

# Topological Data Analysis and Clustering Algorithms in Machine Learning

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Mathematical Engineering - İTÜ





2 Hierarchical Clustering

- Topological Data Analysis
- Theoretical Contributions

5 Experimental Contributions



#### Hierarchical Clustering and Zeroth Persistent Homology

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### Introduction



- 3 Topological Data Analysis
- 4 Theoretical Contributions
- 5 Experimental Contributions

# Outline



### Introduction

2 Hierarchical Clustering

Topological Data Analysis

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### 5 Experimental Contributions

# Outline



### Introduction

2 Hierarchical Clustering

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### 5 Experimental Contributions

#### PERSISTENT HOMOLOGY, MATROIDS AND COBORDISMS

İSMAIL GÜZEL AND ATABEY KAYGUN



### "Data has shape, and shape has meaning."

Prof. Gunnar Carlsson



#### Figure: The data taken from SCOPUS

### Questions answered

- What are the similarities and differences between hierarchical clustering and 0-th persistent homology?
- What is the difference from the persistence barcode?
- What about higher dimensional persistent homology?
- What are the experiments on real datasets?



# Hierarchical Clustering

- Unsupervised machine learning algorithm
- Aim: divide the data set into disjoint subsets such that
  - homogeneous in cluster
  - heterogeneous between clusters

- The metric structure of ambient space from data set.
- A nice tree-based representation, called *a dendrogram*





Ismail Guzel (İTÜ)

Ph.D. Thesis















## Compare Dendrograms

- Two Dendrograms
- Two cophenetic matrix

### Mantel Test

- Non-parametric Test
- Like correlation coefficient
- Mantel statistic  $r \in [-1, 1]$



## Silhouette scores

#### Silhouette scores

$$s(x) = \frac{b(x) - a(x)}{\max(a(x), b(x))},$$
  
$$a(x) = d(x, U(x)) \quad \text{and} \quad b(x) = \min_{C \neq U(x)} d(x, C).$$

	Tekirdağ	İstanbul	Balıkesir	Manisa	İzmir	Konya	Antalya
Tekirdağ	0						
İstanbul	132	0					
Balıkesir	379	390	0				
Manisa	511	529	141	0			
İzmir	506	564	176	35	0		
Konya	794	662	551	534	550	0	
Antalya	850	718	505	428	444	322	0



Points	Cohesion	Separation	Silhouette				
Tekirdağ	132	465.3	0.72				
İstanbul	132	494.5	0.73				
Balıkesir	158.5	384.5	0.59				
Manisa	88	428	0.79				
İzmir	105.5	444	0.76				
Konya	0	322	1				
Antalya	0	322	1				
Overall silhouette score is $s \approx 0.80$							

# Simplicial Technology



# Point Cloud to Complex

### Čech Complex

$$\mathscr{C}_{\varepsilon} = \left\{ \sigma \subseteq \mathscr{D} \quad | \quad \bigcap_{x \in \sigma} B_{\varepsilon}(x) \neq \varnothing \right\}, \quad B_{\varepsilon}(x) = \{ y \mid d(x, y) < \varepsilon \}$$

### Vietoris Rips Complex

$$\mathscr{R}_{\varepsilon} = \{ \sigma \subset \mathscr{D} \mid \|x - y\| \leq \varepsilon, \text{ for all } x, y \in \sigma \}$$







## Example: A Simplicial complex $\mathscr{K}$



$$\begin{aligned} & \mathscr{C}_0 = \{ v_0, v_1, v_2, v_3, v_4, v_5 \}, \\ & \mathscr{C}_1 = \frac{\{ [v_0, v_1], [v_1, v_2], [v_2, v_0], [v_2, v_3], \\ & [v_3, v_4], [v_4, v_5], [v_3, v_5] \} \\ & \mathscr{C}_2 = \{ [v_3, v_4, v_5] \}. \end{aligned}$$

$$0 \xrightarrow{\partial_3} \mathscr{C}_2 \xrightarrow{\partial_2} \mathscr{C}_1 \xrightarrow{\partial_1} \mathscr{C}_0 \xrightarrow{\partial_0} 0$$

