Reeb Graphs and Their Variants

Theory and Applications

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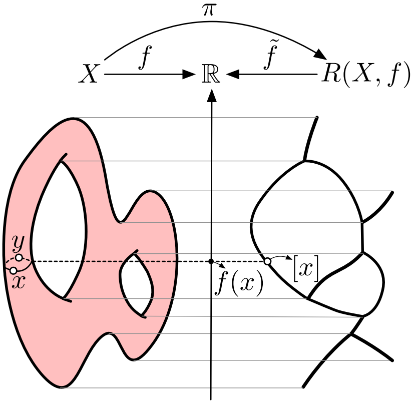
Overview

- Reeb graphs and their variants
- Applications
- Theoretical questions surrounding Reeb graphs and mapper graphs
- Measure theoretic Reeb graphs: robust topological data analysis

Reeb Graphs and Their Variants

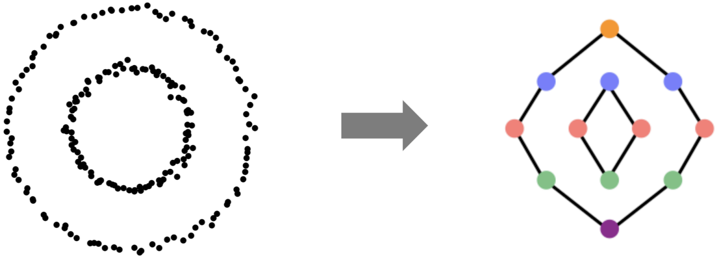
Reeb graph: a topological skeleton of data

- $(\mathbb{X}, f)$: a topological space with a continuous function $f : \mathbb{X} \to \mathbb{R}$.
- Reeb graph (Reeb [1946]): quotient space $R(\mathbb{X}, f) := \mathbb{X}/\!\sim_f$
- For $x, y \in \mathbb{X}$, $x \sim_f y$ iff x and y belong to the same connected component of the level set $f^{-1}(f(x))$.
- Reeb space: for $f : \mathbb{X} \to \mathbb{R}^d$, $R(\mathbb{X}, f) := \mathbb{X}/\!\sim_f$.

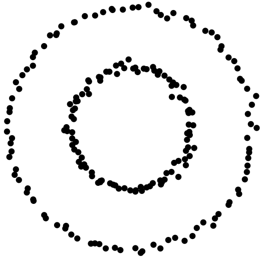


Mapper graph: a discrete approximation of a Reeb graph

- Singh et al. [2007]: Visualize the skeleton of (high-dimensional) point cloud data
- Main idea: turn point cloud data into a graph capturing both clusters and cluster relations.
- Parameters: number of cover elements of the range of the function, amount of overlaps, parameters associated with the clustering, etc.

