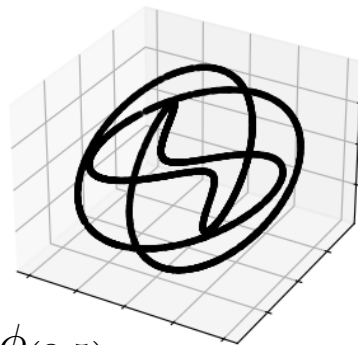
is $\mathcal{O} = \left\{ \begin{pmatrix} \cos 2\theta \\ \sin 2\theta \\ \cos 5\theta \\ \sin 5\theta \end{pmatrix} \mid \theta \in \mathbb{R} \right\}$



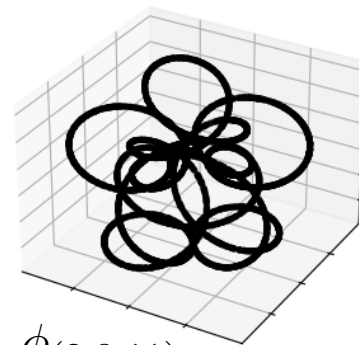
$\phi(1,0)$



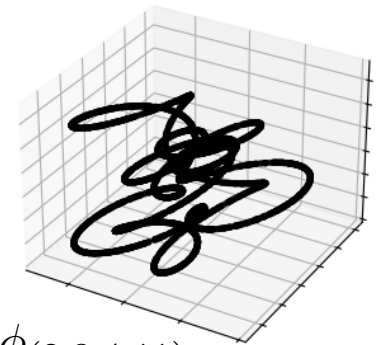
$\phi(2,5)$



$\phi(3,5)$



$\phi(2,3,11)$



$\phi(2,3,4,11)$

Definition: Let $G \rightarrow \text{GL}_n(\mathbb{R})$ 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 $\text{SO}(2)$ are “circles”.

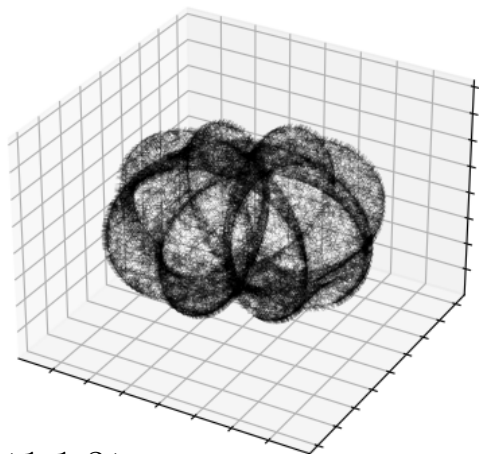
Example: Orbits of T^2 are “tori”. For instance, the orbit of $(1, 0, 1, 0, 1, 0)$ under the representation

• $T^2 \longrightarrow \text{GL}_6(\mathbb{R})$

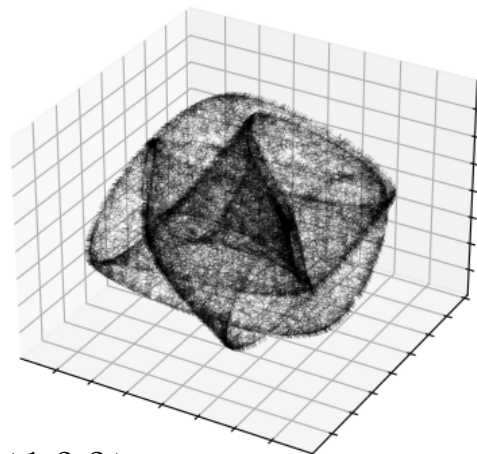
$$\theta \mapsto \begin{pmatrix} \cos \theta & -\sin \theta & 0 & 0 & 0 & 0 \\ \sin \theta & \cos \theta & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos \theta & -\sin \theta & 0 & 0 \\ 0 & 0 & \sin \theta & \cos \theta & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos 3\theta & -\sin 3\theta \\ 0 & 0 & 0 & 0 & \sin 3\theta & \cos 3\theta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