### Homology

The  $k^{th}$  homology group of  $\mathcal{K}$  is defined by

$$H_k(K) := \frac{\ker(\partial_k)}{\dim(\partial_{k+1})}$$

$$\beta_0 = \dim(\ker(\partial_0)) - \dim(\operatorname{im}(\partial_1)) = 6 - 5 = 1$$

$$\beta_1 = \dim(\ker(\partial_1)) - \dim(\operatorname{im}(\partial_2)) = 2 - 1 = 1$$

### Vietoris-Rips Filtration

Filtration of a simplicial complex K is a collection of subcomplexes  $\mathbb{K} = \{K_{\varepsilon} : \varepsilon \in \mathbb{R}^+\}$  that satisfy  $K_{\varepsilon_1} \subseteq K_{\varepsilon_2}$  whenever  $\varepsilon_1 \leq \varepsilon_2$ .















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## Persistent Homology

Filtered Vietoris-Rips complex

$$R_{\mathcal{E}_1} \hookrightarrow R_{\mathcal{E}_2} \hookrightarrow \cdots \hookrightarrow R_{\mathcal{E}_i} \hookrightarrow \cdots \hookrightarrow R_{\mathcal{E}_j} \hookrightarrow \cdots \hookrightarrow R_{\mathcal{E}_{max}}$$

After applying the homology functor,

$$H_k(R_{\varepsilon_1}) o H_k(R_{\varepsilon_2}) o \cdots o H_k(R_{\varepsilon_i}) o \cdots o H_k(R_{\varepsilon_j}) o \cdots o H_k(R_{\varepsilon_{max}})$$

For every pair  $\varepsilon_i, \varepsilon_j$ 

$$\psi^k_{arepsilon_i,arepsilon_j}: H_k(R_{arepsilon_i}) o H_k(R_{arepsilon_j})$$

#### Definition

The k-th persistent homology group is

$$PH_k := \operatorname{im} \psi_{\varepsilon_i,\varepsilon_j}^k.$$

#### Go Forward

## Persistent Homology - Big Picture



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$$D = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$
 Rank = 2



$$D = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$
 Rank = 2



$$D_{\alpha,\beta} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix}$$
 Rank = 2





$$\partial_1 = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \qquad \partial_0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$



$$D = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$
 Rank = 3  
$$D_{\beta,\gamma} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$
 Rank = 3  
$$D_{\alpha,\gamma} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

## Homological Distance

Given a point cloud *P*, construct the Rips Complex

$${\mathcal R}_{arepsilon}({\mathcal P}) = \{ \sigma \subset {\mathcal P} \mid \|x-y\| \leq arepsilon, ext{ for all } x, y \in \sigma \}$$

*R*<sub>\varepsilon\_1</sub> ⊆ *R*<sub>\varepsilon\_2</sub> for a given pair \varepsilon\_1 and \varepsilon\_2 values with \varepsilon\_1 ≤ \varepsilon\_2
For the pair \varepsilon\_1 < \varepsilon\_2 we have the natural map in homology.</li>

$$\psi^k_{\varepsilon_1,\varepsilon_2}: H_k(R_{\varepsilon_1}) \to H_k(R_{\varepsilon_2})$$

• Take two cycles  $lpha,\ eta\in H_k(\mathscr{R}_{arepsilon_1})$ 

•  $\alpha' := \psi_{\varepsilon_1, \varepsilon_2}^k(\alpha)$  and  $\beta' := \psi_{\varepsilon_1, \varepsilon_2}^k(\beta)$  by padding  $\alpha$  and  $\beta$  with suitable number of 0's.

## Homological Distance

- Add  $\alpha'$ ,  $\beta'$  and  $\alpha', \beta'$  together to the differential matrix  $\mathscr{D}^t$  at  $\varepsilon_2$ .
- Calculate rank of the differential matrices.
- Check whether  $\psi^k_{\varepsilon_1,\varepsilon_2}(\alpha)$  and  $\psi^k_{\varepsilon_1,\varepsilon_2}(\beta)$  are linearly dependent.

