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# $p$ -Wasserstein Distance between High-Dimensional Point Clouds via Persistent Homology

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# Research background: topological data analysis (TDA)

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- “Topological”: to extract, analyze and make use of the topological and geometric structures underlying data
- “Data”: high-dimensional point clouds = metric spaces
- Topological features capture the global structure of the data and provide useful information on the connectedness and clusters
- **How can high-dimensional point clouds be compared based on their topological structures?**

# Project Overview

## Introduction

## Persistent Homology

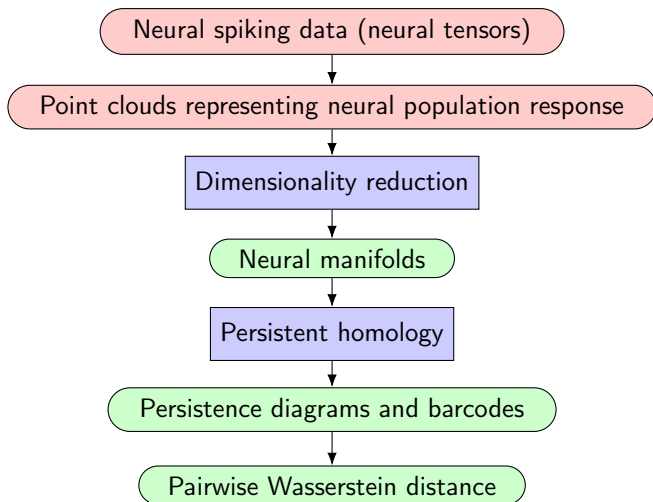
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# Advantages of TDA

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The major advantages for using TDA to analyze high-dimensional point clouds:

- 1 TDA provides qualitative information which is required for data analysis.
- 2 Compared to straightforward geometric methods, TDA is less sensitive to the actual choice of metrics.
- 3 Studying geometric objects using TDA does not depend on the coordinates.

# Simplicial complex

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## Definition 1 (Simplicial complex)

*An abstract simplicial complex is a pair  $(V, \Delta)$ , where  $V$  is a finite set, and  $\Delta$  is a family of non-empty subsets of  $V$  such that*

$$\tau \in \Delta \text{ and } \sigma \subseteq \tau \implies \sigma \in \Delta. \quad (1)$$

$\tau \in \Delta$  is face of  $\Delta$ . The dimension of a face  $\tau$  is  $|\tau| - 1$ .

(Intuition) A simplicial complex  $\Delta$  in  $\mathbb{R}^n$  is a collection of simplices in  $\mathbb{R}^n$  such that

- 1 Every face of a simplex of  $\Delta$  is in  $\Delta$ .
- 2 The intersection of any two simplices of  $\Delta$  is a face of each.

# An example of a simplicial complex

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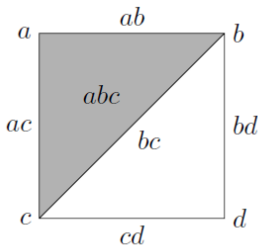
References

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Suppose the family of sets

$\emptyset, \{a\}, \{b\}, \{c\}, \{d\}, \{a, b\}, \{a, c\}, \{b, c\}, \{b, d\}, \{c, d\}, \{a, b, c\}$

form a simplicial complex  $E_1$ .



**Figure:** Geometric realizatoin of the simplicial compelix  $E_1$ .

# Simplicial chain complex

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## Definition 2 (Simplicial chain complex)

*The simplicial chain complex of a simplicial complex  $\Delta$ , denoted with  $\tilde{C}(\Delta)$ , is defined as:*

$$\dots \xrightarrow{\partial_{n+2}} \tilde{C}_{n+1}(\Delta) \xrightarrow{\partial_{n+1}} \tilde{C}_n(\Delta) \xrightarrow{\partial_n} \tilde{C}_{n-1}(\Delta) \xrightarrow{\partial_{n-1}} \dots$$