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

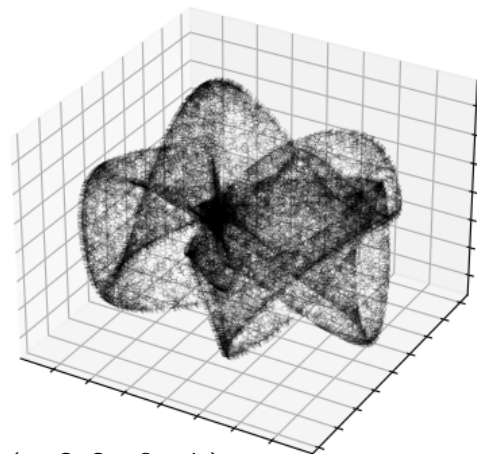
$$\text{is } \mathcal{O} = \left\{ \begin{pmatrix} \cos \theta + \cos \mu \\ \sin \theta + \sin \mu \\ \cos \theta + \cos 2\mu \\ \sin \theta + \sin 2\mu \\ \cos 3\theta + \cos \mu \\ \sin 3\theta + \sin \mu \end{pmatrix} \mid (\theta, \mu) \in \mathbb{R}^2 \right\}$$



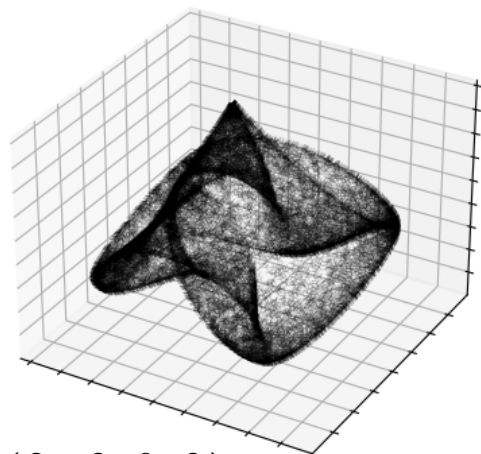
$$\phi \begin{pmatrix} 1 & 1 & 3 \\ 1 & 2 & 1 \end{pmatrix}$$



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



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



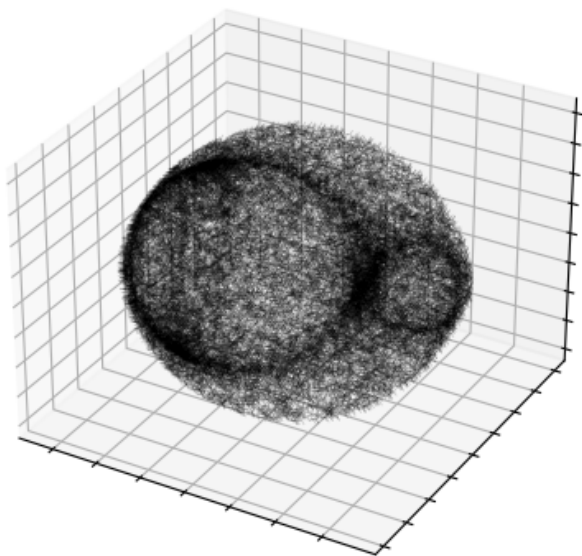
$$\phi \begin{pmatrix} 2 & -2 & 0 & 2 \\ 1 & 1 & -1 & 2 \end{pmatrix}$$

Definition: Let $G \rightarrow GL_n(\mathbb{R})$ 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 $\mathcal{O} = \{\phi(g)x_0 \mid g \in G\}$.

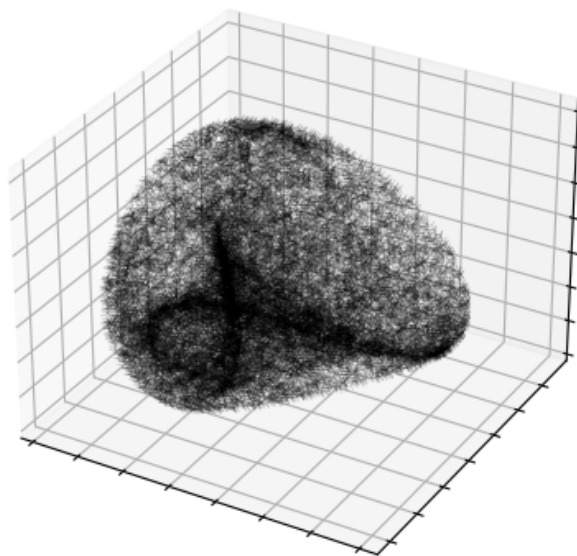
Example: Orbits of $SO(2)$ are “circles”.