#### Homological Distance

*k*-th homological cophenetic distance  $D_k(\alpha, \beta)$  between homology classes  $\alpha$  and  $\beta$  is defined as  $\inf \left\{ \eta - \varepsilon \ge 0 \mid \psi_{\varepsilon,n}^k(\alpha), \psi_{\varepsilon,n}^k(\beta) \text{ non-zero and lin. dep.} \right\}$ 

### Experiments

#### A synthetic point cloud

- $D\in \mathbb{R}^2$  and |D|=20 ,
- Uniform distribution over [0,1),
- Labeled with the first 20 letters.

**Input:** A point cloud *D*, |D| = 20 and a list  $\varepsilon = \{\varepsilon_1 = 0, 0.05, \dots, 0.95, \varepsilon_{max} = 1\}$ . **Output:** Dendrograms

#### begin

 $\begin{array}{l} \mathsf{HomDist} = [ ]_{20 \times 20} \\ \mathscr{R}_{\varepsilon}(P) \longleftarrow \mathsf{Vietoris-Rips filtration} ; \\ \mathsf{for } each \varepsilon \ \mathsf{do} \\ & | \ \mathsf{for } every \ \alpha_i, \alpha_j \in H_0(\mathscr{R}_{\varepsilon}) \ \mathsf{do} \\ & | \ \mathsf{HomDist}_{i,j} \longleftarrow \inf\{\varepsilon | check \ lin. \ dep.\} ; \\ & \mathsf{end} \end{array}$ 

#### end

 $E(D) \leftarrow EuclideanDist(D);$   $Dend_1 \leftarrow HierarchicalClustering(HomDist(D));$   $Dend_2 \leftarrow HierarchicalClustering(E(D));$  $Compare(Dend_1, Dend_2)$ 

end

## Two dendrograms with single-linkage



Experimental Contributions

### Tanglegram with the entanglement of 0.01



## Barcode and Enriched Barcode



### Turkish Cities and Mantel Statistics



- 24 Türkiye cities
- Single-linkage
- Different metrics
- Dendrograms

Metrics	Bray-Curtis	Cosine	Manhattan	Euclidean	Minkowski	Homological
Bray-Curtis	1.00	0.64	0.96	0.90	0.90	0.90
Cosine		1.00	0.61	0.52	0.69	0.59
Manhattan			1.00	0.96	0.87	0.97
Euclidean				1.00	0.75	0.98
Minkowski					1.00	0.78
Homological						1.00

### Turkish Cities and Mantel Statistics



- 24 Türkiye cities
- Single-linkage
- Different metrics
- Dendrograms

Metrics	Bray-Curtis	Cosine	Manhattan	Euclidean	Minkowski	Homological
Bray-Curtis	1.00	0.64	0.96	0.90	0.90	0.90
Cosine		1.00	0.61	0.52	0.69	0.59
Manhattan			1.00	0.96	0.87	0.97
Euclidean				1.00	0.75	0.98
Minkowski					1.00	0.78
Homological						1.00



Table: Datasets used and their properties.

Dataset	#Instances	#Attributes	Supervised	#Classes
Turkish Cities	82	2	No	-
lris	150	4	Yes	3
Cancer Coimbra	116	10	Yes	2
Synthetic (total separation)	100	100	Yes	4
Synthetic (with mixture)	100	2	Yes	4

## Silhouette Scores

#### Synthetic Perfect



#### Synthetic Mixed



## Silhouette Scores

#### Cancer Coimbra







### A comparison of metrics on Mixed Synthetic datasets.

#### Synthetic Dataset

Metric	F1	Acc.	Hom.	Comp.	M.Info	Rand
Bray-Curtis	1.00 A	1.00 A	1.00 A	1.00 A	1.38 A	1.00 A
Cosine	0.83 A	0.91 A	0.72 C	0.77 S	1.38 C	0.87 A
Manhattan	1.00 S	1.00 S	1.00 S	1.00 S	0.99 S	1.00 S
Euclidean	1.00 A	1.00 A	1.00 A	1.00 A	1.38 A	1.00 A
Minkowski	1.00 C	1.00 C	1.00 C	1.00 C	1.38 C	1.00 C
Homological	0.98 A	0.99 A	0.95 A	1.00 S	1.31 A	0.98 A