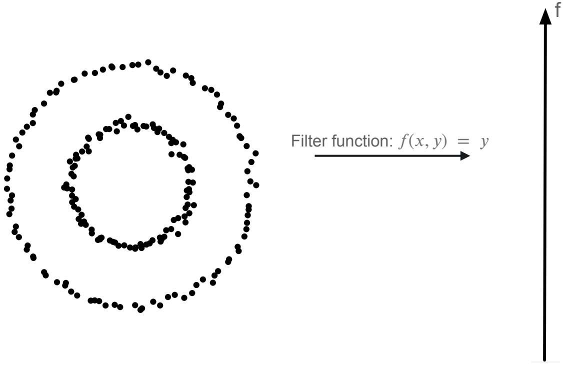


Mapper Graphs

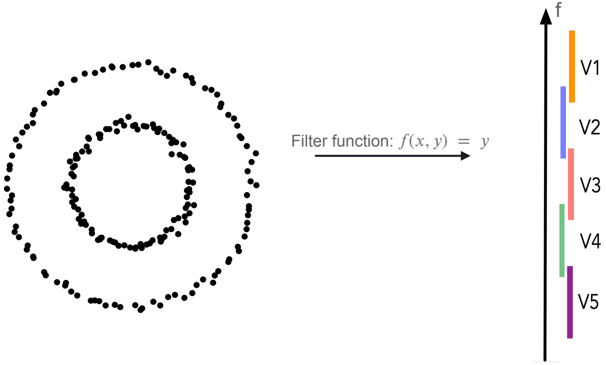


Filter function: $f(x, y) = y$

Mapper Graphs

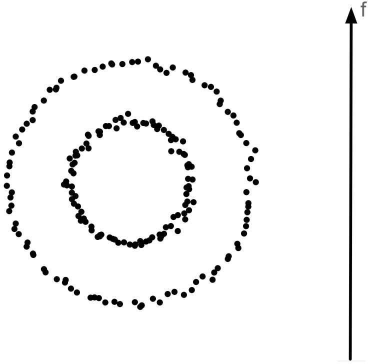


Mapper Graphs

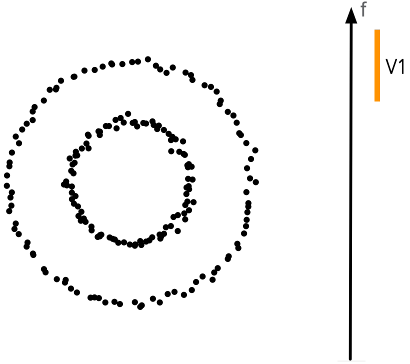


$\{V_\ell\}$: cover of image(f)

Mapper Graphs



Mapper Graphs



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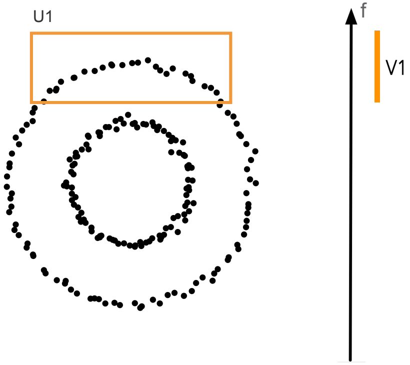
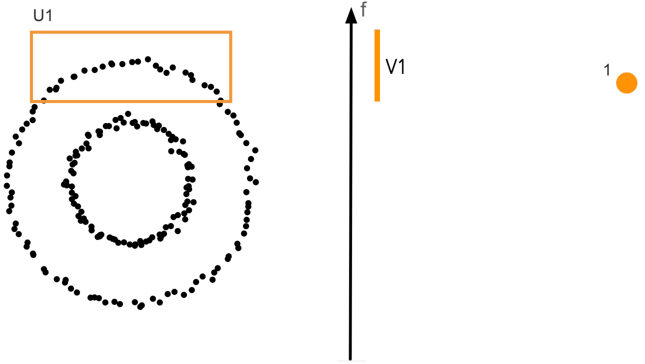
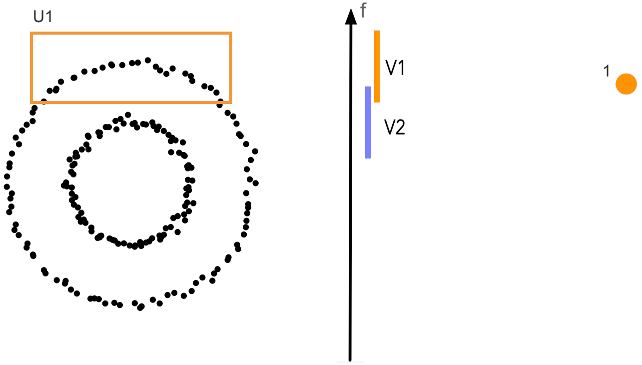


