Statistical Shape Analysis using Topological Data Analysis

Part I: Introduction to Topological Data Analysis

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Idea of Topological Data Analysis (TDA)

Data have shape,

shape has meaning,

meaning brings value

Idea of Topological Data Analysis (TDA)

Data have shape,

$\rightarrow$ Modeling

shape has meaning,

$\rightarrow$ Inference/Learning

meaning brings value

$\rightarrow$ Collaboration

Contents of Today's Lecture

1. Part I: Introduction to TDA
2. Part II: Representations and Modeling
3. Part III: Applications
   - Fingerprint Data
   - Time Series Data
   - Material and Tumor Images

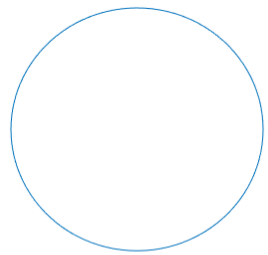
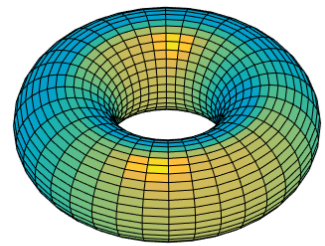
Outline

Topology and Topological Data Analysis (TDA)

- Topology and topological invariance
- TDA analyzes the "shape" of data
- Uses techniques from topology; homology and persistent homology
- Homology analyzes topological spaces

Betti Numbers

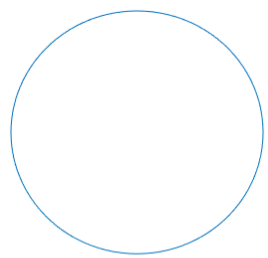
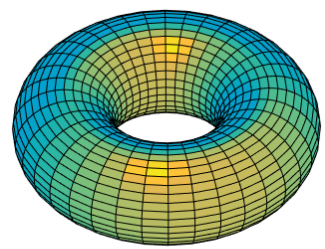
Betti number β_k, counts the number of k-dimensional holes

		
Dim. 0 (Conn. comp.)	1	1
Dim. 1 (Loops)	1	2
Dim. 2 (Voids)	0	1

Euler Characteristic

Euler characteristic χ is defined

$$\begin{aligned}\chi &= \sum_{i=0}^{d}(-1)^i\beta_i \\ &= \text{num. of vertices} - \text{num. of edges} + \text{num. of faces}\end{aligned}$$

		
Dim. 0 (Conn. comp.)	1	1
Dim. 1 (Loops)	1	2
Dim. 2 (Voids)	0	1
Euler characteristic	$1-1+0=0$	$1-2+1=0$

Toy Example

- How many of holes are there? What would be the Euler characteristics?

	A	B	U	⊠	◎
Dim. 0 (Conn. comp.)					
Dim. 1 (Loops)					
Dim. 2 (Voids)					
Euler characteristic					

Shape of Data?

- Shape $\longrightarrow$ Data $\longrightarrow$ Complex

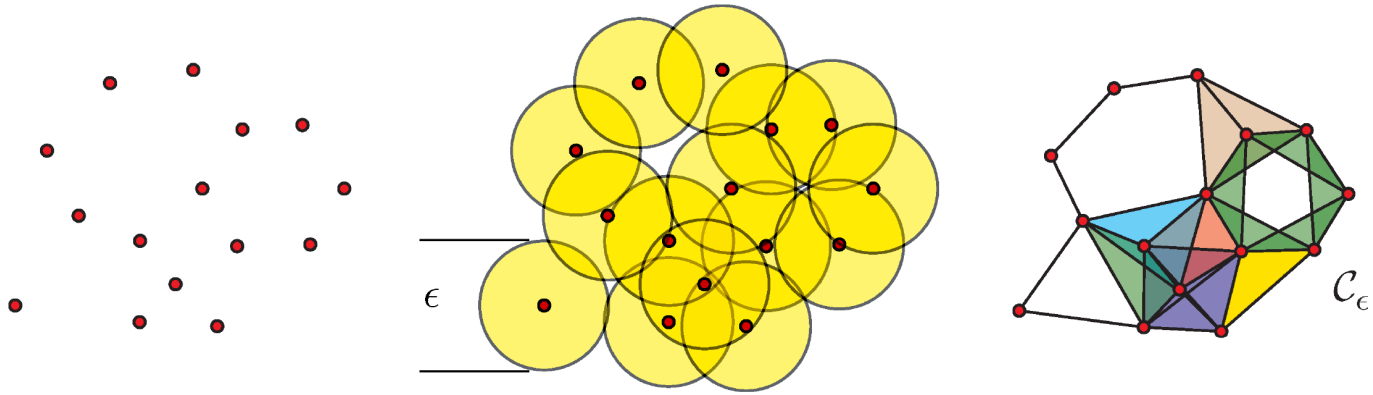


Figure: Example of Čech complex. Figure from Ghrist (2008)

- Čech complex is defined by the intersection between those balls
- If there are m balls of diameter ϵ that share the intersection region, then the corresponding m data points form an $m-1$-simplex (simplex will be covered within a few slides)
- Čech complex at the filtration value ϵ is a union of those simplexes and is represented as $\mathcal{C}_\epsilon$

Nerve Theorem

- Is it okay to analyze the complex instead of the topological space?
- A simplicial complex from an open covering of a topological space preserves topological properties

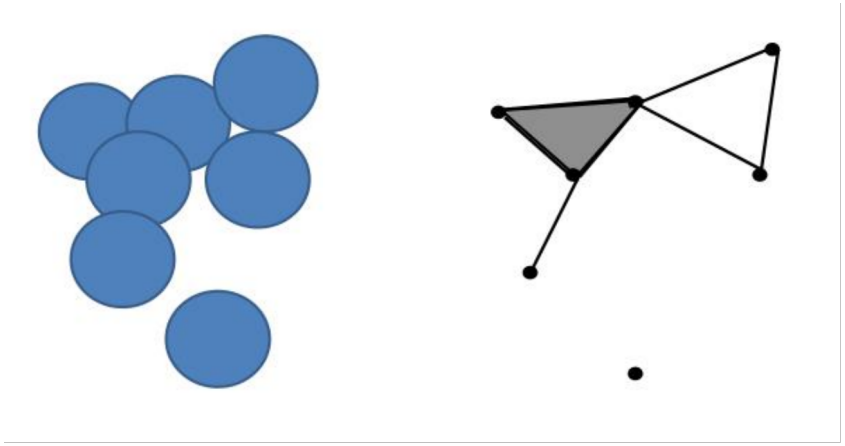


Figure: Figure from `https://www.slideserve.com/mandy/sampling-conditions-and-topological-guarantees-for-shape-recons`

- Čech complex satisfies the nerve theorem: if we sample enough data from a topological space $\mathcal{X}$ and construct the Čech complex, then the complex reflects the topology of $\mathcal{X}$

Vietoris-Rips Complex

- Drawback of the Čech complex is that it is computationally expensive
- Vietoris-Rips (Rips) complex is defined by pairwise distances
- For given ϵ, m data points whose pairwise distances are smaller than ϵ form a $(m-1)$-simplex
- Rips complex of X given ϵ is a union of the simplexes and expressed $\mathcal{R}_\epsilon$

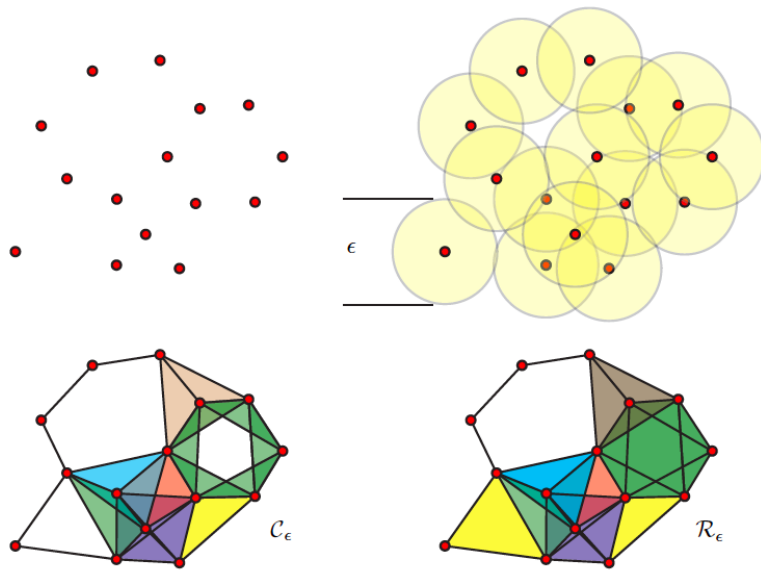


Figure: Figure from Ghrist (2008)

Čech vs. Rips Complexes

- Rips complex does not satisfy the nerve theorem
- Rips complex still carries topological properties of point cloud data. For all $\epsilon > 0$, the following relationships hold:

$$\mathcal{C}(X, \epsilon) \subset \mathcal{R}(X, \epsilon) \subset \mathcal{C}(X, 2\epsilon).$$

- Rips complex contains topological information of the Čech complexes somewhere between $\mathcal{C}(X, \epsilon)$ and $\mathcal{C}(X, 2\epsilon)$ and used as a good alternative to the Čech

Simplices and Simplicial Complexes

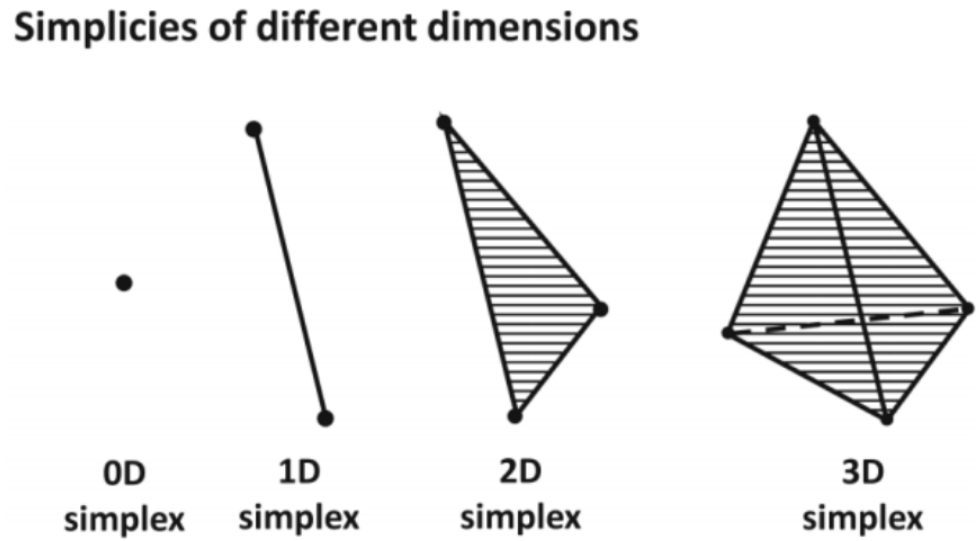


Figure: Figure from Wang et al. (2019)

- Simplices are building blocks of a simplicial complex: vertices (0-simplex), edges (1-simplex), triangles (2-simplex), tetrahedra (3-simplex), and higher-dimensional simplices

Simplices and Simplicial Complexes (2)

- In the construction of the simplicial complex, simplices are glued together in a way that two adjacent simplices share their faces