### A comparison of metrics on Cancer datasets.

#### Real Dataset

Metric	F1	Acc.	Hom.	Comp.	M.Info	Rand
Bray-Curtis	0.56 S	0.56 S	0.02 A	0.14 S	0.02 A	0.50 S
Cosine	0.55 C	0.55 C	0.01 S	0.12 S	0.01 S	0.50 C
Manhattan	0.53 S	0.53 S	0.02 A	0.13 A	0.02 A	0.50 S
Euclidean	0.54 W	0.54 W	0.02 A	0.13 A	0.02 A	0.50 W
Minkowski	0.53 S	0.53 S	0.02 A	0.13 A	0.02 A	0.50 S
Homological	0.61 W	0.61 W	0.03 W	1.00 S	0.02 W	0.52 W

## BAP, TÜBİTAK, Michigan State University, Other Works

#### BASARIM2022

#### Classification of Stochastic Processes with Topological Data Analysis

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#### SIAM Data Mining: TDA, ML

A Case Study on Identifying Bifurcation and Chaos with CROCKER Plots

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#### Abstract

The CHOCKSR plot is a coarsened but easy to visualize representation of the data in a one-parameter varying family operastence barcodes. In this paper, we use the CROCKER plot to vise changes in the periodence under a varying hidreadon parameter. We perform experiments to support our methods using the the Lyapunov exponent.

Erzincan Üniversitesi Fen Bilimleri Enstittsü Dergisi 2022, 15(ÖZEL SAYI I), 1-13 ISSN: 1307-9085, e-ISSN: 2149-4584 Araştırma Makalesi Erzincan University Journal of Science and Technology 2022, 15(SPECIAL ISSUE I), 1-13 DOI: 10.18185/erzifbed.1199660 Research Article

#### Attitudes and Behaviors of Turkish Consumers Regarding the Olive Oil Consumption

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#### MDPI

#### Article

Phenolic Constituents, Antioxidant and Antimicrobial Activity and Clustering Analysis of Propolis Samples Based on PCA from Different Regions of Anatolia

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Experimental Contributions

## BAP, TÜBİTAK, Michigan State University, Other Works

#### BASARIM2022

#### SIAM Data Mining: TDA, ML



## Future Work

#### On this thesis

- Apply real-world dataset for the first degree of homology.
- Visualization tools for the first degree of homology.
- Apply to the categorical dataset.
- Deal with problems about computational power and memory.

#### Other tasks

- Relation between Lyapunov exponent and persistent homology
- Two dimension bifurcation and CROCKER
- Classification Alpha-stable processes via TDA

# **Thank You!**



## Seperation of complex

#### Chain Complex

A chain complex of a simplicial complex  $\mathscr{K}$  is a sequence of abelian groups or modules  $\mathscr{C}_k$  connected by homomorphisms  $\partial_k : \mathscr{C}_k \to \mathscr{C}_{k-1}$  such that  $\partial_{k-1} \circ \partial_k = 0$  for  $k \in \mathbb{Z}$ .

$$\dots \xrightarrow{\partial_{k+2}} \mathscr{C}_{k+1} \xrightarrow{\partial_{k+1}} \mathscr{C}_k \xrightarrow{\partial_k} \dots$$
$$\partial_k \sigma = \sum_{i=0}^k (-1)^i [v_0, v_1, \dots, \hat{v}_i, \dots, v_k]$$



#### Homology and Betti Number

The  $k^{th}$  homology group of a simplicial complex K is defined by

$$\mathcal{H}_k(\mathcal{K}) := \frac{\ker(\partial_k)}{\operatorname{im}(\partial_{k+1})}$$

The dimension of the  $k^{th}$  homology group of K is called the  $k^{th}$  Betti number  $\beta_k(K)$ .



## Well-defined Persistence barcode

• Persistence modules

$$V_1 \rightarrow V_2 \rightarrow \cdots \rightarrow V_r \rightarrow \cdots \rightarrow V_s \rightarrow \cdots \rightarrow V_n$$

• Decompose persistence module into interval modules,

$$0 \rightarrow 0 \rightarrow \cdots \rightarrow 0 \rightarrow \mathbb{Z}_2 \rightarrow \cdots \rightarrow \mathbb{Z}_2 \rightarrow 0 \rightarrow \cdots 0$$

- A persistence module V indexed by  $T \subset \mathbb{R}$  is q tame if for any v < s in T, the rank of the linear map  $v_r^s : V_r \to V_s$  is finite.
- If  $\mathbb V$  is a q-tame persistence module, then it has a well-defined persistence barcode.

