Deep Learning with Topological Signatures

Persistent Homology and Machine Learning

Filip Jekić

MATF/ASW

Table of contents

1. Introduction
2. TDA
3. A Network Layer for Topological Signatures
4. Classification of Social Network Graphs

Introduction

Analysing high-dimensional data

How to infer topological and geometrical information from data?

- Methods from algebraic topology in machine learning
- Topological data analysis - TDA

Linear Regression

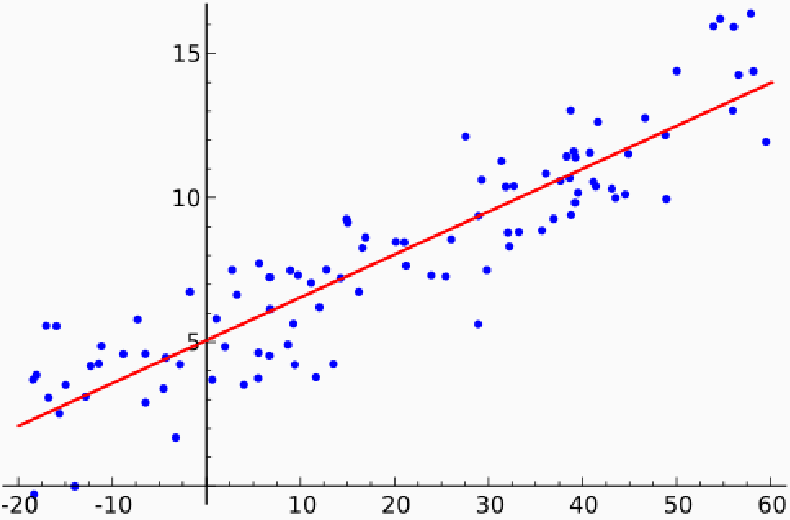


Figure 1: https://en.wikipedia.org/wiki/Linear_regression

Three clusters

Figure 2: http://ayasdi.com/wp-content/uploads/2015/01/GC-Pic-21.png

Three clusters

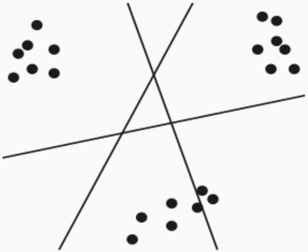


Figure 3: http://ayasdi.com/wp-content/uploads/2015/01/GC-Pic-31.png

Circle

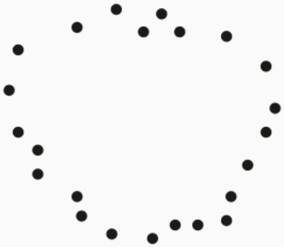


Figure 4: http://ayasdi.com/wp-content/uploads/2015/01/GC-Pic-41.png

Y-shape

Figure 5: http://ayasdi.com/wp-content/uploads/2015/01/GC-Pic-51.png

How to fit them all?

There is a large number of possible shapes

- Impossible to create templates for all
- A flexible way of representing all shapes is needed
- TDA gives a solution

Example: Returning customers in retail

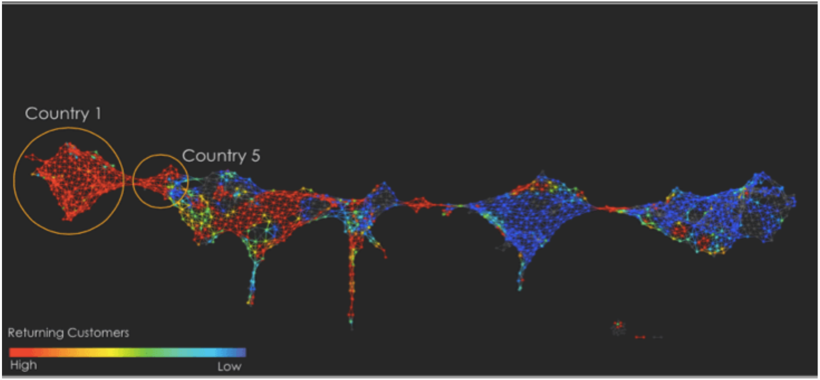


Figure 6: ayasdi.com/wp-content/uploads/2015/01/GC-Pic-111.png

Why Topology?