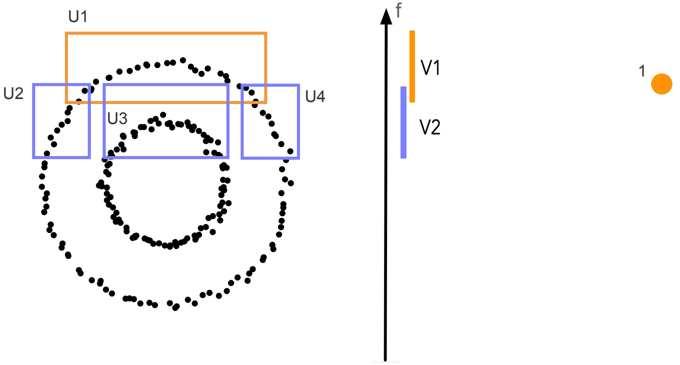
Mapper Graphs



Mapper Graphs



Mapper Graphs



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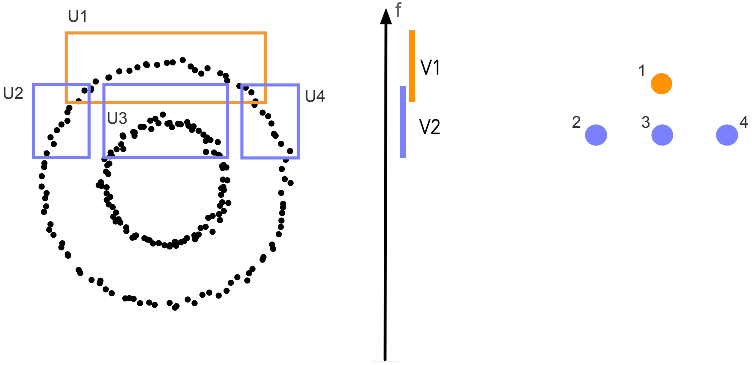
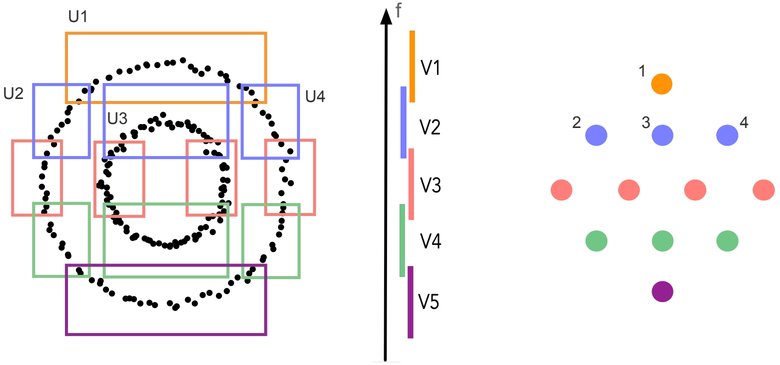