The simplicial chain complex of  $E_1$ ,  $C(E_1)$  is

$$\begin{array}{ccccccccc} 0 & \longrightarrow & \tilde{C}_2(E_1) & \xrightarrow{\partial_2} & \tilde{C}_1(E_1) & \xrightarrow{\partial_1} & \tilde{C}_0(E_1) & \xrightarrow{\partial_0} & \tilde{C}_{-1}(E_1) & \longrightarrow & 0 \\ & & \downarrow \cong & & \downarrow \cong & & \downarrow \cong & & \downarrow \cong & & \\ 0 & \longrightarrow & \mathbb{F} & \xrightarrow{\partial_2} & \mathbb{F}^5 & \xrightarrow{\partial_1} & \mathbb{F}^4 & \xrightarrow{\partial_0} & \mathbb{F} & \longrightarrow & 0 \end{array}$$

# Simplicial homology of degree $k$

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## Definition 3 (Simplicial homology of degree $k$ )

- *Cycle group,*

$$Z_k(\Delta; \mathbb{F}) = \ker(\partial_k) = \{Z \in \tilde{C}_k(\Delta; \mathbb{F}) : \partial_k(Z) = 0\}$$

- *Boundary group,*

$$B_k(\Delta; \mathbb{F}) = \text{im}(\partial_{k+1}) = \{Z \in \tilde{C}_k(\Delta; \mathbb{F}) : \partial_{k+1}(x), \quad x \in \tilde{C}_{k+1}(\Delta; \mathbb{F})\}$$

- *Simplicial homology group is the quotient group,*

$$H_k(\Delta; \mathbb{F}) := \ker(\partial_k) / \text{im}(\partial_{k+1}) \quad (2)$$

$$= Z_k(\Delta; \mathbb{F}) / B_k(\Delta; \mathbb{F}) \quad (3)$$

(Intuition) The simplicial homology gives an algebraic measure on the amount of cycles that are not the boundaries.



# $k$ -th Betti number

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## Definition 4 ( $k$ -th Betti number)

The  $k$ -th Betti number of the simplicial complex  $\Delta$  is

$$\beta_k(\Delta; \mathbb{F}) := \dim H_k(\Delta; \mathbb{F}) \quad (4)$$

$$= \dim \ker(\partial_k) - \dim \operatorname{im}(\partial_{k+1}). \quad (5)$$

- *elements in  $\ker(\partial_k)$  are called  $k$ -cycles.*
- *elements in  $\operatorname{im}(\partial_k)$  are called  $k$ -boundaries.*
- *$k$ -cycles that are not boundaries represent  $k$ -holes, which means that the  $k$ -th Betti number  $\beta_k(\Delta; \mathbb{F})$  is the number of  $k$ -holes.*

# An example for cycles and boundaries

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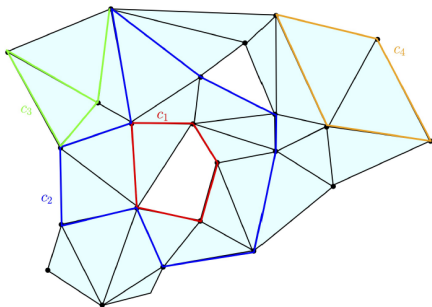
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**Figure:** A 2-dimensional simplicial complex  $K$ .

- $c_1, c_2, c_4$  are 1-cycles.
- $c_3$  is a 1-chain but not a 1-cycle.
- $c_4$  is the 1-boundary, namely the boundary of the 2-chain obtained as the sum of the two triangles surrounded by  $c_4$ .

# Persistent homology

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- ① The main idea of *persistence*: from a fixed value of the threshold  $\varepsilon$  to all the different values of  $\varepsilon$  at once.
- ② As  $\varepsilon$  increases, we add simplices to the complexes and detect which features “persist.”
- ③ It is robust with regards to perturbations in the input data.

# $p$ -persistent $k$ -th homology group

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## Definition 5 (Filtered simplicial complex)

*The simplicial complex  $\Delta$  with such a sequence of subcomplexes,  $\emptyset \subseteq \Delta^1 \subseteq \Delta^2 \subseteq \dots \subseteq \Delta^m = \Delta$ , is called filtered simplicial complex.*

## Definition 6 ( $p$ -persistent $k$ -th homology group)

*Given a filtered complex, the  $p$ -persistent  $k$ -th homology group  $H_k^{i,p}$  of for the  $i$ -th subcomplex  $\Delta^i$  is*

- $$H_k^{i,p} = Z_k^i / (B_k^{i+p} \cap Z_k^i)$$

Note that this is simply the definition of homology group of degree  $k$  in Definition 3 with the additional notion of persistence.

