Homological Inference of Embedding Dimensions in Neural Networks

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Overview

1. Motivation
   - The manifold of data
   - The manifold of a neural network
2. Simplicial structures
   - Simplicial complexes
   - Persistent homology
3. Counting betti numbers
   - Experiments with connected abelian Lie group assumption
   - Outlook

Manifolds and Lie groups

Smooth manifold

Let X be a topological space. A pair $(X, \mathcal{A})$, consisting of a second countable Hausdorff space X and a differentiable structure on X given by $\mathcal{A} = (U_i, \varphi_i)_{i \in I}$, the family of pair-wise compatible coordinate charts such that $X = \bigcup_{i \in I} U_i$, is said to be a differentiable manifold. If $\varphi(U) \subseteq \mathbb{R}^n$ for all $(U, \varphi) \in \mathcal{A}$, then we say $\dim X = n$.

Lie group

A Lie group is a smooth manifold G equipped with a group structure so that the maps $\mu : (x, y) \mapsto xy$, $G \times G \to G$ and $\iota : x \mapsto x^{-1}$ are smooth.

The manifold of data

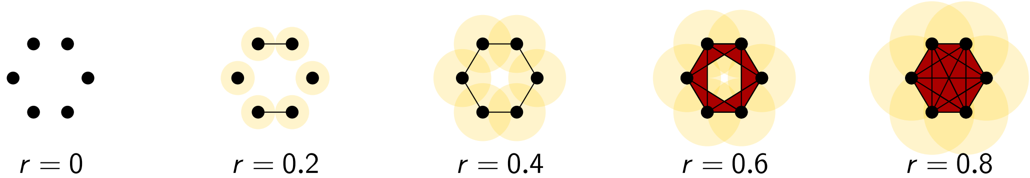
Manifold assumption

A set of points in Euclidean space $\mathbb{R}^d$ is underlain by a manifold, which can be embedded in ibid. Euclidean space and on which the points lie.

Decomposition of connected abelian Lie groups

Every connected commutative (abelian) Lie group G is isomorphic to a product space $\mathbb{R}^p \times \mathbb{T}^q \cong G$ with $p + q = \dim G$.

The manifold of data



Idea:

1. Estimate a suitable structure.
2. Estimate one of its invariants.
3. Relate the invariant to the dimension.

How many dimensions do I need to represent the manifold that I suspect underlies the above set of points?

How many and which neurons are needed to represent this manifold?

The manifold of a neural network

$$
\begin{tikzcd}
 & & M \arrow[dll, bend right, "x^{(0)}"'] \arrow[dl, bend right, "x^{(1)}"'] \arrow[d, dashed, "x^{(2)}"] \arrow[dr, bend left, "x^{(3)}"] \arrow[drr, bend left, "x^{(L)}"] & & \\
x^{(0)}(M) \arrow[r, "\varphi^{(0)}"] & x^{(1)}(M) \arrow[r, "\varphi^{(1)}"] & x^{(2)}(M) \arrow[r, "\varphi^{(2)}"] & x^{(3)}(M) \arrow[r, dotted, "\varphi^{(L)}"] & x^{(L)}(M)
\end{tikzcd}
$$

Coordinate systems $x^{(l)} := \varphi^{(l-1)} \circ \cdots \circ \varphi^{(1)} \circ \varphi^{(0)} \circ x^{(0)}$ of a deep neural network induced by change of coordinate charts $\varphi^{(l)} : x^{(l)}(M) \mapsto (\varphi^{(l)} \circ x^{(l)})(M)$ learned by the neural network acting on the data.

Following Michael Hauser and Asok Ray: Principles of Riemannian Geometry in Neural Networks.

Realise a good representation

Question: How can we adjust the neuromanifold to fit the data manifold?

1. Take suitable assumptions on the dataset and its manifold.
2. Measure invariants on the filtration of a dataset to get a descriptor.
3. Infere possible manifolds from these measured invariants.
4. Relate the invariants to the dimension of the manifold.
5. Seek for approximate solutions if assumptions may not hold.