Mapper Graphs



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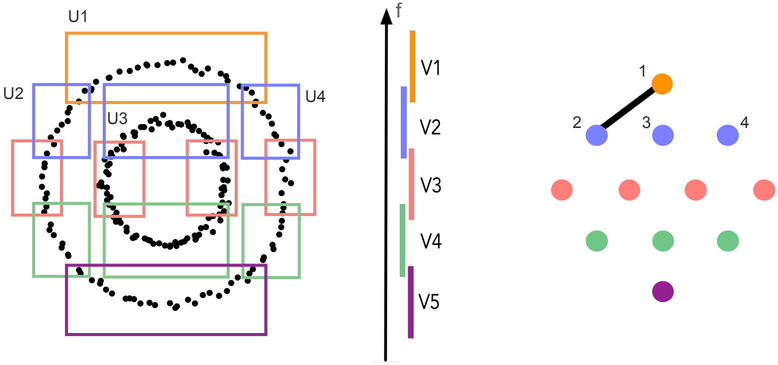
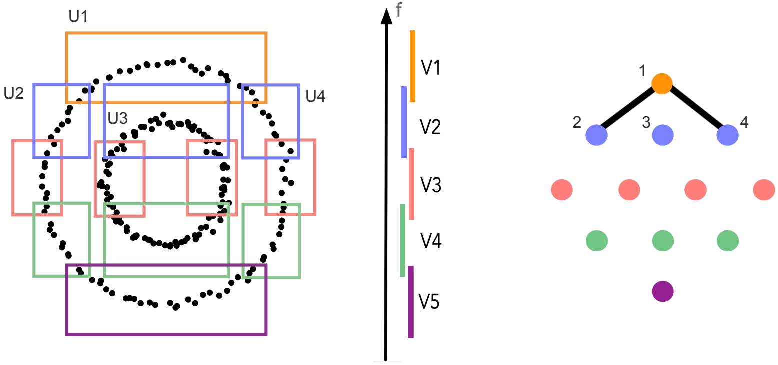
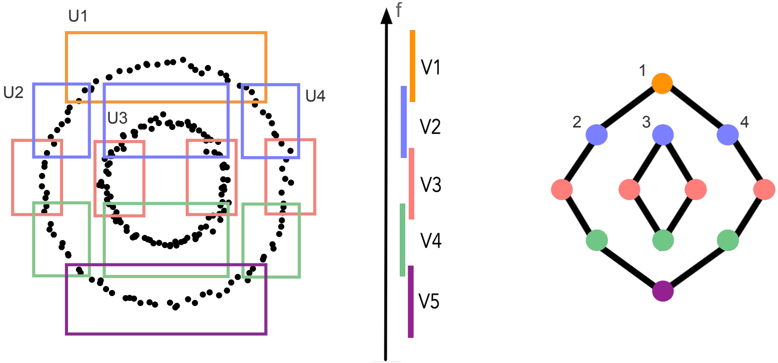


Mapper Graphs



Mapper Graphs



Reeb graph: variants

- Mapper construction, mapper graph: Singh et al. [2007]
- α-Reeb graph: Chazal and Sun [2014]. Cover of range space with open intervals of length at most α.
- Multiscale mapper: Dey et al. [2016]. Consider a hierarchical family of covers and the maps between them.
- Multinerve mapper: Carriére and Oudot [2018]. Compute the multinerve of a connected cover.
- Joint Contour Net (JCN): Carr and Duke [2013], Geng et al. [2014]. A PL mapping over a simplicial mesh with multiple real-valued functions.
- Extended Reeb graph: Barral and Biasotti [2014]. Use cover elements from a partition of the domain without overlaps.
- Enhanced mapper graph: Brown et al. [2021]. Consider additionally the inverse map of intersections among cover elements.
- Ball mapper: Dlotko [2019]