# Classification Theorem

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## Theorem 7 (Classification Theorem)

*For a finite persistence module  $\mathcal{M}$  with coefficients in the field  $F$ ,*

$$H_*(\mathcal{M}; F) \cong \underbrace{\bigoplus_i x^{t_i} F(x)}_{\text{free module}} \oplus \underbrace{\left( \bigoplus_j x^{r_j} (F(x)/(x^{s_j} F[x])) \right)}_{\text{torsion module}} \quad (6)$$

- bijection between {free elements} and {homology generators with birth at  $t_i$  and persist forever}
- bijection between {torsion elements} and {homology generators with birth at  $r_j$  and death at  $r_j + s_j$ }.

# Barcode as the persistence analogue of Betti number

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- The classification theorem gives the fundamental characterization of **persistence barcode**.
- $H_*^{i \rightarrow j}(\mathcal{C}_*^i; F)$  gives the number of intervals that contain  $i$ .
- As with Betti number, the barcode for  $H_k$  does not give the actual structure of the homology group, but just a continuously parameterized rank.
- The barcode is useful in that it can qualitatively filter out topological noise (since they are “short-lived” features) and capture significant topological features (features that persist over increasing values of  $\varepsilon$ ).

# Distances between points in $\mathbb{R}^d$ : $L_p$ Distances

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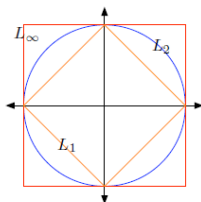
References

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$$L_2 \text{ distance: } d_2(x, y) = \|x - y\|_2 = \left( \sum_{i=1}^d (|a_i - b_i|^2) \right)^{1/2}. \quad (7)$$

$$L_1 \text{ distance: } d_1(x, y) = \|x - y\|_1 = \sum_{i=1}^d (|a_i - b_i|). \quad (8)$$

$$L_\infty \text{ distance: } d_\infty(x, y) = \|x - y\|_\infty = \max_{i=1}^d |a_i - b_i|. \quad (9)$$



# Distances between metric spaces: Hausdorff and Gromov-Hausdorff distances

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## Definition 8 (Hausdorff distance)

*Suppose  $A, B \subseteq X$  are closed sets of the same metric space.*

$$d_H(A, B) = \inf\{\varepsilon > 0 \mid A \subseteq B^\varepsilon \text{ and } B \subseteq A^\varepsilon\}, \quad (10)$$

*where  $A^\varepsilon$  denotes the  $\varepsilon$ -thickening of  $A$ .*

## Definition 9 (Gromov-Hausdorff distance)

*Suppose  $A, B$  are two closed metric spaces (can be distinct).*

$$d_{GH}(A, B) = \inf_{f,g} \{d_H(f_{A \rightarrow X}(A), g_{B \rightarrow X}(B))\}, \quad (11)$$

*where  $f_{A \rightarrow X}$  denotes an isometric embedding of  $A$  into some metric space  $X$  and  $g_{B \rightarrow X}$  denotes an isometric embedding of  $B$  into some metric space  $X$ . The infimum is taken over all possible such embeddings.*



# Distances between metric spaces: Hausdorff and Gromov-Hausdorff distances

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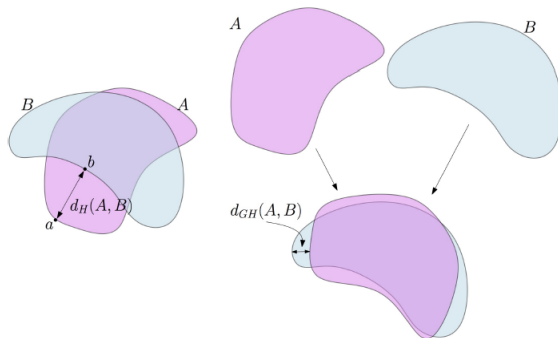
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**Figure:** Comparison between Hausdorff and Gromov-Hausdorff distances. Adapted from (Chazal and Michel, 2021).