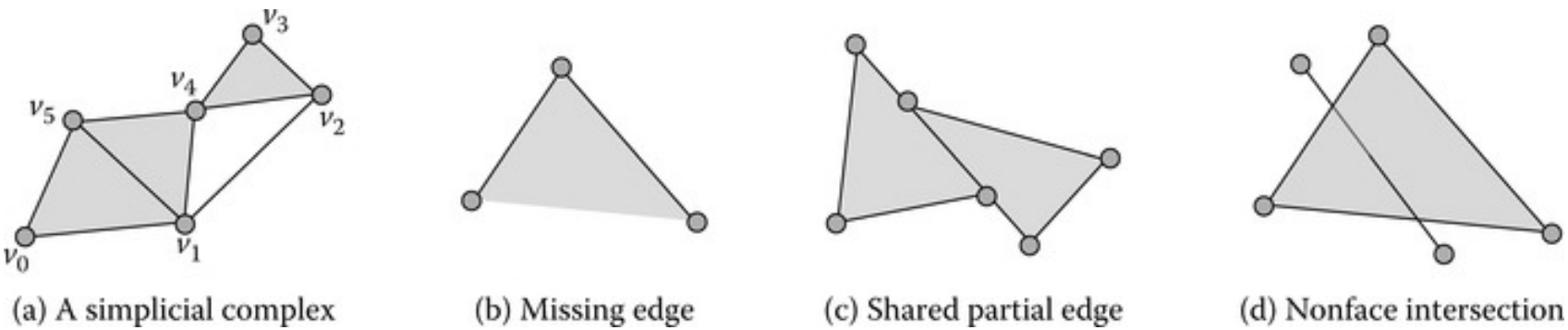


Figure: Figure from Atallah and Blanton (2009)

Homology

- Homology enables to analyze a topological space $\mathcal{X}$ by examining its k-dimensional holes

$$H_k = \ker(\partial_k)/\mathrm{im}(\partial_{k+1}) = \mathsf{Z}_k/\mathsf{B}_k$$

- The rank of $H_k(\mathcal{X})$ is the Betti number β_k
- Computation of homology is done by simple linear algebra

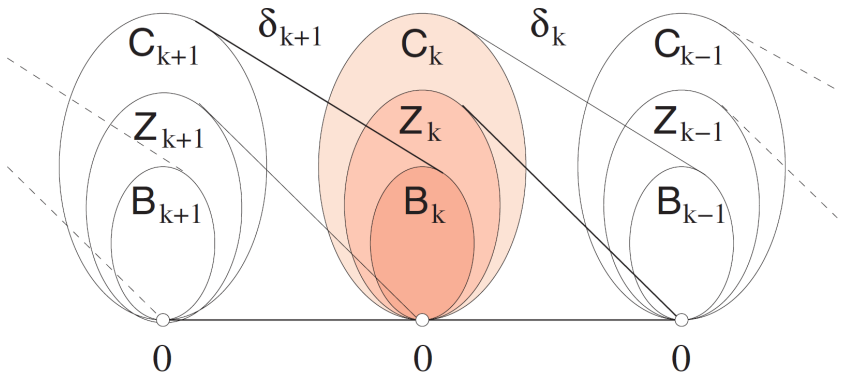


Figure: Chain, cycle, and boundary groups. Figure from Zomorodian and Carlsson (2005)

Is Homology Enough?

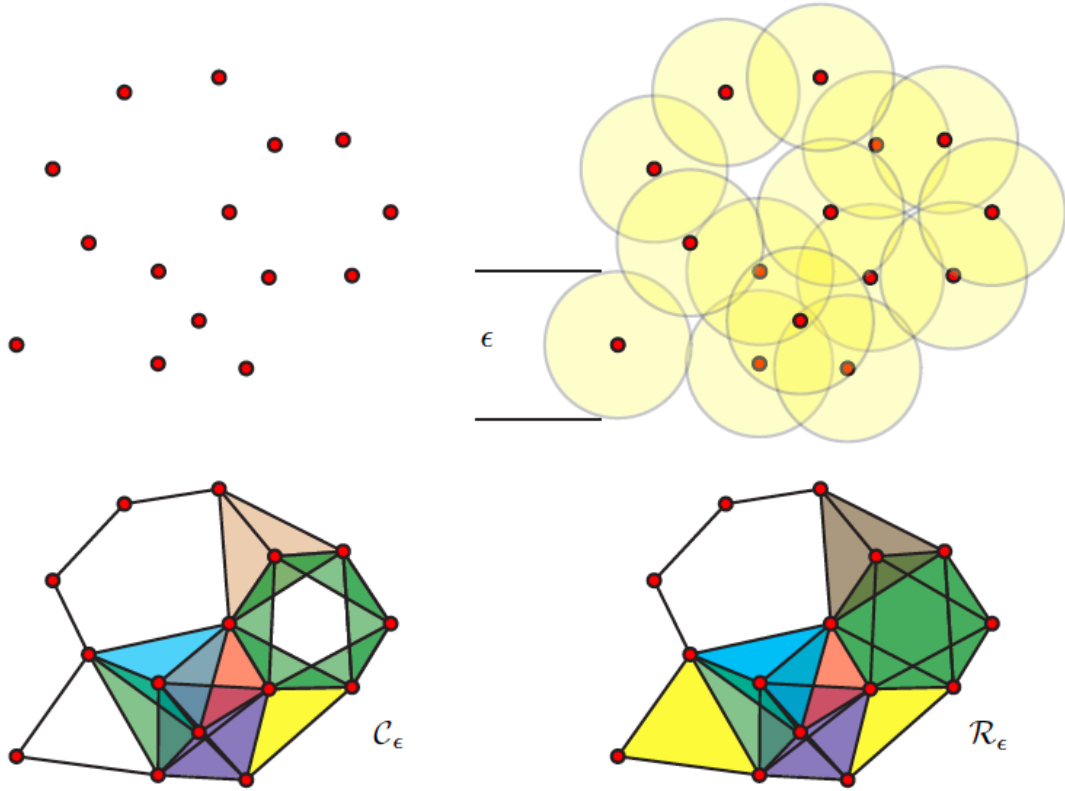


Figure: Figure from Ghrist (2008)

- Question: which ϵ do we need to use to reveal the underlying shape?

Persistent Homology

- Persistent homology keeps track of the homology of a sequence of topological spaces
- Let $\emptyset = \mathcal{X}_0 \subseteq \mathcal{X}_1 \subseteq \cdots \subseteq \mathcal{X}_n = \mathcal{X}$ be a non-decreasing sequence of topological spaces
- The inclusion of $\mathcal{X}_i$ in $\mathcal{X}_j$ for $0 \leq i \leq j \leq n$ induces a homomorphism between the homology groups, $\iota_k(i,j) : H_k(\mathcal{X}_i) \to H_k(\mathcal{X}_j)$

$$0 = H(\mathcal{X}_0) \to H(\mathcal{X}_1) \to \cdots \to H(\mathcal{X}_n) = H(\mathcal{X})$$

- Some topological features in a topological space $\mathcal{X}_s$ may born or die along the sequence. The image of the homomorphism include such information
- k-dimensional (i,j) persistent homology groups is the image of the homomorphism $\iota_k(i,j) : H_k(\mathcal{X}_i) \to H_k(\mathcal{X}_j)$
- The parameter that controls the sequential changes (ϵ) is called the filtration

Techniques from Topology: Persistent Homology (2)

- Tracks evolution of homology as ϵ (filtration) changes
- Persistence homology results are given as an interval of [Birth, Death]
- In general, true topological properties persist for a wide range of filtrations

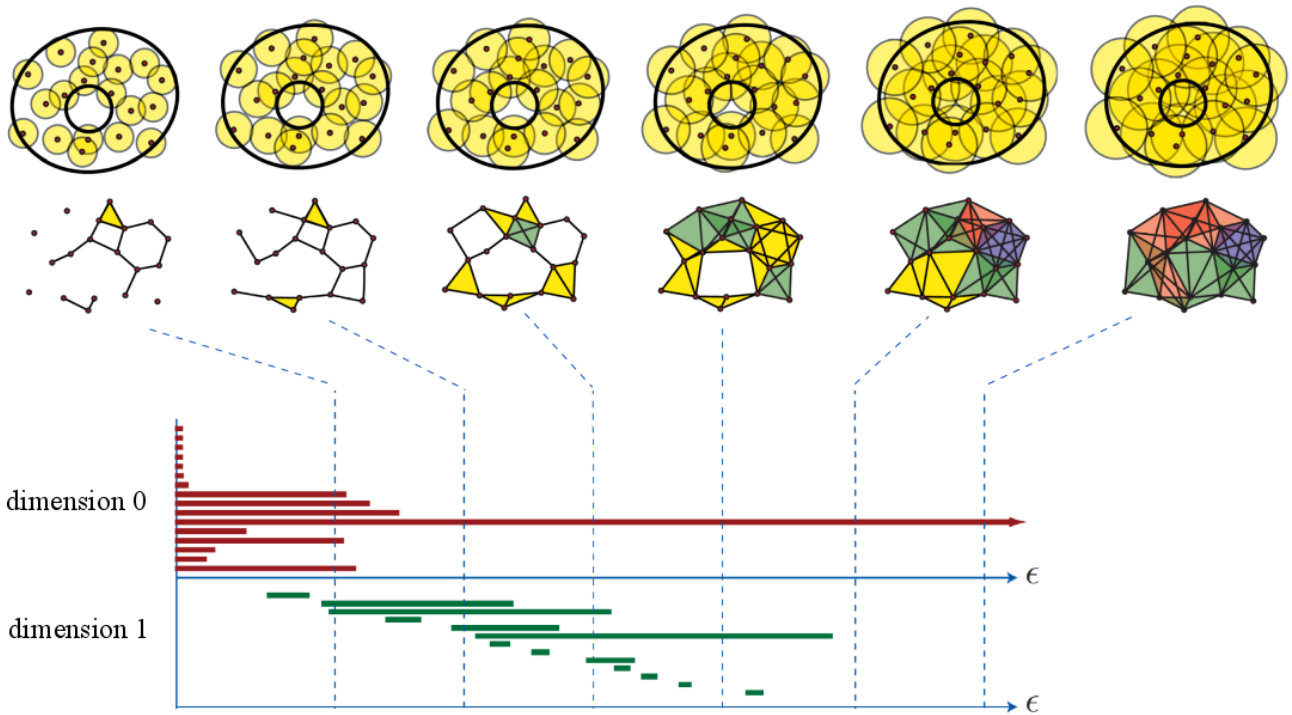
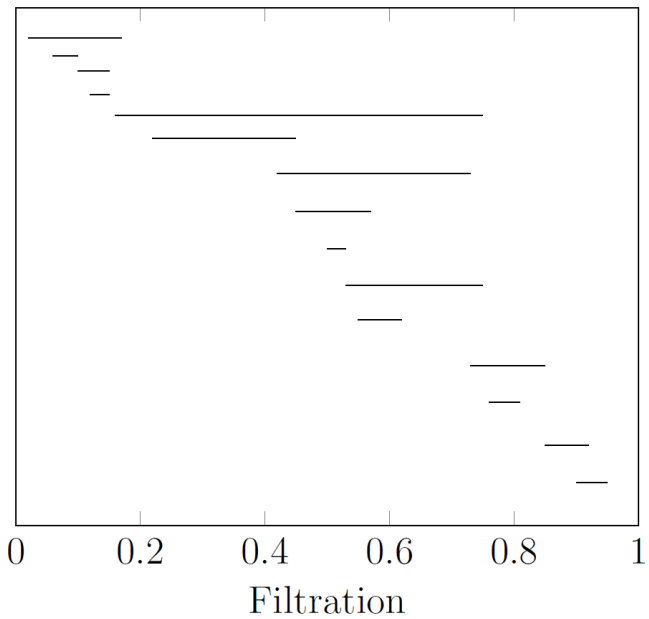