Example: Orbits of T^2 are “tori”.

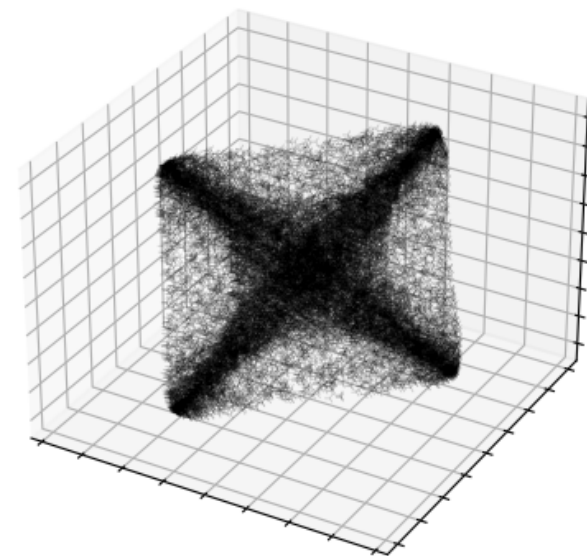
Example: Orbits of $SO(3)$ and $SU(2)$ are “spheres”.



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



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



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

Let G be a Lie group, $0 \in G$ the identity element and $\mathfrak{g} = T_0G$ the tangent space.

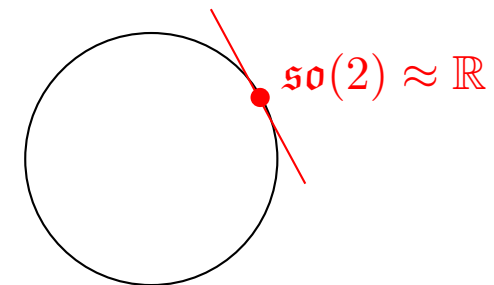
There exists an **exponential map**, denoted $\exp: \mathfrak{g} \rightarrow G$. It is smooth. When G is connected and compact, it is surjective.

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.

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

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



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

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

Caution: In general, $\exp(t_1X_1 + t_2X_2 + t_3X_2) \neq \exp(t_1X_1) \exp(t_2X_2) \exp(t_3X_3)$.

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

It is a bilinear map $\mathfrak{g} \times \mathfrak{g} \rightarrow \mathfrak{g}$ 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 $SO(3)$, one has $[X_1, X_2] = X_3$, $[X_2, X_3] = X_1$ and $[X_1, X_3] = -X_2$, where

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

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 III/III: the correspondence group \sim algebra 11/22

Lie algebras allow to study representations from an infinitesimal viewpoint.

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

$$\begin{array}{ccc} G & \xrightarrow{\phi} & GL_n(\mathbb{R}) \\ \uparrow \text{exp} & & \uparrow \text{exp} \\ \mathfrak{g} & \xrightarrow{d\phi} & \mathfrak{gl}_n(\mathbb{R}) \quad = n \times n \text{ matrices} \end{array}$$

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

$$\begin{array}{ccc} G & \xrightarrow{\phi} & SO(n) \\ \uparrow \text{exp} & & \uparrow \text{exp} \\ \mathfrak{g} & \xrightarrow{d\phi} & \mathfrak{so}(n) \quad = \text{skew-symmetric } n \times n \text{ matrices} \end{array}$$

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

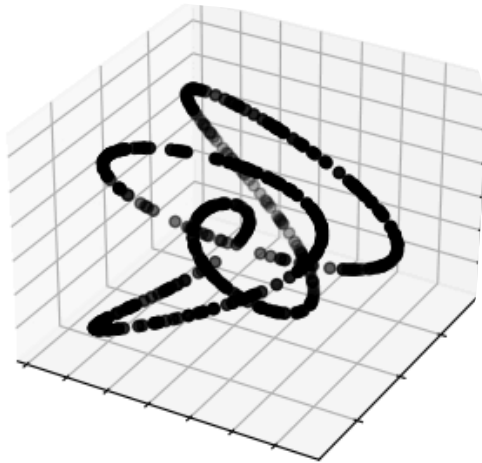
1. Lie group - Lie algebra correspondence
2. Closest Lie algebra problem
3. Examples