# Distances between topological features: Bottleneck distance

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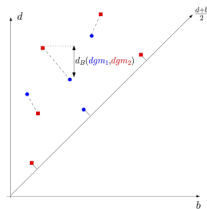
References

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## Definition 10 (Bottleneck distance)

$$d_B(dgm_1, dgm_2) = \inf_M \left\{ \max_{(x,y) \in M} \|x - y\|_\infty \right\}, \quad (12)$$

where the infimum is taken over all possible matchings  $M$ .



**Figure:** A perfect matching and the Bottleneck distance between the blue and red persistent diagrams. Adapted from (Chazal and Michel, 2021).

# Distances between topological features: distance

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## Definition 11 ( $p$ -Wasserstein distance)

*Given  $p \geq 1$ , the  $p$ -Wasserstein distance between a pair of persistence diagrams  $dgm_1$  and  $dgm_2$  is defined by*

$$W_p(dgm_1, dgm_2) = \left( \inf_M \sum_{(x,y) \in M} \|x - y\|_\infty^p \right)^{1/p}, \quad (13)$$

*where the infimum is taken over all possible matchings  $M$ .*

As  $p$  tends to infinity, the Wasserstein distance approaches the bottleneck distance.

# Application to neural data: Data collection

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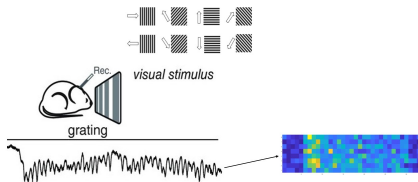
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- Moving visual stimuli of artificial gratings are flashed in front of the mouse.
- Each visual stimuli are shifting in 8 directions over time.
- Neuron output is recorded with electrodes and encoded in peristimulus (PSTH) diagrams.
- Each PSTH diagram shows the firing rate of one neuron over time for 8 directions. Brighter pixels indicate higher firing rates.



**Figure:** Visualising neural data from lab experiments.

# Neural tensors

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## Definition 12 (Neural population response)

*Suppose  $\mathcal{S}$  is a set of  $S$  visual stimuli (e.g., images)*

*$\mathcal{S} = \{s_1, s_2, \dots, s_S\}$ , each moving over a time interval of  $T$  in  $d$  directions. The neural population response of a set of  $N$  neurons to a stimulus  $m_i$  over time is  $\mathcal{N} = \{\vec{n}_1, \vec{n}_2, \dots, \vec{n}_N\}$ , where  $\vec{n}_i \in \mathbb{R}^{dT}$ .*

## Definition 13 (Neural tensors)

*Each neural tensor encodes the neural population response of a set of neurons to a set of moving visual stimulus over the time and directions of the movement. It is thus a 3-way tensor of dimension  $N$ -by- $S$ -by- $dT$ .*

# Build point clouds from neural tensors

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The neural spiking data set used in this project is represented by a 3-way tensor of dimension 698-by-6-by-264, where the dimensions represent:

- 1 698 neurons
- 2 6 types of visual stimuli
- 3 264 number of pixels in the PSTH diagram

Thus we have

- Six point clouds each corresponds to the neural population response towards one type of stimuli, which we denote as  $X_1, X_2, \dots, X_6$ .
- Each point cloud  $X_i$  consists of 698 points in  $\mathbb{R}^{264}$ .

# Step 1 dimensionality reduction: implementation

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- The Manifold Hypothesis states that real-world high-dimensional data lie on low-dimensional manifolds embedded within the high-dimensional space. (DeepAI, 2019)
- Neural spiking data is high-dimensional, but the neural connections constrain the possible patterns of population activity (Okun et al., 2015, Sadtler et al., 2014, Tsodyks, 1999) and that the possible patterns are confined to a low-dimensional manifold (Stopfer, Jayaraman, and Laurent, 2003, Yu et al., 2009).
- We reduced the dimensionality of each point cloud from the space of  $\mathbb{R}^{264}$  to  $\mathbb{R}^3$  using diffusion map implemented with pydiffmap package (Eastman et al., 2017)

# Step 1 dimensionality reduction: results

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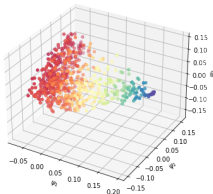
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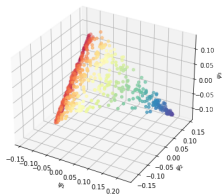
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Embedding given by first three DCs.