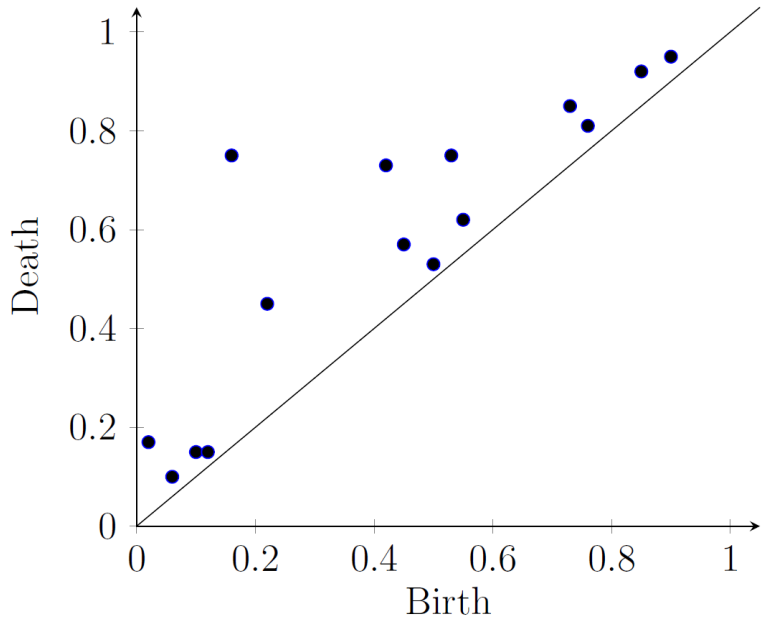
Figure: Figure from Ghrist (2008)

Summary of Persistent Homology Result

- Barcode plot: as a straight line of Birth———Death
- Persistence diagram: as a point of (Birth, Death)



(a) Barcode Plot



(b) Persistence Diagram

Popular Packages for Persistent Homology

- Python
  - Dionysus 2
  - GUDHI
  - scikit-tda
  - ripser
  - giotto-tda
- R
  - TDA

Pipeline

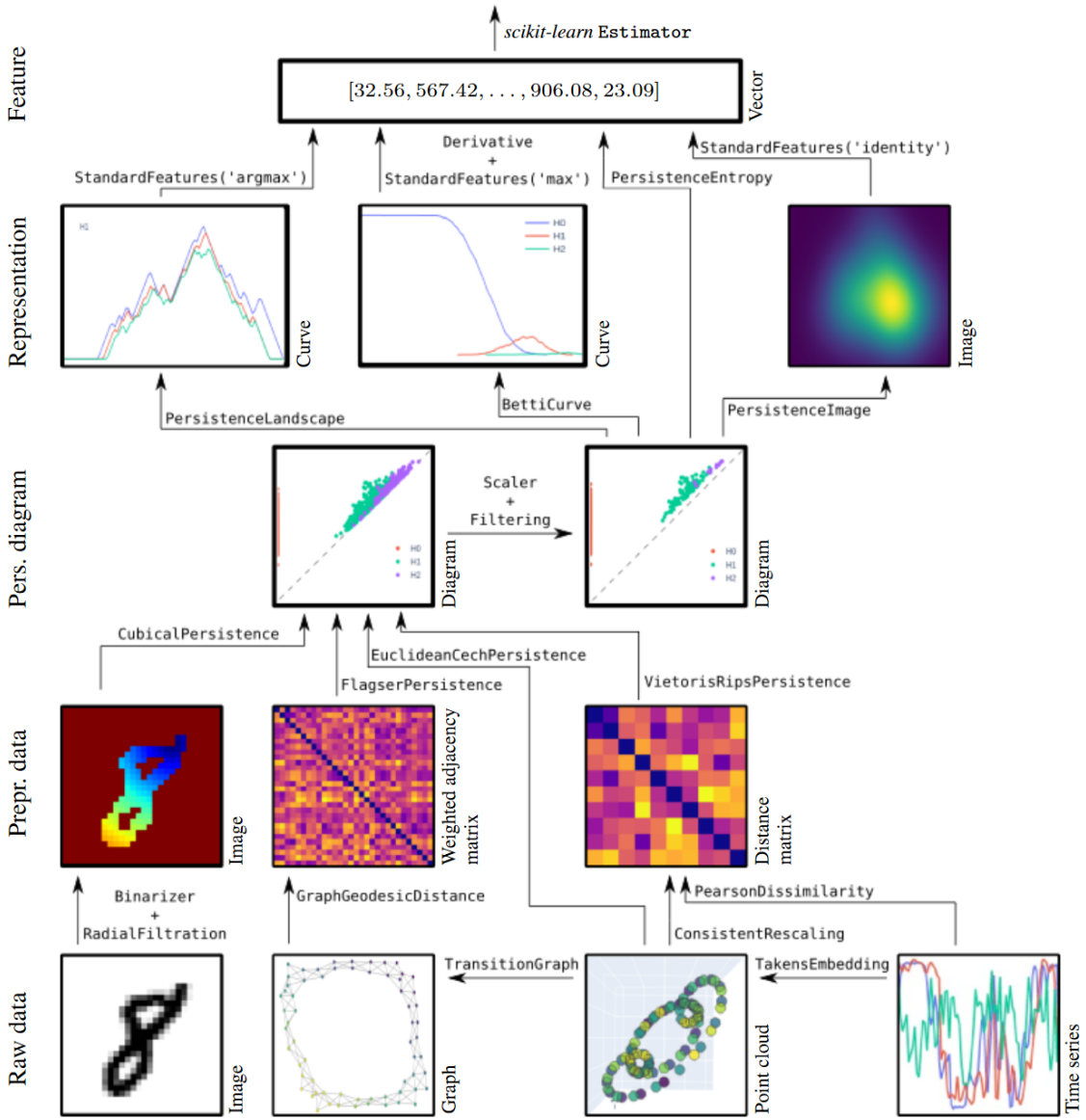


Figure 1: Non-exhaustive depiction of *giotto-tda* capabilities. Arrows represent operations available as `transformers` and paths potential `pipelines`.

Outline

Examples of Point Cloud Data

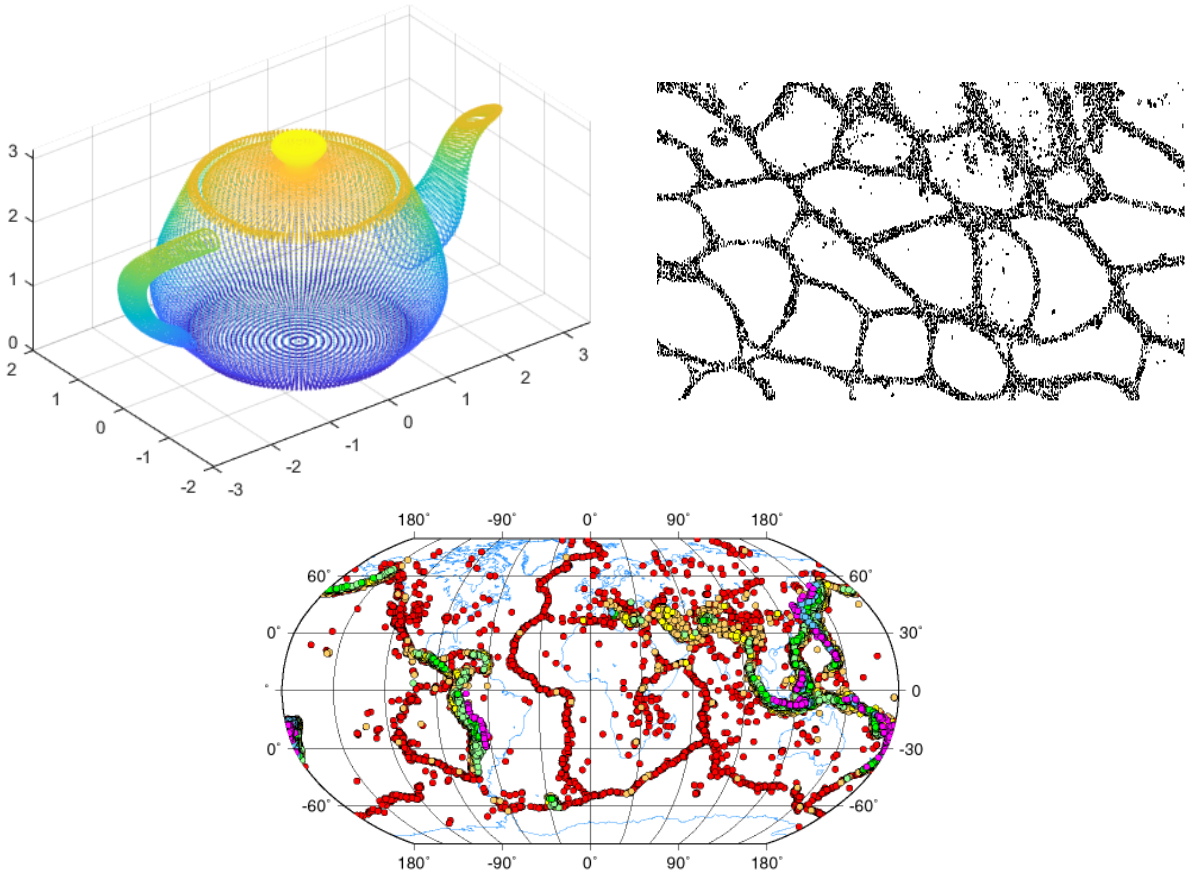


Figure: Figures from MATLAB (2016) (top-left), Mula et al. (2013) (top-right), and Pidwirny (2006) (bottom)

Limitations of Čech complex on Point Cloud Data

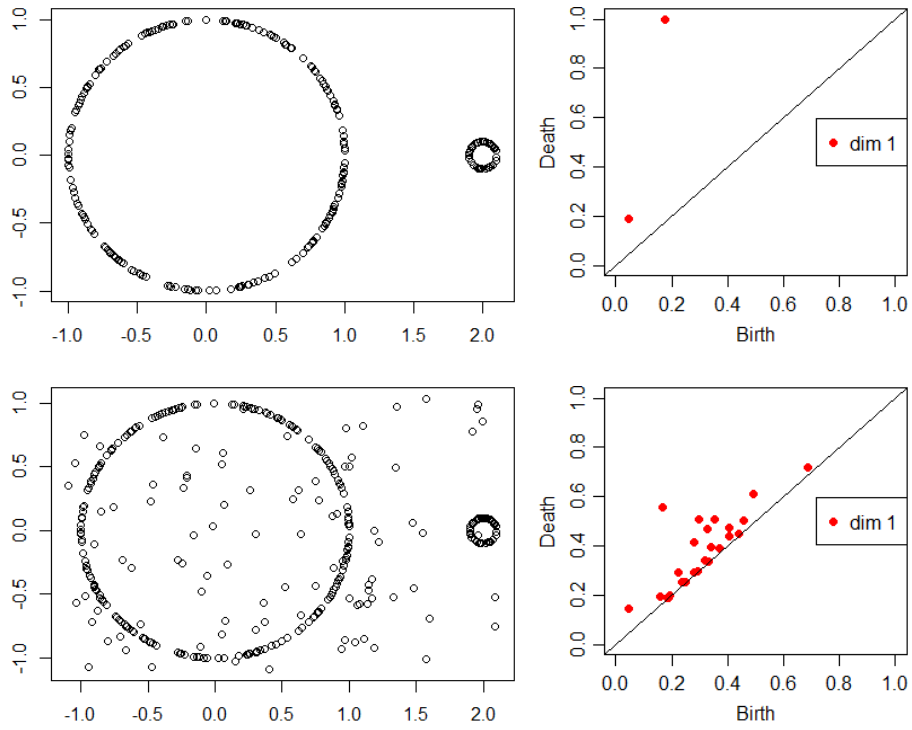
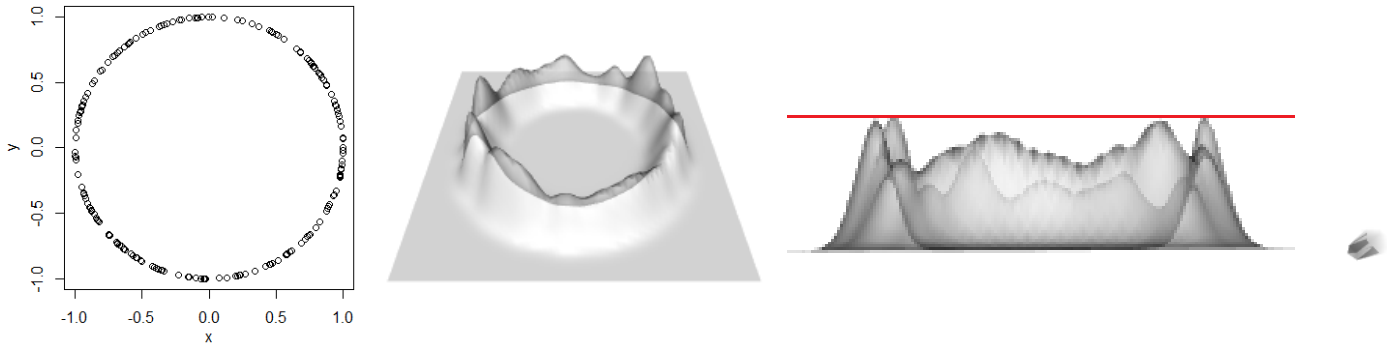