- Topology studies shapes in a coordinate free way
- Topology studies the properties of shapes that are invariant under “small” deformations
- Topology methods give compressed representations of shapes

TDA

Persistent Homology

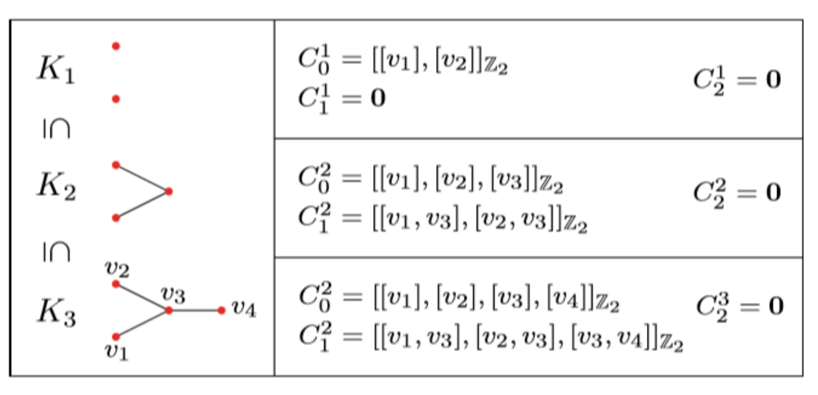
- Allows us to track topological changes in data at multiple scales
- Topological components (connected components, holes, etc.) appear and dissapear
- Their lifespan - (birth, death)
- Multiset - topological signature

Applications

- Manifold analysis of natural image patches
- Analysis of activity patterns of the visual cortex
- Interpretability of Convolutional Neural Networks
- Clustering
- Network classification

Scikit-TDA:
Topological Data Analysis Python libraries
https://scikit-tda.org/

Filtration



K_1 $\subseteq$	$C_0^1 = [[v_1], [v_2]]_{\mathbb{Z}_2}$ $C_1^1 = \mathbf{0}$ $C_2^1 = \mathbf{0}$
K_2 $\subseteq$	$C_0^2 = [[v_1], [v_2], [v_3]]_{\mathbb{Z}_2}$ $C_1^2 = [[v_1, v_3], [v_2, v_3]]_{\mathbb{Z}_2}$ $C_2^2 = \mathbf{0}$
K_3 (v_1, v_2, v_3, v_4)	$C_0^2 = [[v_1], [v_2], [v_3], [v_4]]_{\mathbb{Z}_2}$ $C_1^2 = [[v_1, v_3], [v_2, v_3], [v_3, v_4]]_{\mathbb{Z}_2}$ $C_2^3 = \mathbf{0}$

Figure 7: Example of a filtration

Chain complex

$$
\begin{array}{ccccccccc}
\cdots & \xrightarrow{\partial_3} & C_2^1 & \xrightarrow{\partial_2} & C_1^1 & \xrightarrow{\partial_1} & C_0^1 & \xrightarrow{\partial_0} & \mathbf{0} \\
 & & \downarrow \iota & & \downarrow \iota & & \downarrow \iota & & \\
\cdots & \xrightarrow{\partial_3} & C_2^2 & \xrightarrow{\partial_2} & C_1^2 & \xrightarrow{\partial_1} & C_0^2 & \xrightarrow{\partial_0} & \mathbf{0} \\
 & & \vdots \ \iota & & \vdots \ \iota & & \vdots \ \iota & & \\
\cdots & \xrightarrow{\partial_3} & C_2^m & \xrightarrow{\partial_2} & C_1^m & \xrightarrow{\partial_1} & C_0^m & \xrightarrow{\partial_0} & \mathbf{0}
\end{array}
$$