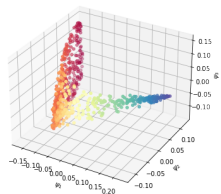
(a) Three-dimensional embedding of  $X_1$ .

Embedding given by first three DCs.



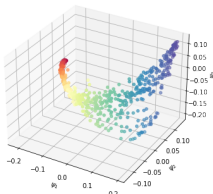
(b) Three-dimensional embedding of  $X_2$ .

Embedding given by first three DCs.



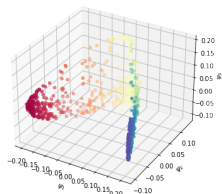
(c) Three-dimensional embedding of  $X_3$ .

Embedding given by first three DCs.



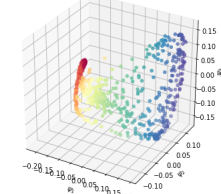
(d) Three-dimensional embedding of  $X_4$ .

Embedding given by first three DCs.



(e) Three-dimensional embedding of  $X_5$ .

Embedding given by first three DCs.



(f) Three-dimensional embedding of  $X_6$ .



## Step 2 persistent homology: implementation

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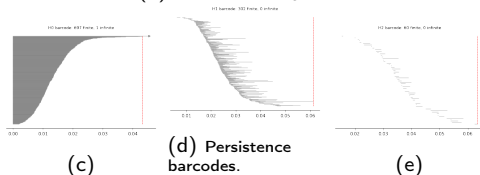
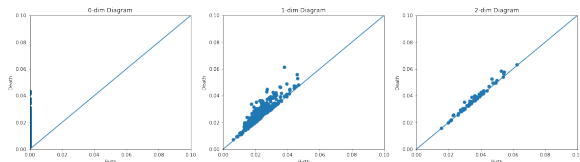
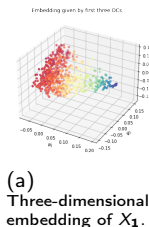
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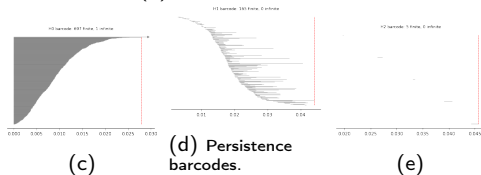
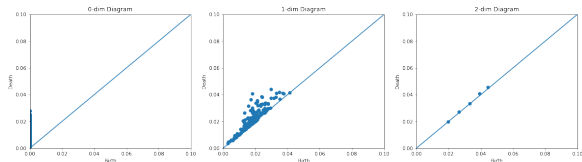
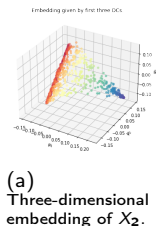
- We applied persistent homology to extract the topological features from the six embeddings respectively.
- We used the package ripser (Tralie, Saul, and Bar-On, 2018) to obtain the respective persistence diagrams from the embeddings.
- Using the (birth, death)-intervals from each persistence diagram, we then wrote code to draw the equivalent persistence barcode representation.

# Step 2 persistent homology: results



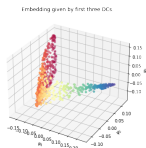
**Figure:** Results for applying persistent homology on the three-dimensional embedding of  $X_1$ .

# Step 2 persistent homology: results

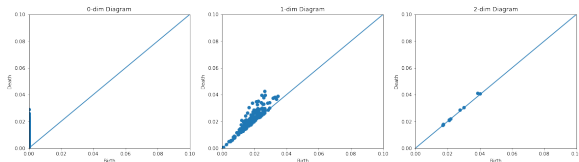


**Figure:** Results for applying persistent homology on the three-dimensional embedding of  $X_2$ .

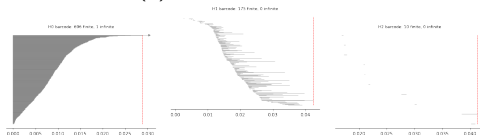
# Step 2 persistent homology: results



(a) Three-dimensional embedding of  $X_3$ .