Figure: Data without noise (top row) and with noise (bottom row)

- Persistence is related to the size of the feature
- Small-sized features do not persist for a long range of filtrations
- Sensitive to noise

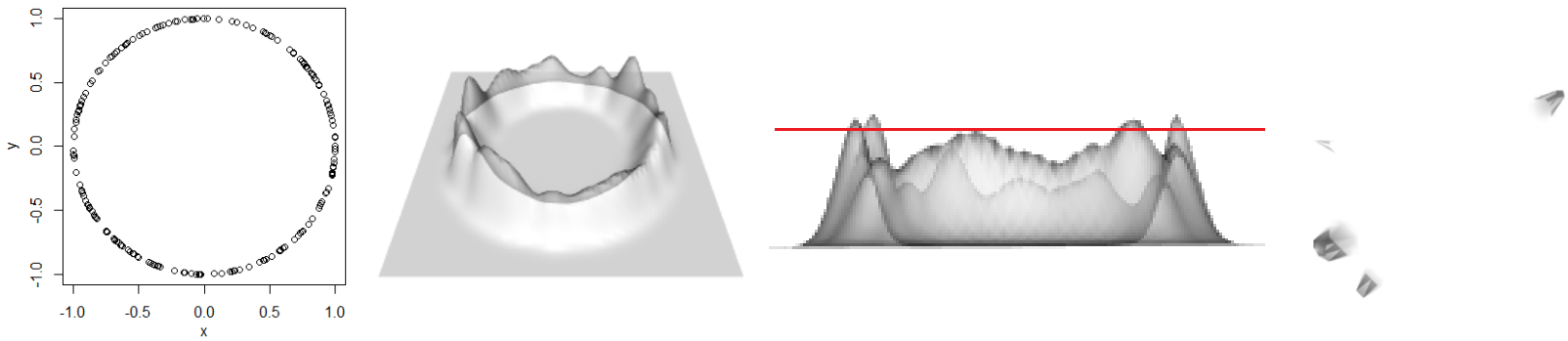
Robust Estimation using Smoothing Function



(a) Scatterplot (b) Manifold

- Transform a discrete point cloud into a continuous manifold via a smoothing function
- Set a filtration as a level of manifold
- Optimal smoothing parameter selection
- Lose size information

Robust Estimation using Smoothing Function



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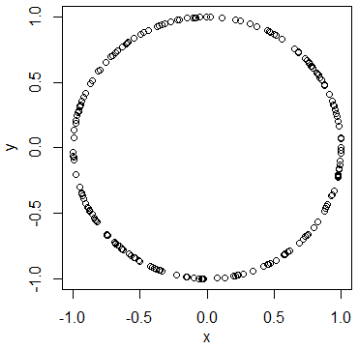

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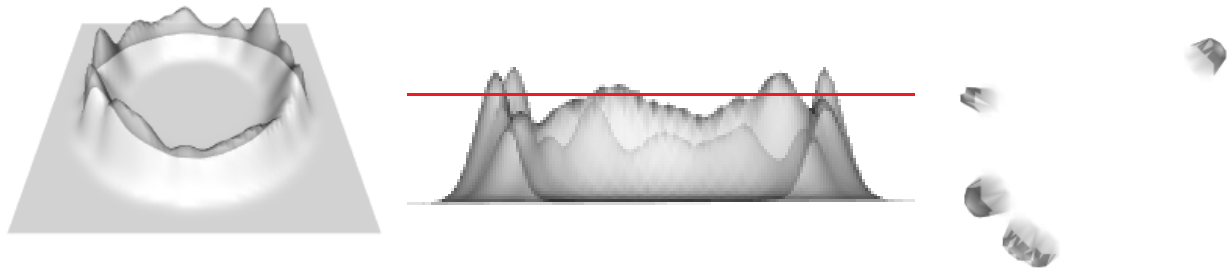

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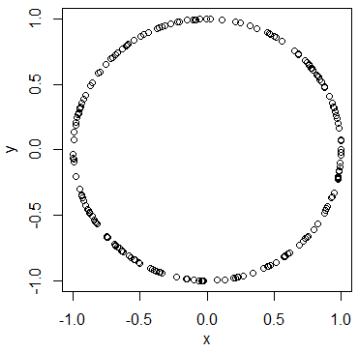

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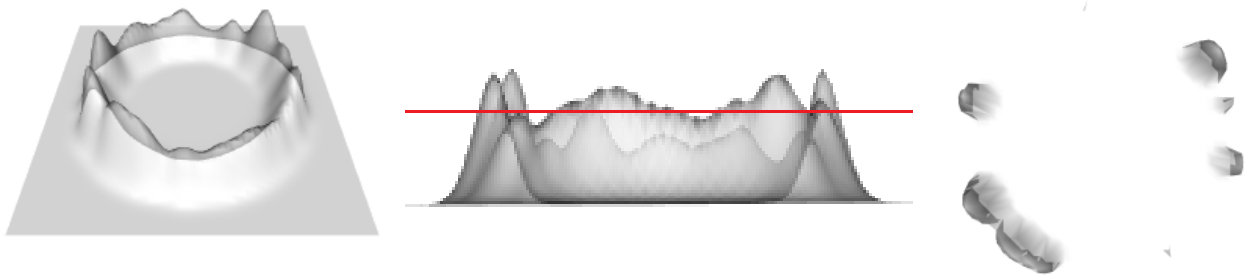

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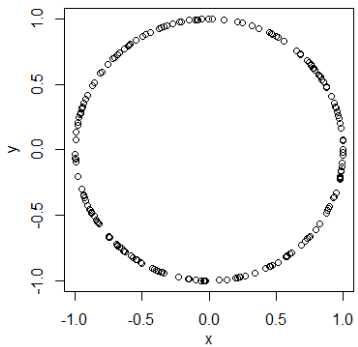

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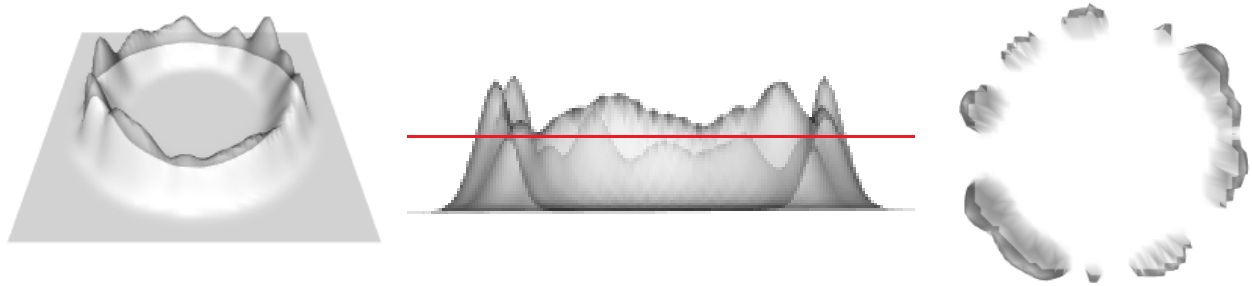

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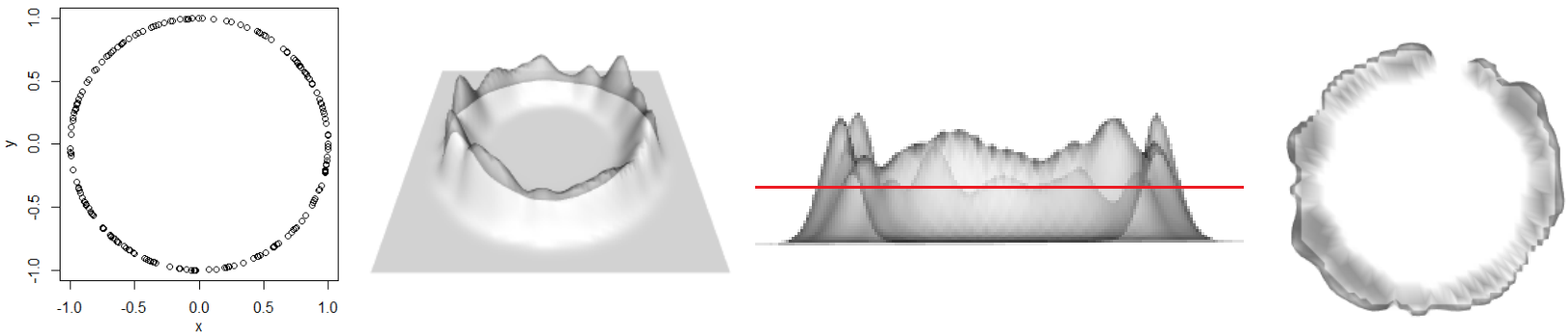

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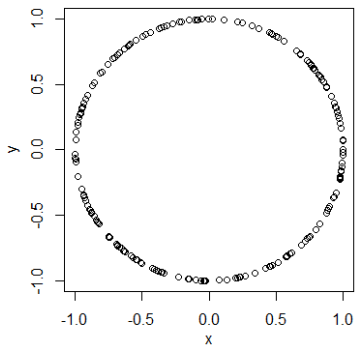

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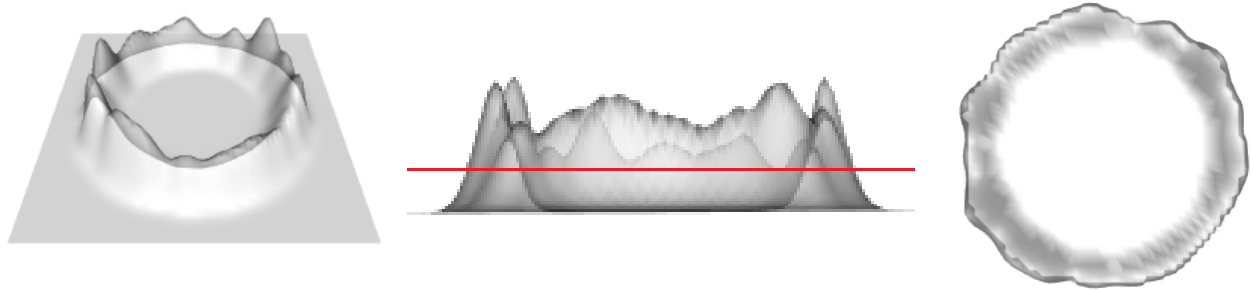