Formulation of our problem - infinitesimal viewpoint^{13/22 (1/2)}

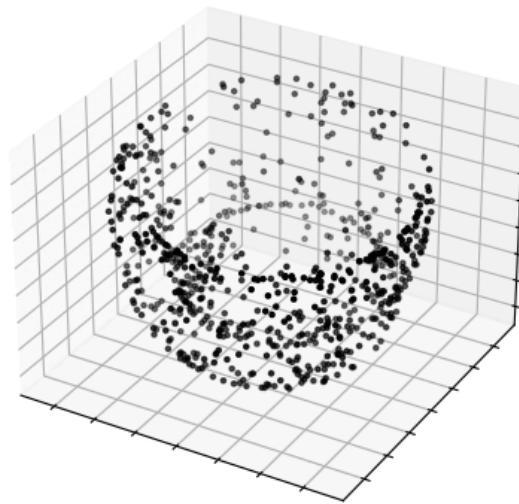
Input: A point cloud $X = \{x_1 \dots, x_N\} \subset \mathbb{R}^n$.

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

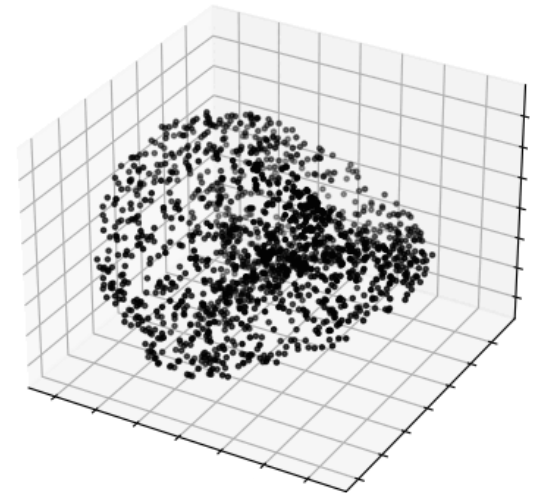
Orbit of $SO(2)$ in \mathbb{R}^6



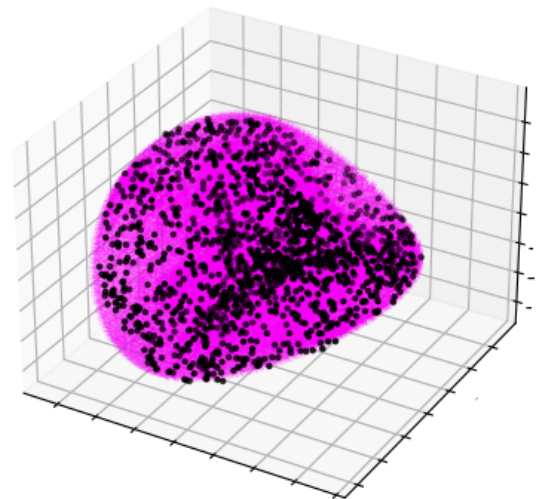
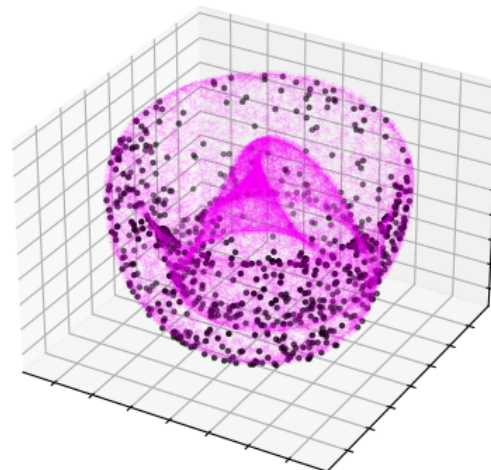
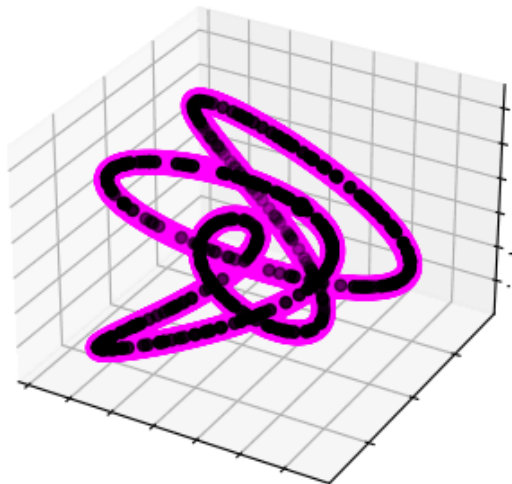
Orbit of T^2 in \mathbb{R}^6