Figure 8: Chain complex of a filtration

Persistent Homology Groups

$$H_n^{i,j} = \ker \partial_n^i / (\operatorname{im} \partial_{n+1}^j \cap \ker \partial_n^i)$$

$$\beta_n^{i,j} = \operatorname{rank} H_n^{i,j}$$

Topological signatures

Filtration from sublevel sets of $f : C_0 \longrightarrow \mathbb{R}$:

$$f([v_0, \ldots, v_n]) = \max\{f([v_i]) \ : \ 0 \leq i \leq n\}$$

Defined filtration: $K_0 = \emptyset$ and $K_i = f^{-1}((-\infty, a_i])$

Persistence diagram

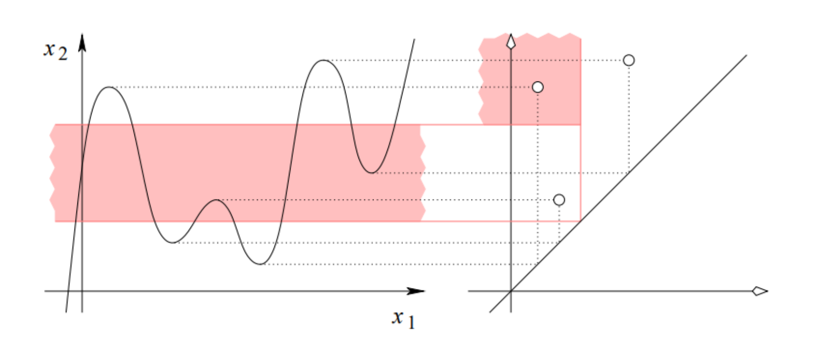


Figure 9: Persistent Homology — a Survey, Herbert Edelsbrunner and John Harer

A Network Layer for Topological Signatures

Projection of Persistence Diagrams

- $\mu = (\mu_0, \mu_1) \in \mathbb{R} \times \mathbb{R}^+$
- $\sigma = (\sigma_0, \sigma_1) \in \mathbb{R}^+ \times \mathbb{R}^+$
- $\nu \in \mathbb{R}^+$

$$s_{\mu,\sigma,\nu}((x_0, x_1)) =$$

$$\begin{cases} \exp(-\sigma_0^2(x_0 - \mu_0)^2 - \sigma_1^2(x_1 - \mu_1)^2), & \text{for } x_1 \in [\nu, \infty) \\ \exp(-\sigma_0^2(x_0 - \mu_0)^2 - \sigma_1^2(\ln \frac{x_1}{\nu}\nu + \nu - \mu_1), & \text{for } x_1 \in (0, \nu) \\ 0, & \text{for } x_1 = 0 \end{cases}$$

The Network Layer

- $N \in \mathbb{N}$
- $\theta = (\mu_i, \sigma_i)_{i=0}^{N} \in ((\mathbb{R} \times \mathbb{R}^+) \times (\mathbb{R}^+ \times \mathbb{R}^+))^N$
- $\nu \in \mathbb{R}^+$

$$S_{\theta,\mu} : \mathbb{D} \longrightarrow (\mathbb{R}_0^+)^N$$

$$S_{\theta,\mu}(D) = (S_{\mu_i,\sigma_i,\nu}(D))_{i=0}^{N-1}$$

Properties of the layer

- $s_{\mu,\sigma,\nu}$ is continuous in x_1
- $s_{\mu,\sigma,\nu}$ is differentiable on $\mathbb{R} \times \mathbb{R}^+$
- $S_{\mu_i,\sigma_i,\nu}$ is a finite sum of $s_{\mu_i,\sigma_i,\nu}$
- $S_{\theta,\mu}$ is a concatenation

It follows that this network layer is trainable via backpropagation

Classification of Social Network Graphs

Dataset

- Problem of graph classification
- Vertices are unlabeled and edges are undirected
- Reddit-5k: 5 classes, 5k graphs
- Reddit-12k: 12 classes, 12k graphs

- Sample: Discussion graph
- Label: Subreddit (e.g. worldnews, video, etc.)

Filtration

Construction of a simplicial complex from a graph (V, E):

$$K_0 = \{[v] \in V\}$$

$$K_1 = \{[u, v] : \{u, v\} \in E\}$$

Filtration is based on vertex degree:

$$f([v_0] = \mathrm{deg} v_0 / \mathrm{max}_{v \in V} \mathrm{deg}(v)$$

and lifted on K_1 by taking the maximum

Network architecture - input

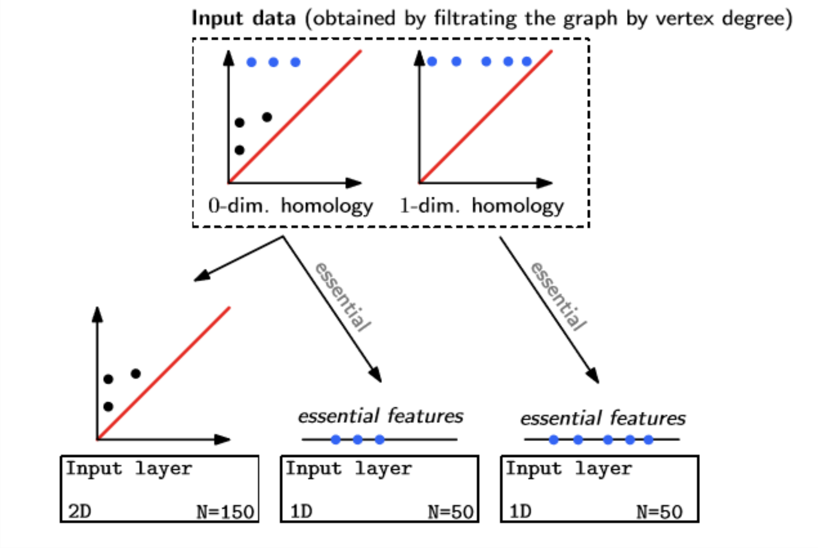


Figure 10: Deep Learning with Topological Signatures - Hofer et al.

Network architecture - middle layers

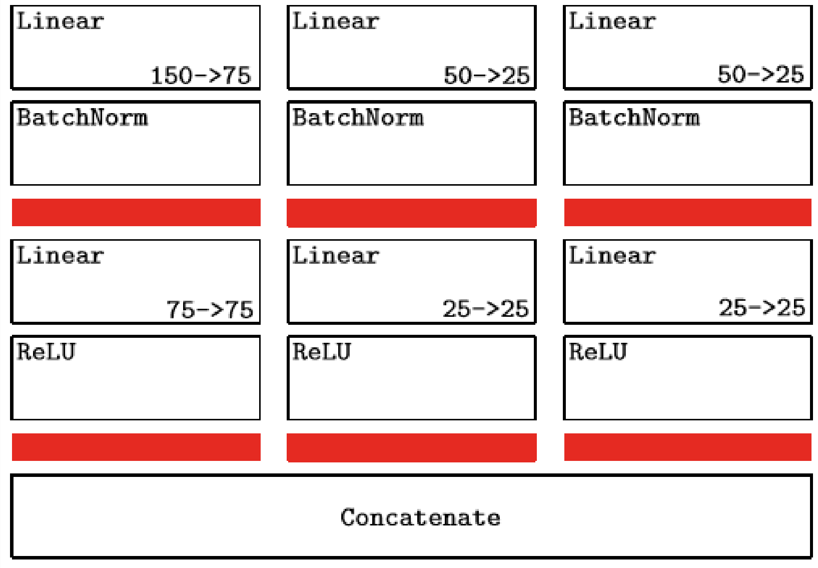


Figure 11: Deep Learning with Topological Signatures - Hofer et al.

Network architecture - output

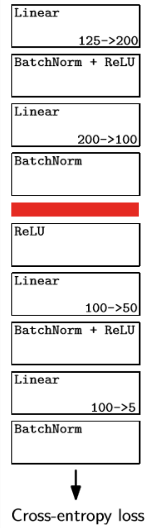


Figure 12: Deep Learning with Topological Signatures - Hofer et al.

Results

	reddit-5k	reddit-12k
GK [31]	41.0	31.8
DGK [31]	41.3	32.2
PSCN [24]	49.1	41.3
RF [4]	50.9	42.7
Ours (w/o essential)	49.1	38.5
Ours (w/ essential)	**54.5**	**44.5**

Figure 13: Deep Learning with Topological Signatures - Hofer et al.

References i

H. Edelsbrunner and J. Harer.
Persistent homology - a survey.
Contemporary mathematics, (453):257–282, 2008.

R. Graham, D. Knuth, and O. Patashnik.
Concrete mathematics.
Addison-Wesley, Reading, MA, 1989.

C. Hofer, R. Kwitt, M. Niethammer, and A. Uhl.
Deep learning with topological signatures.
NIPS, 2017.

P. Lum and et al.
Extracting insights from the shape of complex data using topology.
Scientific reports, (3), 2013.