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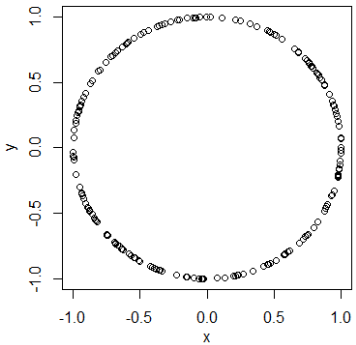

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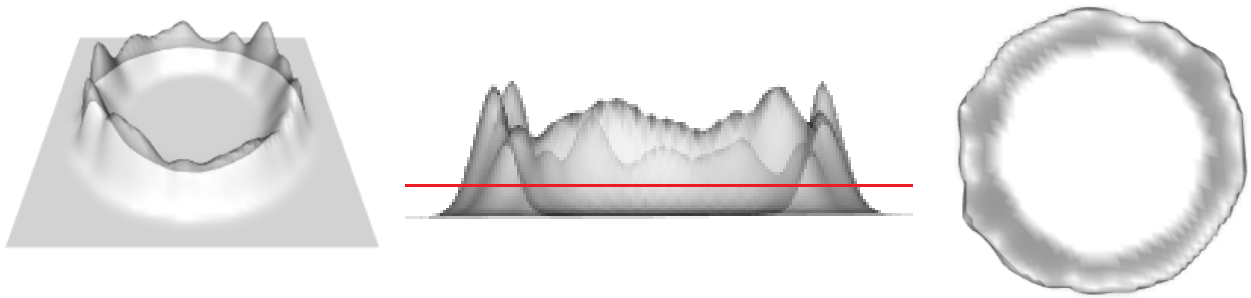

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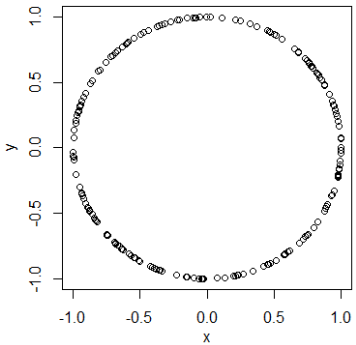

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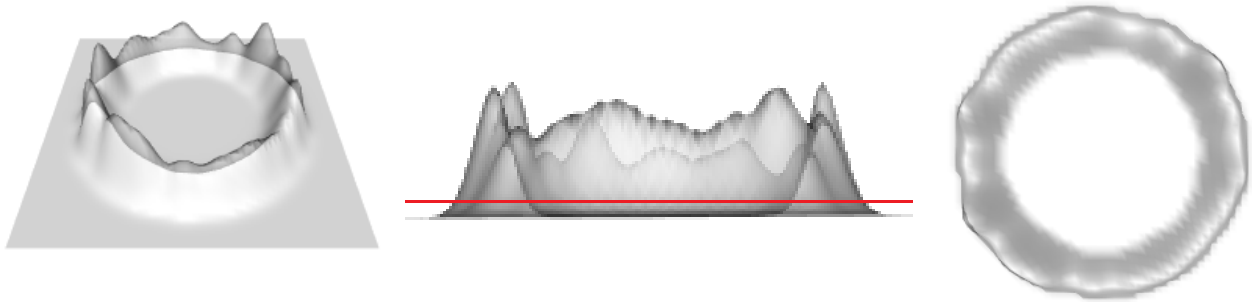

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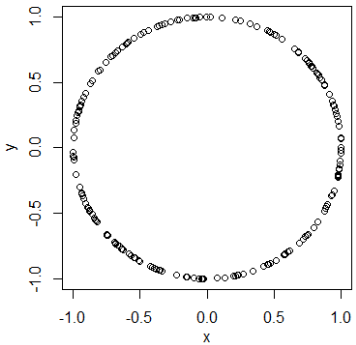

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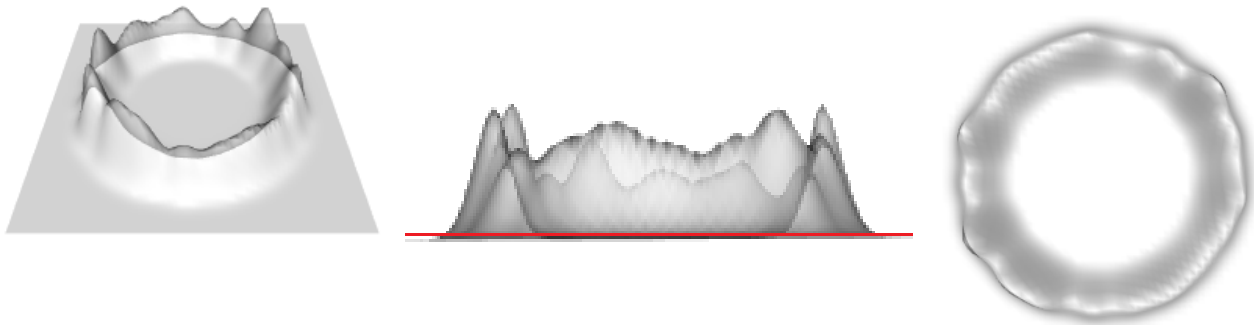

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Various Smoothing Functions

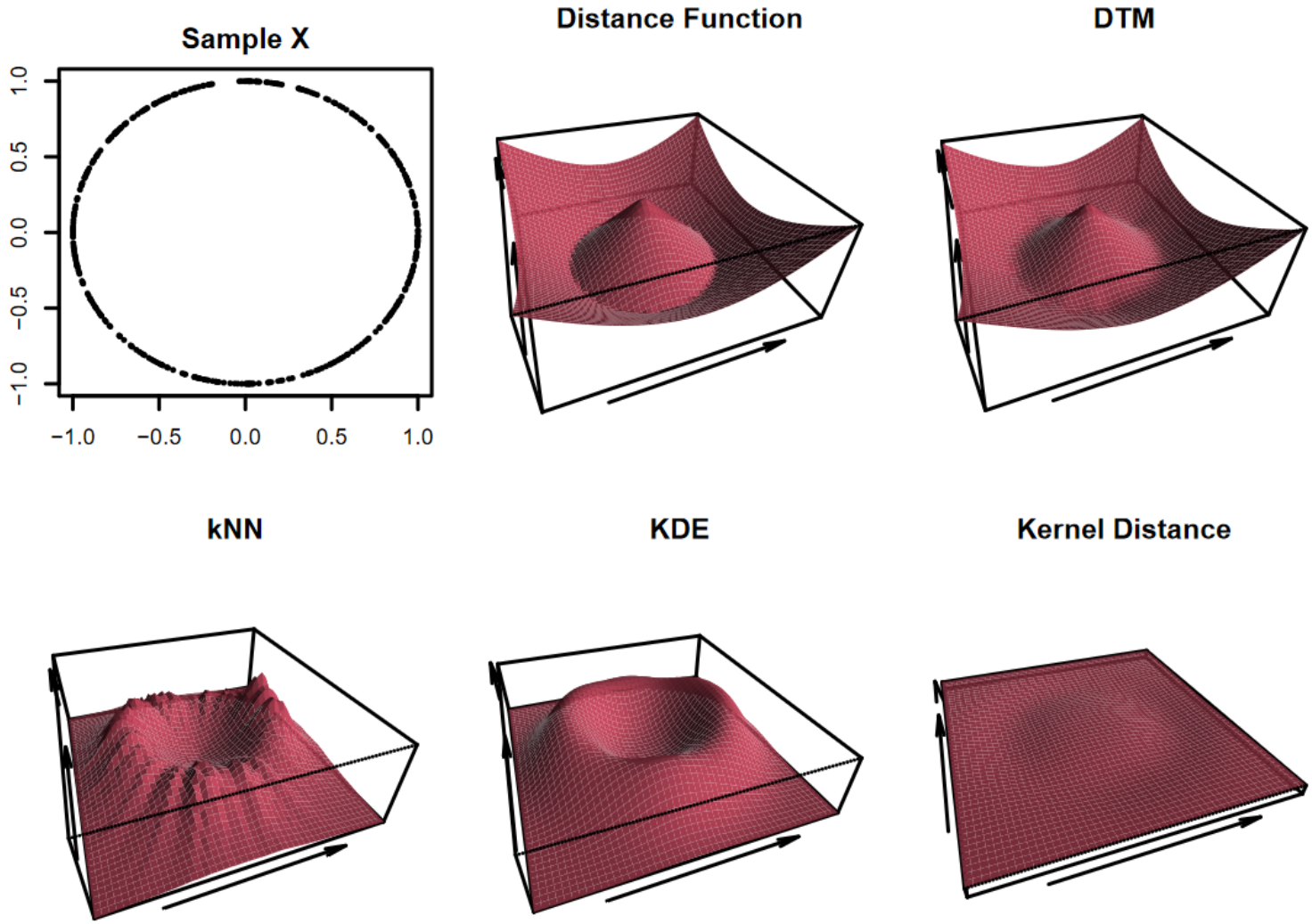


Figure: Figure from Fasy et al. (2014)

Outline

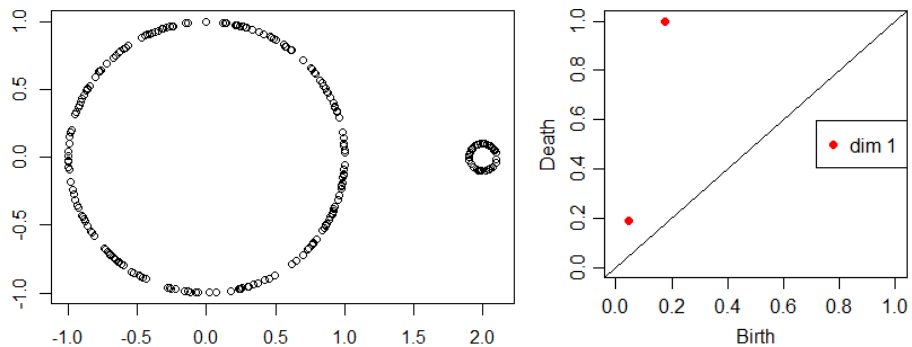
Reliability of Persistent Homology Results

Can persistence diagrams be used to measure geometric or topological differences between spaces?

- Let D_X and D_Y be the persistence diagrams of metric space X and Y
- For given metrics d_1 on persistence diagrams and d_2 on the metric spaces, the stability of persistence diagrams holds when

$$d_1(D_X, D_Y) \leq d_2(X, Y).$$

- If the persistence diagram is stable, then small changes in metric spaces (measured as $d_2(X, Y)$) induce small changes in persistence diagrams (measured as $d_1(D_X, D_Y)$)



Persistence Diagram Distances

- The persistence diagram distances $d_1(D_X, D_Y)$ measure the dissimilarity between diagrams
- The space where persistence diagrams live is unique
  - The persistence diagram distance needs to compare diagrams that include different numbers of points
  - Number of barcodes created varies from dataset to dataset
  - Only half of the 2-dimensional space will be used
- Also, the distances need to satisfy an important property called stability under perturbations.