Building blocks: simplices

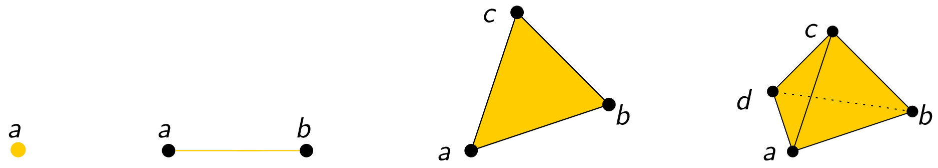
Consider the set of points $X := \{v_0, v_1, \ldots, v_n\} \subset \mathbb{R}^d$. They are said to be **affinely independent** if the points $\{v_0 - v_n, v_1 - v_n, \ldots, v_{n-1} - v_n\}$ are linearly independent. The **convex closure** of these points is a **simplex** and written as

$$[v_0, v_1, \ldots, v_n] = \left\{ \sum_{i=0}^{n-1} \lambda_i (v_i - v_n) \;\middle|\; \sum_{i=0}^{n-1} \lambda_i = 1 \text{ and } \lambda_i \geq 0 \right\}. \tag{1}$$

The dimension of the simplex is n.
The i-th face of a simplex $[v_0, v_1, \ldots, v_n]$ (with an ommitted element $\hat{v}_i$) is defined by

$$d_i[v_0, v_1, \ldots, v_n] = [v_0, v_1, \ldots, \hat{v}_i, \ldots, v_n]. \tag{2}$$

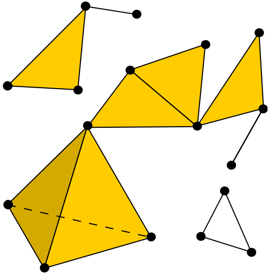
Examples

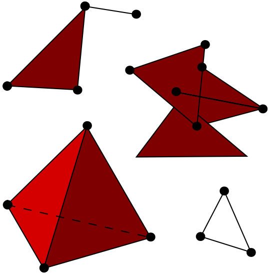


0-simplex (point) | 1-simplex (line segment) | 2-simplex (triangle) | 3-simplex (tetrahedron)

The coefficients λ_i are chosen from the **field** $\mathbb{Z}_2 := \mathbb{Z}/2\mathbb{Z}$, such that we can **neglect the orientation** of the simplices. This is used for highly efficient computations.

Definition of simplicial complexes





A **simplicial complex** K is a finite union of simplices satisfying that every face of a simplex in K is in K and that the non-empty intersection of two simplices in K is a face of each.

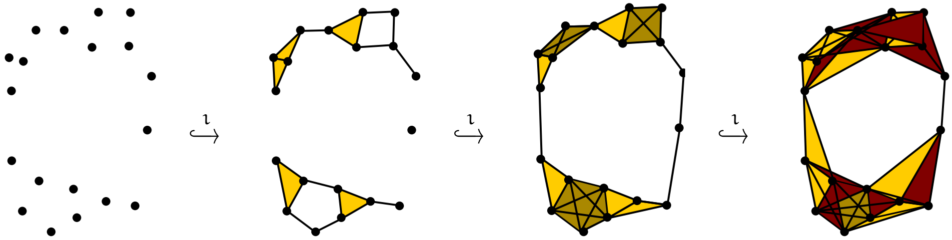
Filtered simplicial complexes

A **filtration** is a nested sequence of complexes K_i, which induce an ordering of the sublevel complexes. These complexes, together with the inclusion $K_i \hookrightarrow K_j$ for $0 \leq i \leq j \leq n$ are called a filtration and denoted by $\mathbb{K}$:

$$\mathbb{K}: \quad \emptyset = K_0 \subseteq K_1 \subseteq \cdots \subseteq K_n = K. \tag{3}$$

The inclusion on the filtration induces a homomorphism of groups $f_k^{i,j} : H_k(K_i) \to H_k(K_j)$, in this case H_k are the k-th homology groups.