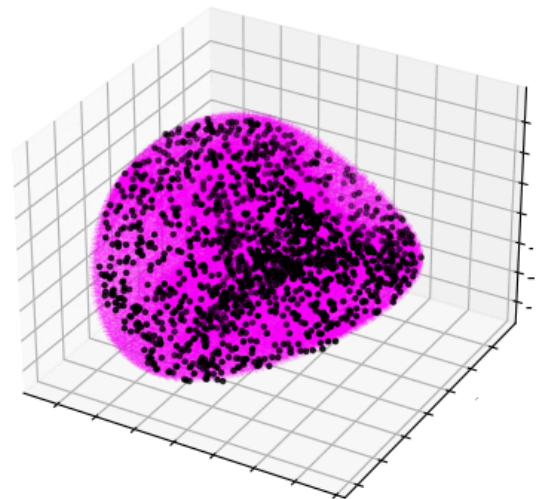
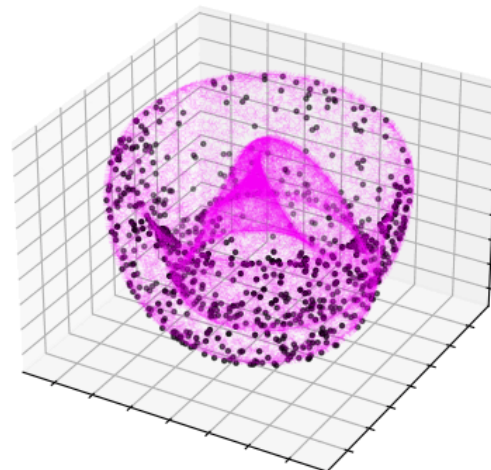
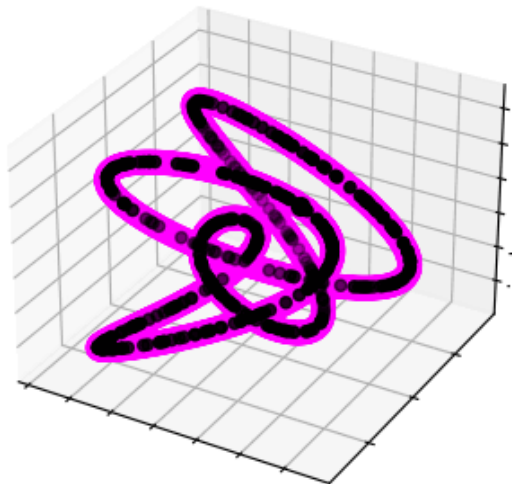
Orbit of $SU(2)$ in \mathbb{R}^7



Input:



Output:



Formulation of our problem - infinitesimal viewpoint^{13/22 (2/2)}

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

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

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

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

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

$$\begin{array}{ccc} G & \xrightarrow{\phi} & \text{SO}(n) \\ \exp \uparrow & & \uparrow \exp \\ \mathfrak{g} & \xrightarrow{d\phi} & \mathfrak{so}(n) \end{array}$$

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

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

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

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

The output, denoted $\widehat{\mathfrak{g}}$, is a d -dimensional linear subspace of $\mathfrak{so}(n)$.

It is spanned by the matrices $\widehat{\mathfrak{g}}_1, \dots, \widehat{\mathfrak{g}}_d$.