Bottleneck Distance

- Let $x_i = (a_i, b_i)$, $y_j = (a_j, b_j)$, and $d(x_i, y_j) = ||x_i - y_j||_\infty = \max(|b_i - b_j|, |a_i - a_j|)$
- Bottleneck distance between persistence diagrams D_X and D_Y is defined as

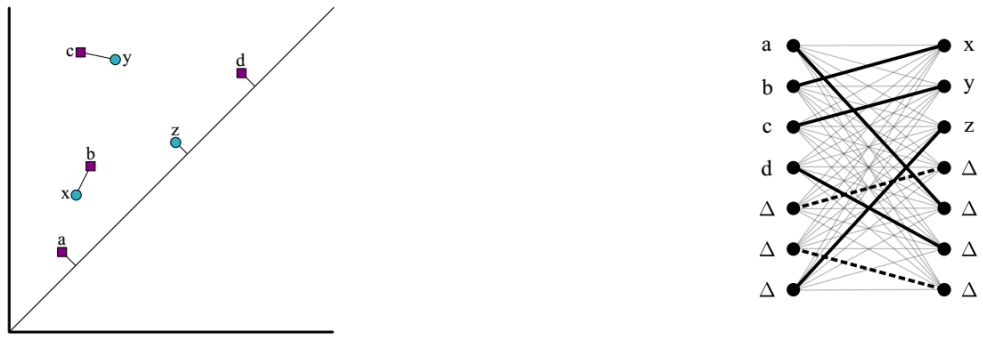
$$W_\infty(D_X, D_Y) = \inf_\gamma \sup_{x \in D_X} ||x - \gamma(x)||_\infty$$

  where γ is the bijections from D_X to D_Y
- Bottleneck distance between two persistence diagrams has an upper bound by L_∞-distance
- The stability of the bottleneck distance is shown in Cohen-Steiner et al. (2007) and Chazal et al. (2012)

Wasserstein Distance

p-Wasserstein distance between D_X and D_Y is given by

$$W_p(D_X, D_Y) = \left(\inf_{\gamma} \sum_{x \in D_X} ||x - \gamma(x)||_\infty^p \right)^{\frac{1}{p}}$$



(a) Two persistence diagrams (b) Weighted graph

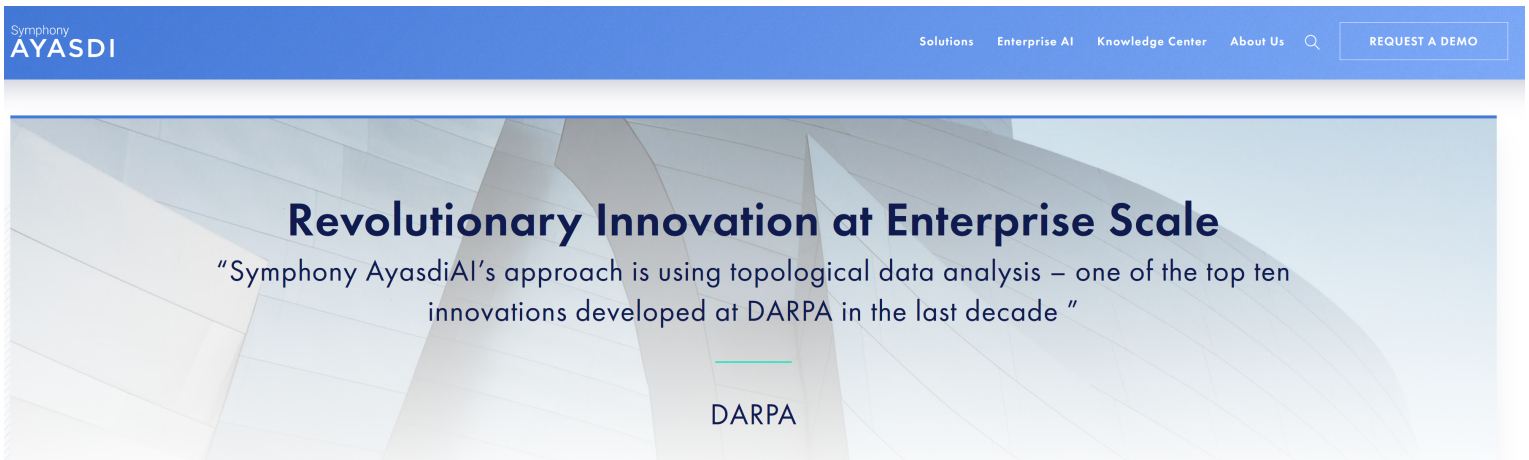
Figure: Two persistence diagrams of purple squares and green circles (left) and the weighted graph for Wasserstein distance computation (right). Figure from Munch et al. (2015).

- Wasserstein distance's stability conditions and results are shown in Cohen-Steiner et al. (2010)

Outline

Mapper Algorithm

- Proposed in Singh et al. (2007)
- The authors, Gunnar Carlsson, Gurjeet Singh, and Facundo Mémoli, who were professors of mathematics at Stanford founded the startup Symphony Ayasdi



Mapper Algorithm

- Data: point cloud data in a metric space
- Define an appropriate filter function
- Put data in overlapping bins
- Find cluster in each bin and construct a network

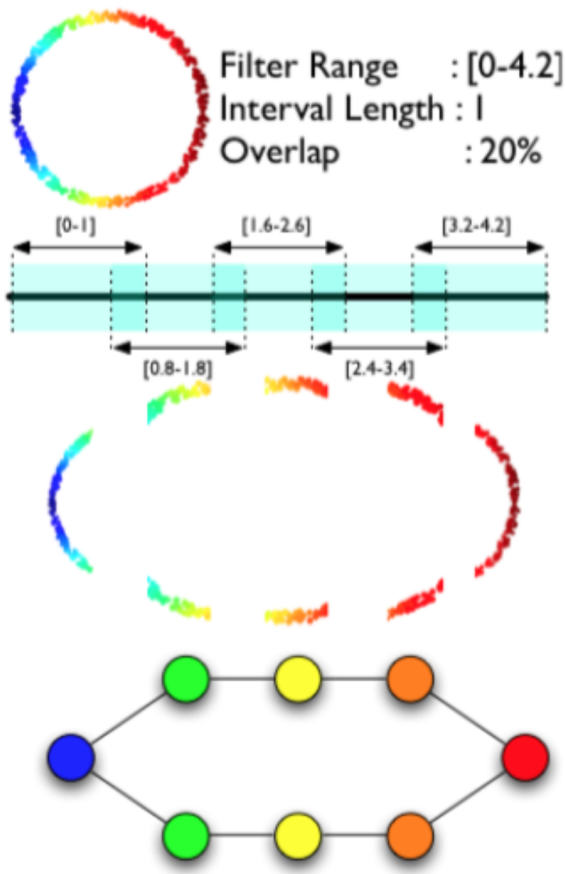


Figure: Figure from Singh et al. (2007)

Mapper Algorithm Toy Example

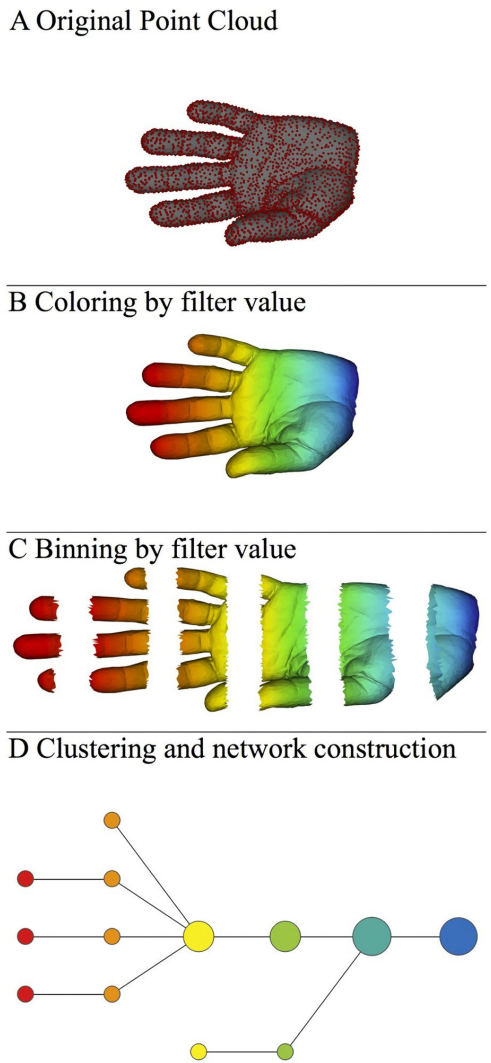


Figure: Figure from Lum et al. (2013)

Mapper Algorithm Toy Example

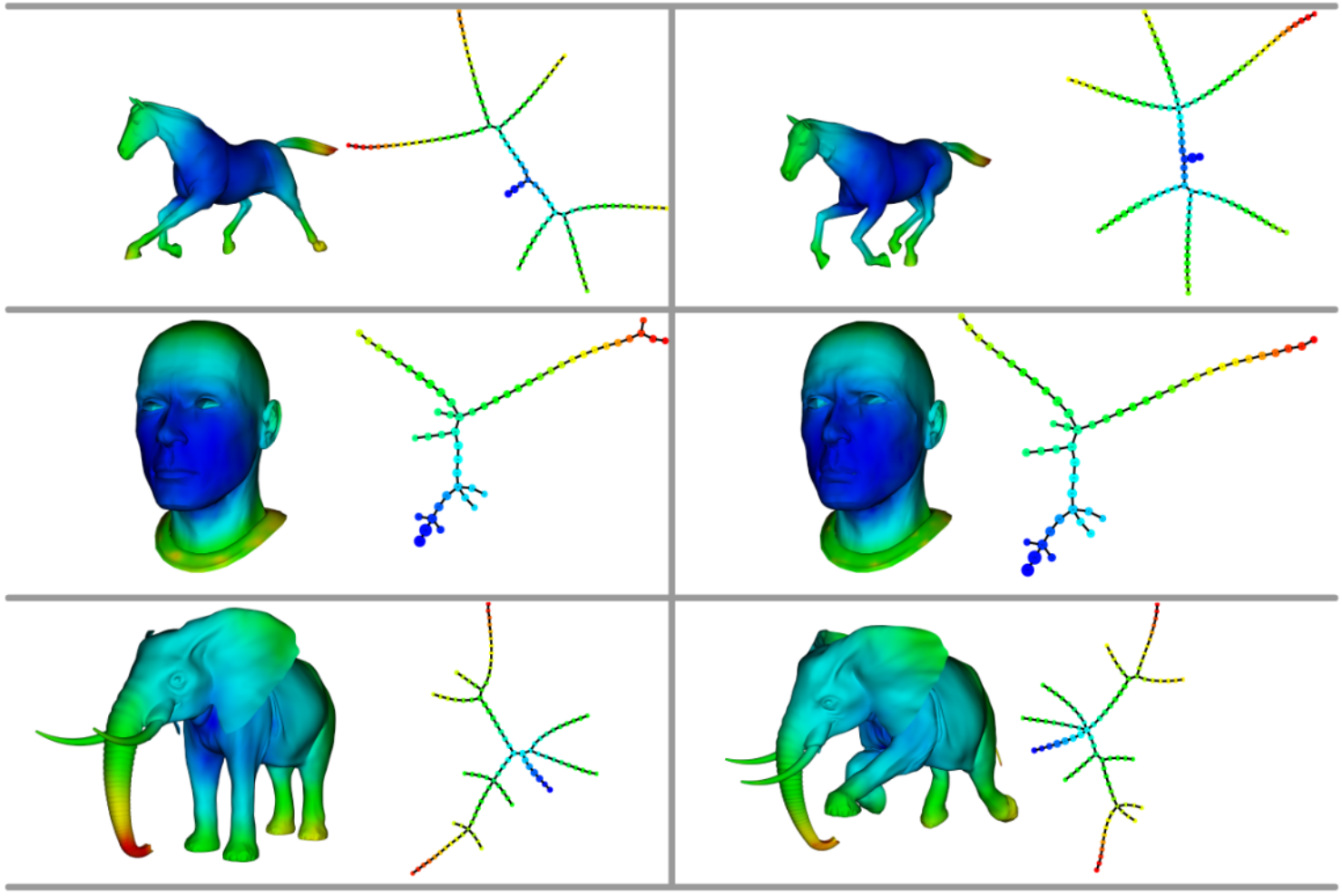


Figure 9: *Refer to Section 5.3 for details. Each row of this image shows two poses of the same shape along with the* `Mapper` *result which is computed as described in Section 5.3. For each* `Mapper` *computation, we used 15 intervals in the range of the filter with a 50% overlap.*