Go Back

## Combinatoric Possibilities

• Check whether  $\psi_{\varepsilon_1,\varepsilon_2}^k(\alpha)$  and  $\psi_{\varepsilon_1,\varepsilon_2}^k(\beta)$  are linearly independent by evaluating the rank of the differential matrix  $\mathscr{D}$  at  $\varepsilon_2$  with appending  $\alpha'$ ,  $\beta'$  and  $\alpha',\beta'$  together.

$$egin{aligned} &r_lpha := ext{rank}(\mathscr{D}_lpha) - ext{rank}(\mathscr{D}) \ &r_eta := ext{rank}(\mathscr{D}_eta) - ext{rank}(\mathscr{D}) \ &r_{lpha,eta} := ext{rank}(\mathscr{D}_{lpha,eta}) - ext{rank}(\mathscr{D}) \end{aligned}$$

with the following cases:

 $\begin{cases} \alpha \text{ and } \beta \text{ both die} & \text{ if } r_{\alpha,\beta} = 0, \\ \alpha \text{ and } \beta \text{ both live} & \text{ if } r_{\alpha,\beta} = 2, \\ \alpha \text{ dies and } \beta \text{ lives} & \text{ if } r_{\alpha,\beta} = 1 \text{ and } r_{\alpha} = 0, \\ \alpha \text{ lives and } \beta \text{ dies} & \text{ if } r_{\alpha,\beta} = 1 \text{ and } r_{\beta} = 0, \\ \alpha \text{ and } \beta \text{ merge} & \text{ if } r_{\alpha,\beta} = 1, r_{\alpha} = 1 \text{ and } r_{\beta} = 1. \end{cases}$ 

## Matroids

#### Definition

A partially ordered set is defined as an ordered pair  $P = (X, \leq)$ . Here, X is called the ground set of P and  $\leq$  is the partial order of P

#### Definition

A matroid  $M = (S, \mathbb{I})$  is a finite ground set S together with a collection of sets  $\mathbb{I} \subset 2^S$  satisfying

- Downward closed:  $A \in \mathbb{I}$  and  $B \subseteq A \Rightarrow B \in \mathbb{I}$
- Exchange property:  $A, B, \in \mathbb{I}$  and  $|B| < |A| \Rightarrow \exists x \in A \setminus B$  such that  $\{x\} \bigcup B \in \mathbb{I}$ .

### Matroids

#### Terminology

- Independent set:  $I \in \mathbb{I}$
- Circuit: Minimal dependent set of M
- Basis: Maximal independent set of M
- Span: Basis B and  $B \subseteq \mathbb{I} \Rightarrow \mathbb{I}$  is a spanning set.
- Ground set  $\mathbb{V}$ : set of vectors spanning  $\mathbb{R}^d$
- Independent set  $\mathbb{I}$ : bases of  $\mathbb{R}^d$  in  $\mathbb{V}$
- Matroid:  $(\mathbb{V},\mathbb{I})$

## The Rank Function of a Matroid

#### Definition

Let *M* be a matroid on a finite ground set *E*. The rank r(X) of a subset  $X \subseteq E$  is the cardinality of the largest independent set contained in *X*. In other words

$$r(X) = \max\{|A| \in N \mid A \subseteq X \text{ and } A \in \mathscr{I}\}$$

## Cobordisms

For two linearly independent pair of homology classes  $\alpha$  and  $\beta$  in  $H_1(R_{\varepsilon})$ , one can see  $\psi_{\varepsilon,\eta}^1(\alpha)$ and  $\psi_{\varepsilon,\eta}^1(\beta)$  are linearly dependent in  $H_1(R_{\eta})$ . We, then, visualize that two classes  $\alpha$  and  $\beta$ merged at time  $\eta$ .



Figure: Cobordism in the merging case from  $S^1 \sqcup S^1$  to  $S^1$  representing two cycles  $\alpha$  and  $\beta$  evolve in  $[\alpha,\beta]$  from  $\varepsilon$  to  $\eta$ .