(b) Persistence diagrams.



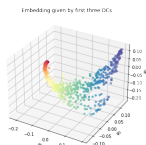
(c)

(d) Persistence barcodes.

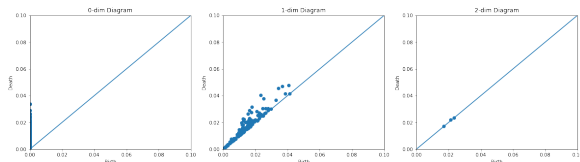
(e)

**Figure:** Results for applying persistent homology on the three-dimensional embedding of  $X_3$ .

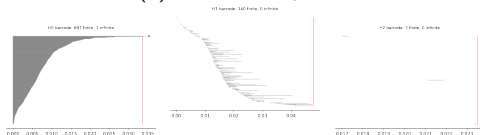
# Step 2 persistent homology: results



(a)  
Three-dimensional  
embedding of  $X_4$ .



(b) Persistence diagrams.



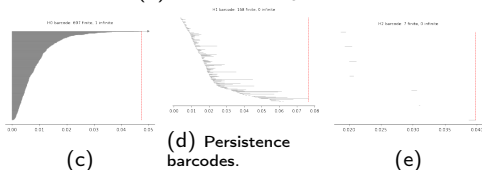
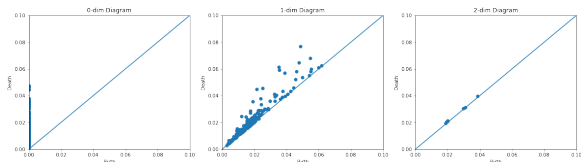
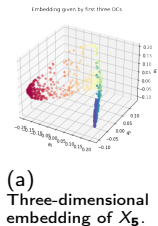
(c)

(d) Persistence  
barcodes.

(e)

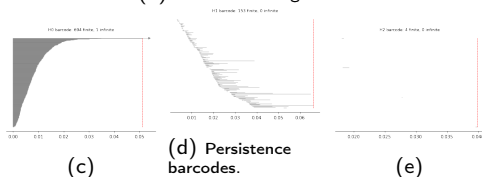
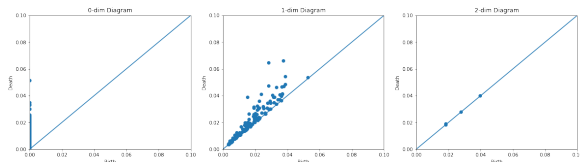
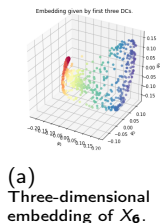
**Figure:** Results for applying persistent homology on the three-dimensional embedding of  $X_4$ .

# Step 2 persistent homology: results



**Figure:** Results for applying persistent homology on the three-dimensional embedding of  $X_5$ .

# Step 2 persistent homology: results



**Figure:** Results for applying persistent homology on the three-dimensional embedding of  $X_6$ .

## Step 3 $p$ -Wasserstein distance: results

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In the last step, we used the gudhi package (The GUDHI Project, 2021) to compute the pairwise Wasserstein distance between the persistence diagrams. The method used is based on (Kerber, Morozov, and Nigmetov, 2016).

$H_0$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$
$X_1$	0.0	2.77	3.05	3.95	3.08	3.42
$X_2$	2.77	0.0	0.43	1.35	1.0	0.84
$X_3$	3.05	0.43	0.0	1.03	0.94	0.66
$X_4$	3.95	1.35	1.03	0.0	1.11	0.72
$X_5$	3.08	1.0	0.94	1.11	0.0	0.51
$X_6$	3.42	0.84	0.66	0.72	0.51	0.0

**Table:** Pairwise Wasserstein distance between persistent diagrams for homology group  $H_0$ .



## Step 3 $p$ -Wasserstein distance: results

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$H_1$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$
$X_1$	0.0	0.46	0.5	0.64	0.64	0.55
$X_2$	0.46	0.0	0.17	0.29	0.36	0.3
$X_3$	0.5	0.17	0.0	0.25	0.33	0.3
$X_4$	0.64	0.29	0.25	0.0	0.27	0.29
$X_5$	0.64	0.36	0.33	0.27	0.0	0.26
$X_6$	0.55	0.3	0.3	0.29	0.26	0.0