Figure: Figure from Singh et al. (2007)

Applications of Mapper

- Financial fraud detection
  - Ayasdi combined Mapper with machine learning algorithms
- Breast cancer subgroups stratification
- Types of NBA players

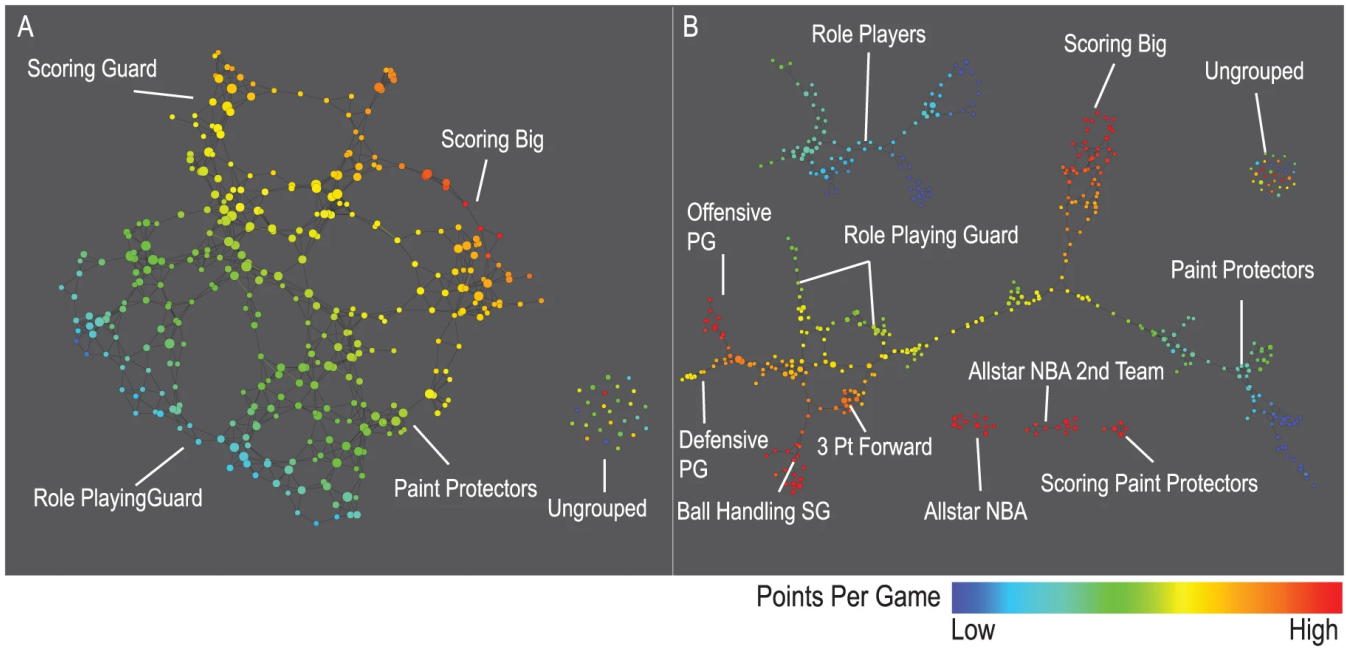


Figure: Figure from Lum et al. (2013)

Applications of Mapper

- Politics

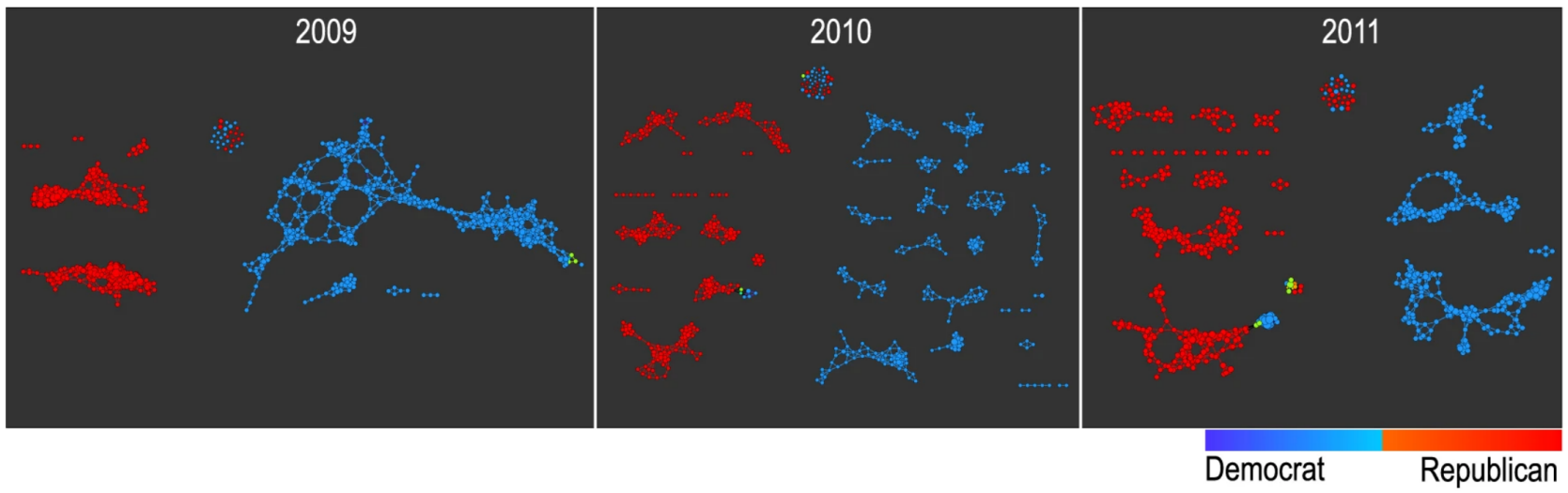


Figure: Figure from Lum et al. (2013)

Usage of Mapper

Packages

- Python
  - Mapper `http://danifold.net/mapper/index.html`
  - KeplerMapper
- R
  - TDAmapper (available via CRAN)
  - Mapper (`https://peekxc.github.io/Mapper/`)

Limitations

- Right filter function?
- How many intervals to use?
- How much buffer to allow?
- Clustering algorithm?

Outline

Motivating Example

- How to identify different shapes?

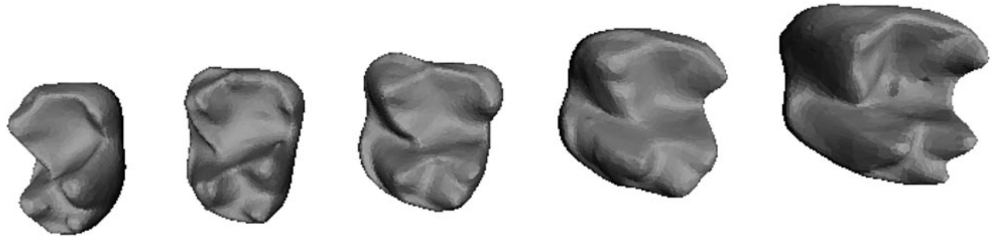


FIG. 1. Images of the meshes of five teeth. A common problem in morphology is to measure distances between these five teeth.

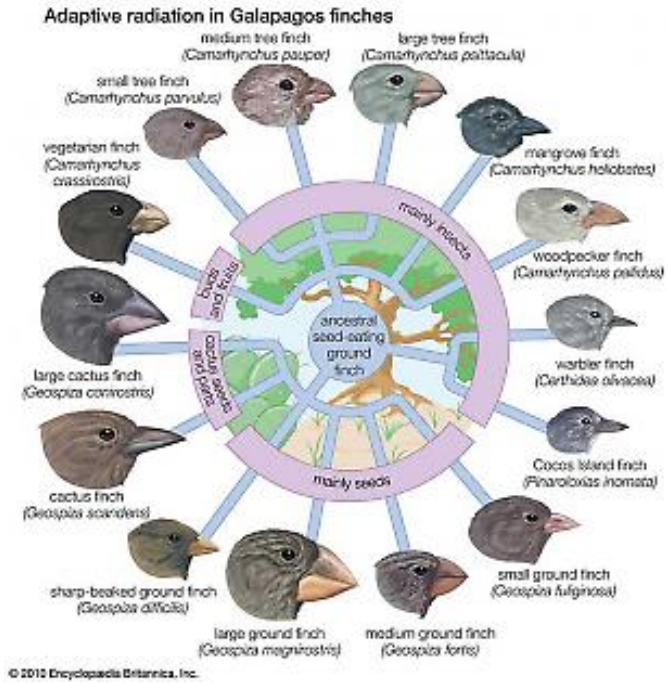


Figure: Figures from Turner et al. (2014) and `http://www.australasianscience.com.au/article/issue-novdec-2018/cultural-evolution-darwin%E2%80%99s-finches.html`

Classical Shape Analysis

- Shape analysis using landmark points

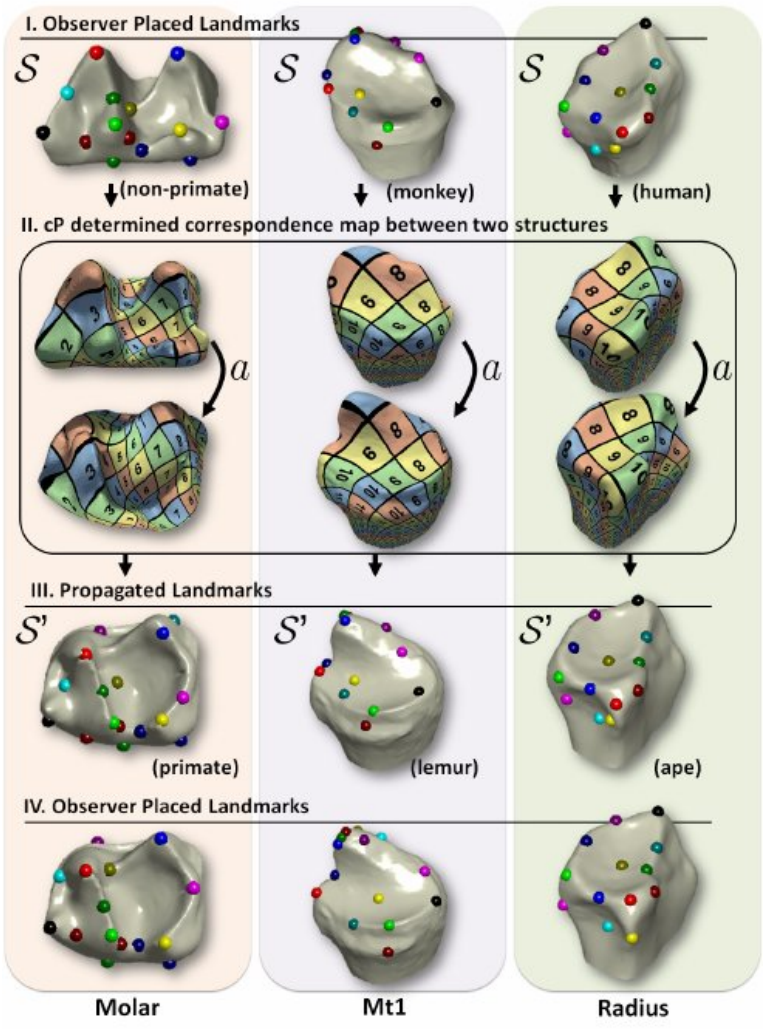


Figure: Figure from Boyer et al. (2011)