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

Lie-PCA operator: $\Lambda: M_n(\mathbb{R}) \rightarrow M_n(\mathbb{R})$ is defined as

$$\Lambda(A) = \frac{1}{N} \sum_{1 \leq i \leq N} \hat{\Pi}[N_{x_i} X] \cdot A \cdot \Pi[\langle x_i \rangle]$$

where

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

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

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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 $\mathfrak{sym}(\mathcal{O}) = \{A \in M_n(\mathbb{R}) \mid \forall x \in \mathcal{O}, Ax \in T_x \mathcal{O}\}$, where $T_x \mathcal{O}$ denotes the tangent space of \mathcal{O} at x . In other words,

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

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

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

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

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

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

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

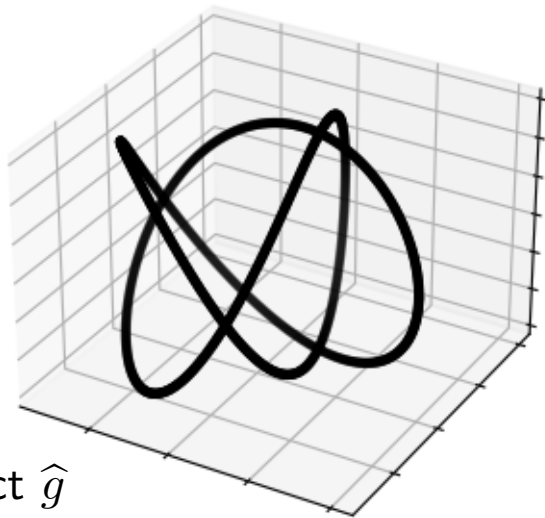
$$\begin{array}{ccc}
 G & \xrightarrow{\phi} & SO(n) \\
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 \end{array}$$

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

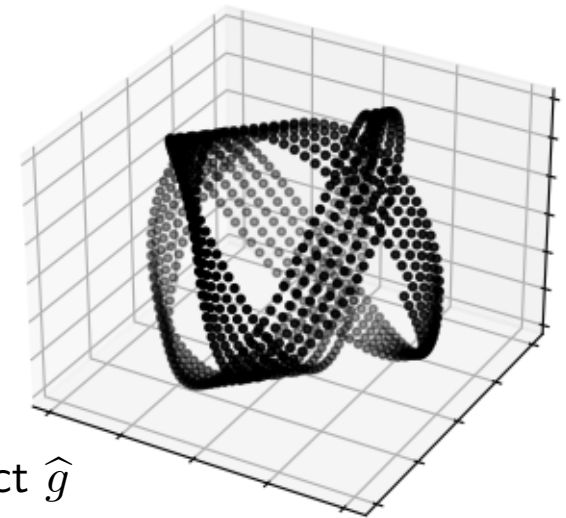
From the Lie algebra: $\mathcal{O} = \{\exp(h)x_0 \mid h \in d\phi(\mathfrak{g})\}$

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

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



exponentiating a non-Lie algebra
may yield large errors



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

$$\langle A, B \rangle = \sum_{i=1}^n \sum_{j=1}^n a_{i,j} b_{i,j} \quad \text{and} \quad \|A\| = \sqrt{\sum_{i=1}^n \sum_{j=1}^n a_{i,j}^2}.$$

Stiefel variety of Lie algebras

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

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

The problem is

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

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

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

The problem is

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

Written explicitly in matrix form, this reads:

Stiefel variety of Lie algebras

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

Grassmannian variety of Lie algebras

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

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

Idea: Fix a compact Lie group G , and restrict the Stiefel $\mathcal{V}^{\text{Lie}}(d, \mathfrak{so}(n))$ 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 $(A_1, \dots, A_d) \in \mathcal{V}^{\text{Lie}}(d, \mathfrak{so}(n))$ for which there exists an orthogonal representation $\phi: G \rightarrow \text{SO}(n)$ such that $d\phi(\mathfrak{g})$ is spanned by (A_1, \dots, A_d) .

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

Definition: We say that two representations $\phi, \phi': G \rightarrow \text{GL}_n(\mathbb{R})$ are *orbit-equivalent* if there exists a matrix $M \in \text{M}_n(\mathbb{R})$ such that $d\phi(\mathfrak{g}) = Md\phi'(\mathfrak{g})M^{-1}$. In particular, their orbits are conjugated. We shall denote by $\text{orb}(G, n)$ 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 $P \in \mathcal{G}^{\text{Lie}}(d, \mathfrak{so}(n))$ for which there exists an orthogonal representation $\phi: G \rightarrow \text{SO}(n)$ such that P is the projection matrix on $d\phi(\mathfrak{g})$.