Filtered simplicial complexes



Vastly used complexes to create a filtration on a point set X are:

Čech complex: $(v_0, v_1, \cdots, v_n) \in \check{C}\mathrm{ech}_r(X) \iff \bigcap_{i=0}^{n} B_r(x_i) \neq \emptyset.$

Vietoris-Rips complex: $(v_0, v_1, \cdots, v_n) \in \mathrm{Rips}_r(X) \iff \|v_i - v_j\| \leq r.$

Isomorphism of homology theories

Isomorphic homology theories

For a triangulable smooth manifold X and a simplicial complex K, forming its triangulation, the following holds for the homology groups from a field of coefficients $\mathbb{F}$:

$$H_k(K;\mathbb{F}) \cong H_k(X;\mathbb{F}) \cong H_k^{\infty}(X;\mathbb{F}) \cong H_{\text{deRham}}^{k}(X;\mathbb{F}). \tag{4}$$

Proof of $H_k(K;\mathbb{F}) \cong H_k(X;\mathbb{F})$: Allen Hatcher: Algebraic Topology.
Proof of $H_k(X;\mathbb{F}) \cong H_k^{\infty}(X;\mathbb{F})$: John Lee: Introduction to smooth manifolds.
Proof of $H_k^{\infty}(X;\mathbb{F}) \cong H_{\text{deRham}}^{k}(X;\mathbb{F})$: John Lee: Introduction to smooth manifolds.

Persistent homology

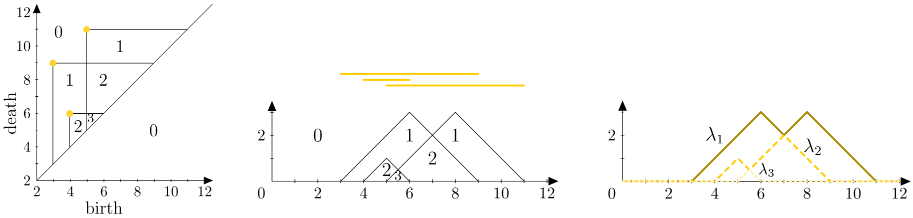
A persistence module is a family of $\mathbb{F}$-vectorspaces $V(s)$ for every real number s together with $\mathbb{F}$-linear maps $f_{st} : V(s) \to V(t)$. These are called structure maps. For each pair $s \leq t$, satisfying that $r \leq s \leq t$, then $f_{rt} = f_{st} \circ f_{rs}$.

Let $\{X(s)\}_{s\in\mathbb{R}}$ be a set of ordered simplicial complexes together with simplicial maps $f_{st} : X(s) \to X(t)$ for each pair $s \leq t$, such that $r \leq s \leq t$ implies $f_{rt} = f_{st} \circ f_{rs}$. An example is the aforementioned filtered simplicial complex. Then the persistence module with coefficients in $\mathbb{F}$ is given by

$$H_\star(X(s);\mathbb{F}), \quad H_\star(f_{st}) : H_\star(X(s);\mathbb{F}) \to H_\star(X(t);\mathbb{F}). \tag{5}$$

Persistent landscapes

Functional representation of persistence diagrams as a sequence of functions $\lambda_k : \mathbb{R} \to [-\infty, \infty]$ with $\lambda_k(x)$ being the kth largest value of $\min(x - b_i, d_i - x)$. It is stable with respect to Bottleneck distance and lies in a Banach space.



Taken from Peter Bubenik: Statistical Topological Data Analysis using Persistence Landscapes.

Commutative abelian Lie groups

Main assumption: $H_k(G) \cong H_k(\mathbb{R}^p \times S^1_1 \times \cdots \times S^1_q)$ with $p + q = \dim G$.
Goal: Sufficiently good representation of the topological structure of input space.

Künneth's Theorem

$$H_k(X \times Y) \cong \bigoplus_{i+j=k} H_i(X) \otimes H_j(Y)), \text{ thus}$$

$$H_k(\mathbb{R}^p \times S^1_1 \times \cdots \times S^1_q) \cong \bigoplus_{i_1+\cdots+i_r=k} H_{i_1}(\mathbb{R}^p) \otimes H_{i_2}(S^1_1) \otimes \cdots \otimes H_{i_r}(S^1_q).$$