PHT and ECT

- Persistent homology transform (PHT) and Euler characteristic transform (ECT) are proposed in Turner et al. (2014)
- Swipe the object in multiple directions and compute persistent homology or Euler characteristics

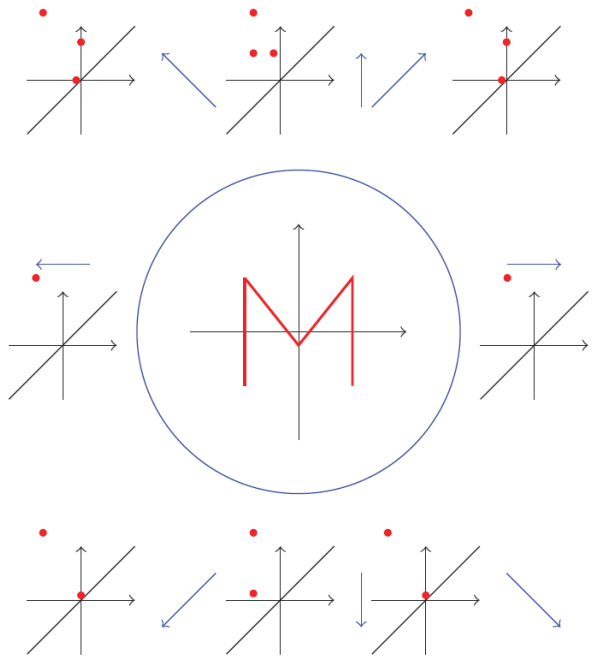


FIG. 5. The 0th dimensional persistence diagrams corresponding to filtrations of the letter M by height functions of eight different directions. The points with ∞ in the second coordinate are represented by a point with second coordinate just above the axes.

Figure: Figure from Turner et al. (2014)

PHT and ECT

- For PHT, persistence diagram is obtained from each direction
- For ECT, an Euler curve is obtaind from each direction
- Both PHT and ECT are injective for two and three dimensional shapes
  - For a given PHT and ECT statistics, there exists a unique corresponding shape
- PHT and ECT enable shape summary without landmarks

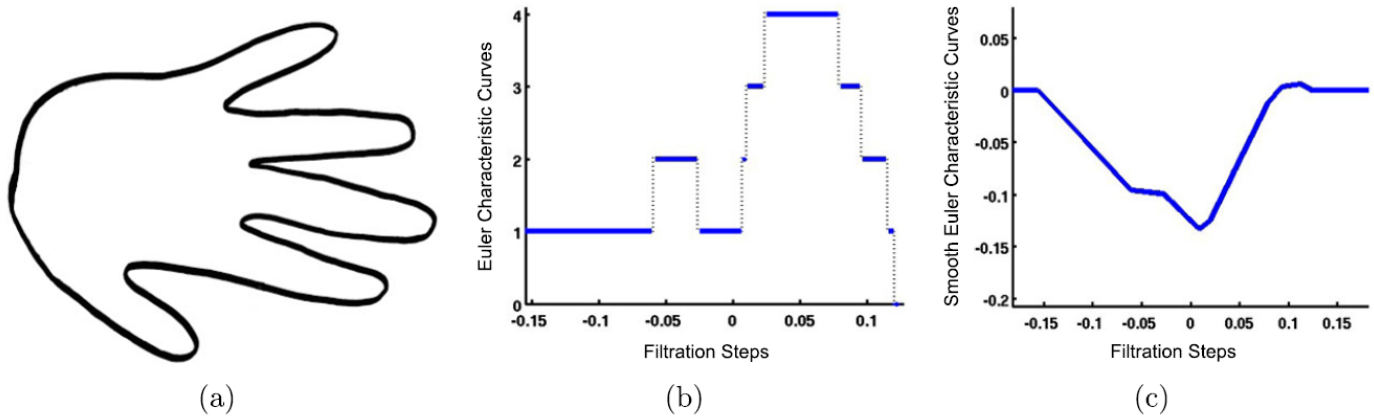
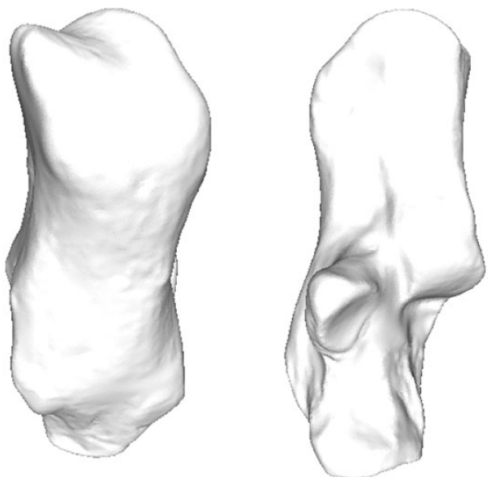


Figure: Figure from Turner et al. (2014)

Applications of PHT

- Would there be variations in heel bones according to genetic variation in species?
- 106 heel bones of extant and extinct primates



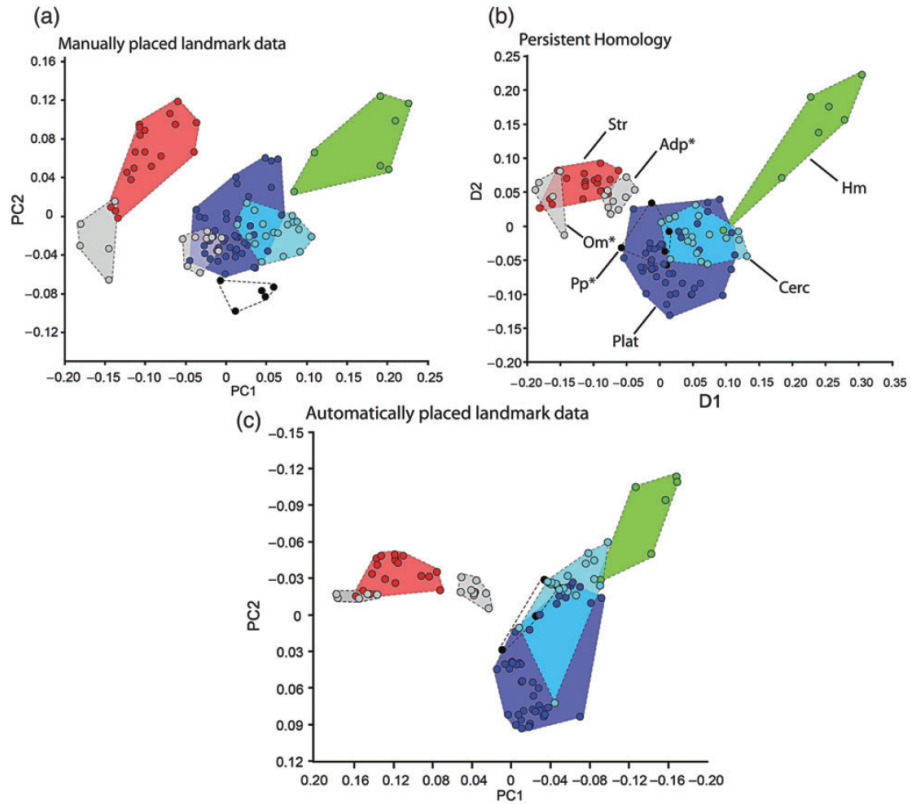


Figure: Figures from Turner et al. (2014)

Applications of (Smoothed) ECT

- Prediction of survival of brain tumor patients using tumor shapes in MRI images
- Smoothed ECT is a good predictor of survival outcomes

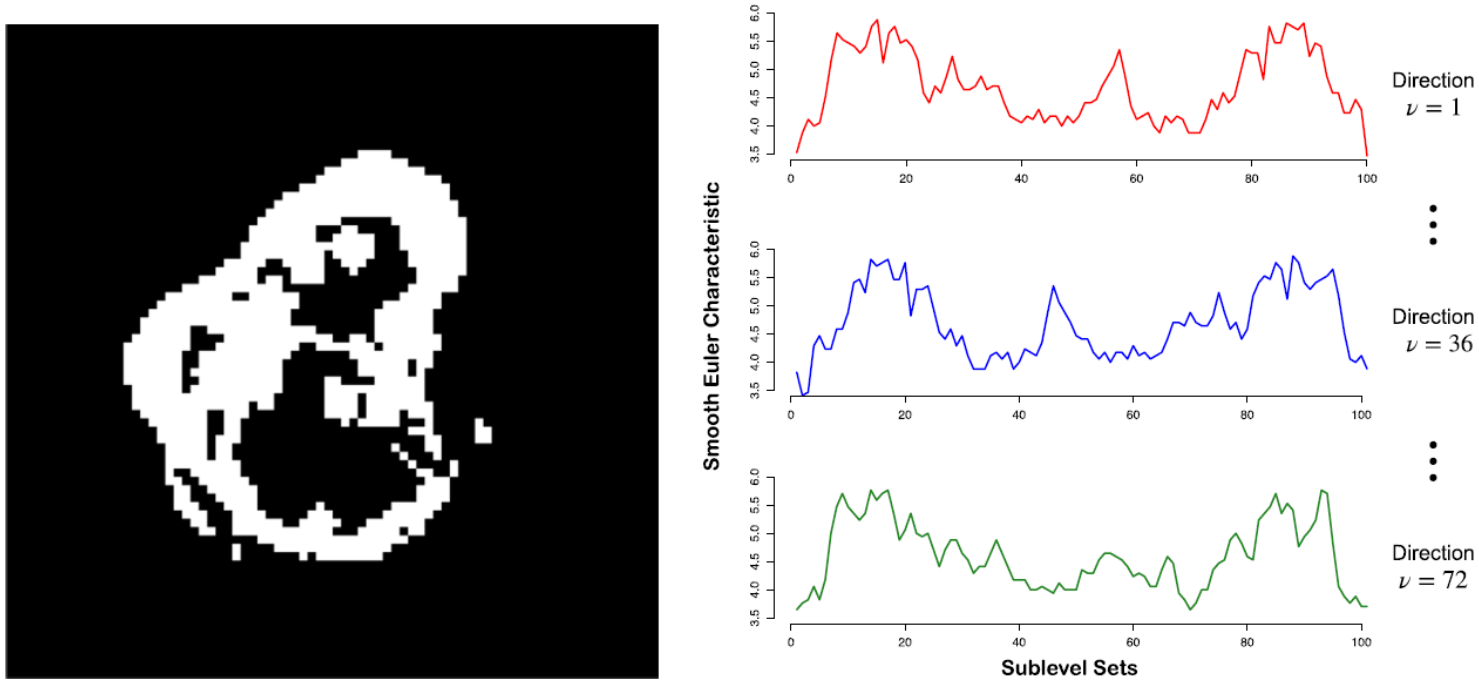


Figure: Figure from Crawford et al. (2020)

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