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 $(A_1, \dots, A_d) \in \mathcal{V}^{\text{Lie}}(d, \mathfrak{so}(n))$ for which there exists an orthogonal representation $\phi: G \rightarrow \text{SO}(n)$ such that $d\phi(\mathfrak{g})$ is spanned by (A_1, \dots, A_d) .

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

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

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

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

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

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

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

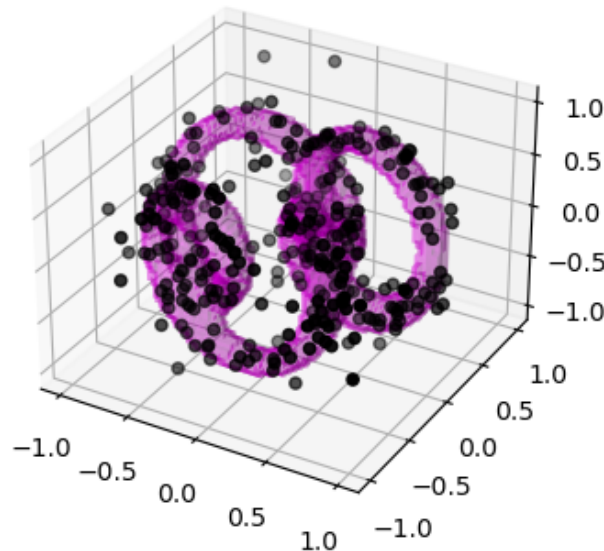
$$\min \left\| \text{proj}[\widehat{\mathfrak{g}}] - \text{proj}[\langle O \text{diag}(B_i^k)_{k=1}^p O^\top \rangle_{i=1}^d] \right\| \quad \text{s.t.} \quad \begin{cases} (B^1, \dots, B^p) \in \text{orb}(G, n), \\ O \in O(n). \end{cases}$$

Remark: This is a discrete-continuous problem.

It splits into N minimization problems over $O(n)$, where N is the cardinal of $\text{orb}(G, n)$.

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

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



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

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

$$\|\text{proj}[\hat{h}] - \text{proj}[\text{sym}(\mathcal{O})]\|_F \leq 9d \frac{\rho}{\lambda} \left(r + 4 \left(\frac{\tilde{\omega}}{r^{l+1}} \right)^{1/2} \right)$$

$$W_2(\mu_{\hat{\mathcal{O}}}, \mu_{\tilde{\mathcal{O}}}) \leq \frac{1}{\sqrt{2}} \frac{W_2(\mu_X, \mu_{\mathcal{O}})}{\sigma_{\min}} + 3\sqrt{dn} \left(\frac{\rho}{\lambda} \right)^{1/2} \left(r + 4 \left(\frac{\tilde{\omega}}{r^{l+1}} \right)^{1/2} \right)^{1/2}$$

where

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

Technical assumptions: Define the quantities

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

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

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

Suppose that ω is small enough, so as to satisfy

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

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

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

Moreover, we suppose that

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

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

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

In this case, the output \hat{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 $\text{SO}(2)$ in \mathbb{R}^n take the form

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

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

The corresponding pushforward Lie algebra is spanned by the matrix

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

In this context, the minimization problem reads

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

This is equivalent to

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

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

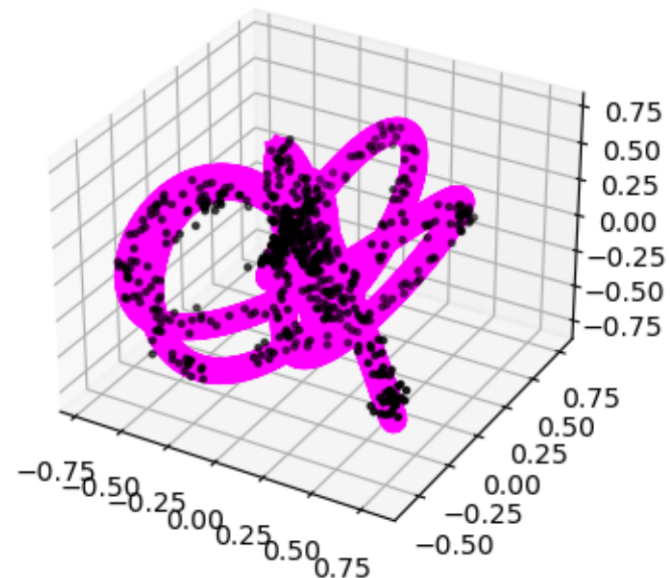
Example: We consider a representation of SO(2) in \mathbb{R}^{10} with frequencies (2, 4, 5, 7, 8) and sample 600 points on one of its orbits, that we corrupt with a Gaussian additive noise of deviation $\sigma = 0.03$.