**Table:** Pairwise Wasserstein distance between persistent diagrams for homology group  $H_1$ .

## Step 3 $p$ -Wasserstein distance: results

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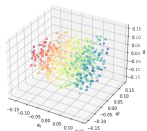
$H_2$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$
$X_1$	0.0	0.06	0.06	0.06	0.06	0.06
$X_2$	0.06	0.0	0.01	0.0	0.01	0.0
$X_3$	0.06	0.01	0.0	0.0	0.01	0.0
$X_4$	0.06	0.0	0.0	0.0	0.0	0.0
$X_5$	0.06	0.01	0.01	0.0	0.0	0.0
$X_6$	0.06	0.0	0.0	0.0	0.0	0.0

**Table:** Pairwise Wasserstein distance between persistent diagrams for homology group  $H_2$ .

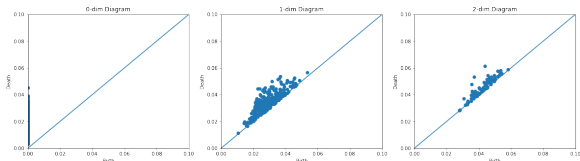
# Extension: comparison with known shapes (2-sphere)

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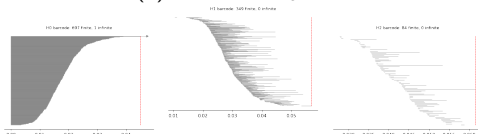
Embedding given by first three DCs



(a) Scatter plot for 2-sphere.



(b) Persistence diagrams.



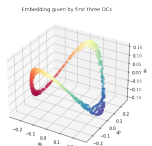
(c)

(d) Persistence barcodes.

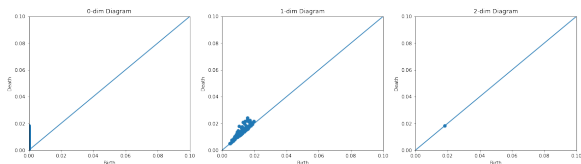
(e)

**Figure:** Results for applying persistent homology on the 2-sphere.

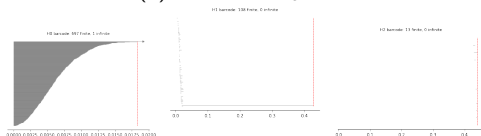
# Extension: comparison with known shapes (torus)



(a) Scatter plot for the three-dimensional torus.



(b) Persistence diagrams.



(c)

(d) Persistence barcodes.

(e)

**Figure:** Results for applying persistent homology on the three-dimensional torus.

## Extension: comparison with known shapes ( $p$ -Wasserstein distance)

Then, we computed the Wasserstein distance between the six point clouds and the known shapes:

$H_0$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$
2-sphere	2.48	4.46	4.64	5.18	4.53	4.83
torus	3.63	1.46	1.31	0.73	1.38	1.06

$H_1$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$
2-sphere	0.62	0.77	0.80	0.87	0.85	0.76
torus	0.74	0.49	0.44	0.34	0.45	0.47

$H_2$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_6$
2-sphere	0.11	0.12	0.12	0.12	0.13	0.12
torus	0.057	0.017	0.018	0.016	0.018	0.016

# Analysis of results

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Based on the results from the above tables of Wasserstein distances, our observations and inferences are as follows.

- 1 Neural population response evoked by stimulus type 1 is significantly different from the other stimulus types.
- 2 The intrinsic dimensionality of this neural data might be even lower than three-dimensional since there is no significant differences in homology groups  $H_2$  for the point clouds.
- 3 The topological structure of the neural population response evoked by stimuli type 1 is more similar to a sphere while those evoked by the other stimuli types are more similar to a torus.

# Conclusions

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- In this project, we proposed a topological approach to compare high-dimensional point clouds and provided a concrete application to neural spiking data.
- Limitations: lab data involve sampling errors such as missing data and inconsistent densities, causing noise to the true underlying geometry of the neural population response.
- Advantages: our approach obtained a useful summary of the global geometric structure of the neural spiking data in terms of how similarly the neurons collectively respond to visual stimuli.

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