Computing dimensions

We get

$$H_0(S^1) = H_1(S^1) = \mathbb{Z}, \tag{6}$$

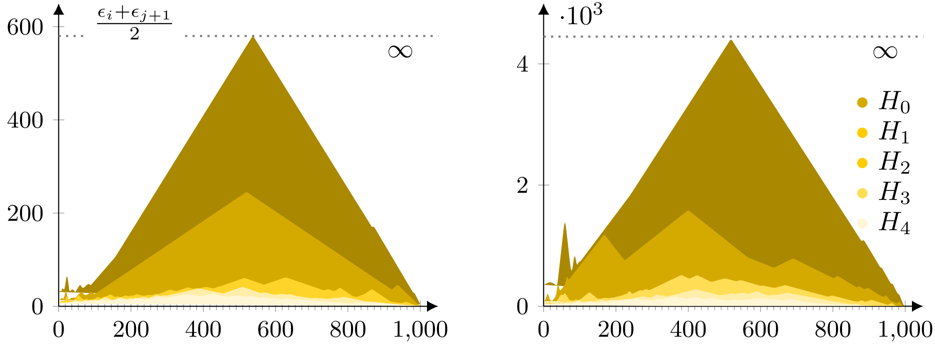
$$H_i(S^1) = 0, \text{ for all } i \geq 2. \tag{7}$$

Applying Künneth's formula only indices for $i_j \in \{0, 1\}$ remain, thus we get

$$H_0(\mathbb{R}^p) \cong \mathbb{Z}, \tag{8}$$

$$H_k(\mathbb{T}^q) \cong H_k(S^1_1 \times \cdots S^1_q) \cong \mathbb{Z}^{\binom{q}{k}}. \tag{9}$$

Experimental results on `cifar10` & `cifar100`



Results for the Betti numbers

	Homology groups					$\approx$ embedding dimension					
	H_0	H_1	H_2	H_3	H_4	p	$q\|H_1$	$q\|H_2$	$q\|H_3$	$q\|H_4$	$\dim U$
`cifar10`	12	16	40	59	50	12	16	$9{\pm}4$	$8{\pm}3$	$7{\pm}15$	$92{\pm}44$
`cifar100`	13	18	34	46	48	13	18	$9{\pm}2$	$8{\pm}10$	$7{\pm}13$	$97{\pm}50$

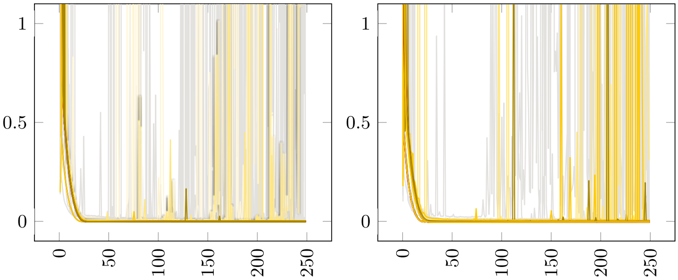
Problem: It becomes apparent, that this can't be a torus. Further, it might be, that the components are not connected. Our theory does give us results for *connected* abelian Lie groups.

Results for the Betti numbers

	Homology groups					≈ embedding dimension					
	H_0	H_1	H_2	H_3	H_4	p	$q\|H_1$	$q\|H_2$	$q\|H_3$	$q\|H_4$	$\dim U$
`cifar10`	12	16	40	59	50	12	16	$9_{\pm 4}$	$8_{\pm 3}$	$7_{\pm 15}$	$92_{\pm 44}$
`cifar100`	13	18	34	46	48	13	18	$9_{\pm 2}$	$8_{\pm 10}$	$7_{\pm 13}$	$97_{\pm 50}$

Solution: Choose a dimension being capable of embedding *n*-tori according to the rank of *every single* persistent homology group.

Losses on cifar10 & cifar100



$$\texttt{cifar10}: \bullet \in [2, 148], \bullet \in [150, 198], \bullet \in [200, 270] \text{ and } \bullet \in [272, 784], \tag{10}$$
$$\texttt{cifar100}: \bullet \in [2, 148], \bullet \in [150, 198], \bullet \in [200, 292] \text{ and } \bullet \in [294, 784]. \tag{11}$$

Outlook

1. **Sliding window embeddings** – investigated by Jose Perea et al. [PersHS2016, SliWi2015] – embed time series as a curve on or a curve dense on a torus. For these embeddings our method is an accurate estimate.
2. For arbitrary datasets we do not yield an exact solution for the binomial coefficient. The assumption of a **connected structure** fails. How could one generalize this?
3. We use vanilla neural networks. If we know the homology groups we want to represent, we can assign a commutative Lie group structure to the neural network itself, so that the **neuromanifold** has the same invariants as the **data manifold**.

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Thank you.

Got interested?
Drop a line to `luciano.melodia@fau.de`
or follow karhunenloeve on GitHub.