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.

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



Let $G = T^d$, the torus of dimension d .

In this case, the output \hat{g} of Lie-PCA is a d -tuple (A_1, \dots, A_d) of skew symmetric $n \times n$ matrices.

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

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

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

The push-forward Lie algebra is spanned by

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

In this context, the minimization problem reads

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

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

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

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

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

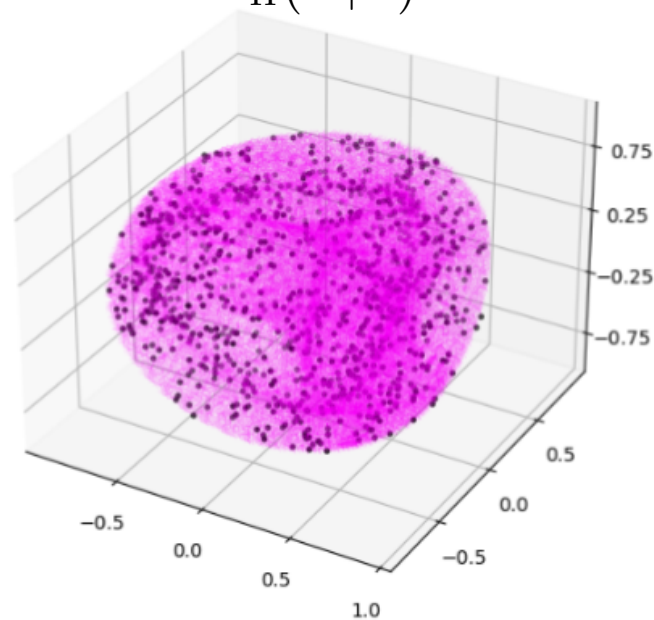
Example: Let X be a uniform 750-sample of an orbit of the representation $\phi_{\begin{pmatrix} 1 & 1 & 2 \\ 1 & 2 & 1 \end{pmatrix}}$ of the torus T^2 in \mathbb{R}^6 .

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

Representation	$\begin{pmatrix} 0 & 1 & 1 \\ 2 & -2 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 2 \\ -2 & 2 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 2 \\ 2 & -2 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & -2 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & -2 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 2 \\ 2 & -2 & 1 \end{pmatrix}$
Cost	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 $\begin{pmatrix} 0 & 1 & 1 \\ 2 & -2 & 1 \end{pmatrix}$, i.e., the representation $\phi_{\begin{pmatrix} 0 & 1 & 1 \\ 2 & -2 & 1 \end{pmatrix}}$. It is equivalent to $\phi_{\begin{pmatrix} 1 & 1 & 2 \\ 1 & 2 & 1 \end{pmatrix}}$.

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



Closest Lie algebra - Case of $SO(3)$ and $SU(2)$ 21/22 (1/2)

For $SO(3)$ and $SU(2)$, 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: $SO(3)$ acts transitively on itself.

The irreps of $SU(2)$ and $SO(3)$ 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	2×10^{-5}	4×10^{-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 $d_H(X|\hat{\mathcal{O}}) \approx 2.658$.

In comparison, $d_H(\hat{\mathcal{O}}|X) \approx 0.543$.

This indicates that the representation is not transitive on X .

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

Closest Lie algebra - Case of $SO(3)$ and $SU(2)$ 21/22 (2/2)

For $SO(3)$ and $SU(2)$, 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: $SO(3)$ acts transitively on itself.

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action $SO(3) \rightarrow SO(3)$ by conjugation (not transitive)

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

action $SO(3) \rightarrow SO(3)$ by translation (transitive)

Conclusion

- First algorithm to find the **representation type** (not only a subspace close to the Lie algebra)
- Implementation for $G = SO(2)$, T^d , $SO(3)$ and $SU(2)$
- 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 $O(n)$ 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
- Group Equivariant Convolutional Networks

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