Reeb graph: variants

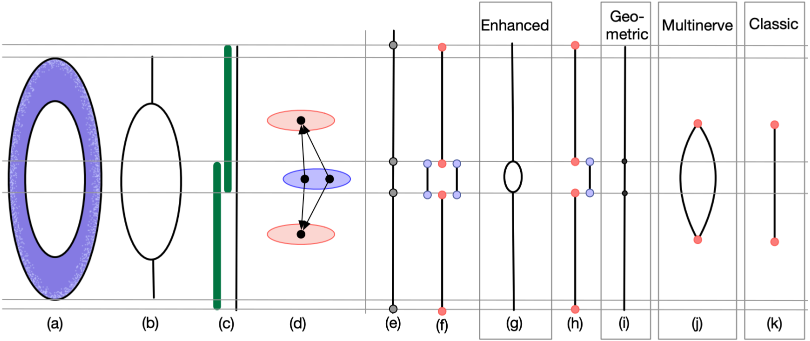


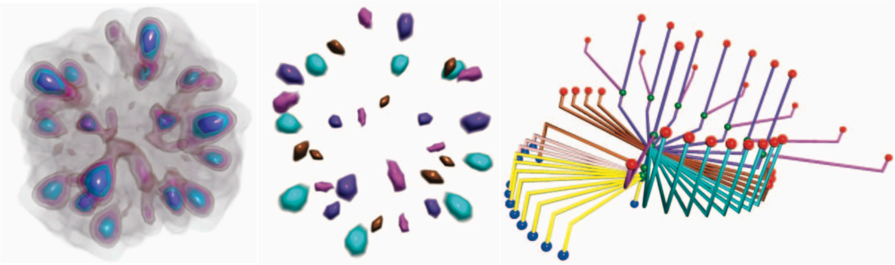
Fig 6. from Brown et al. [2021]
(a) Torus with a height function. (b) Reeb graph. (c) Nice cover.
(d) Visualization of the mapper cosheaf. (e) Stratification of $\mathbb{R}$.
(f) Disjoint union of closed intervals with quotient isomorphic to the enhanced mapper graph. (g) Enhanced mapper graph: Brown et al. [2021].
(i) Geometric mapper graph: Munch and Wang [2016].
(j) Multinerve mapper graph: Carriére and Oudot [2018].
(k) Classic mapper graph: Singh et al. [2007].

Applications

Application: shape skeletonization

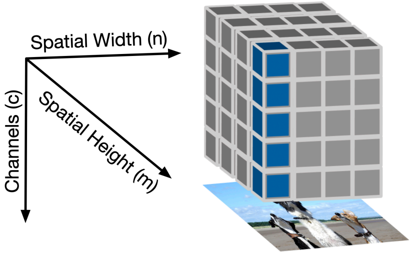
Pascucci et al. [2007]

Application: symmetry detection



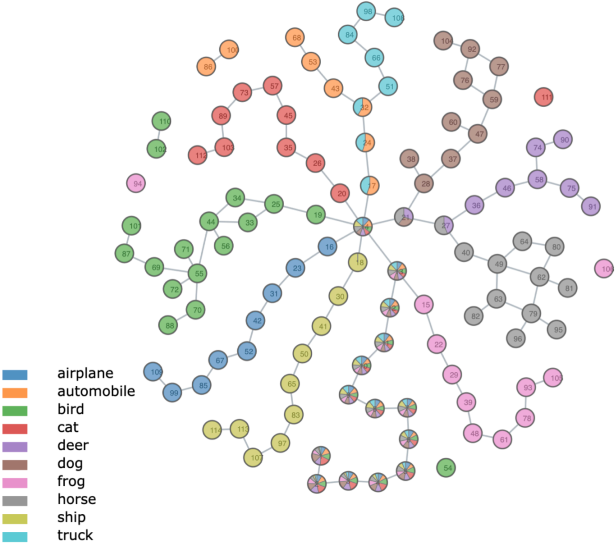
Symmetric patterns identified using contour trees
in electron microscopy data of a protein molecule
Thomas and Natarajan [2011].
See Yan et al. [2021] for a survey.

Application: deep learning



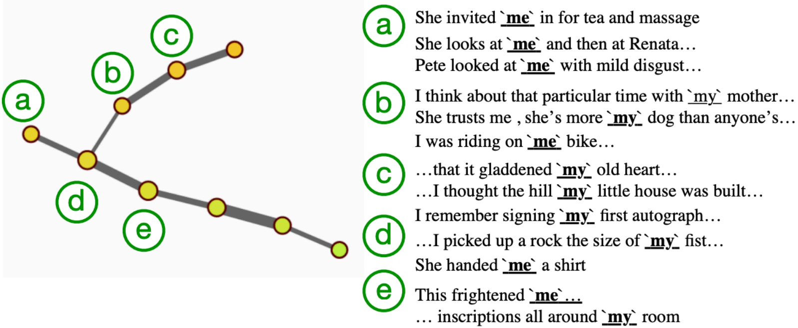
Neuron activations: neuron outputs from a convolutional neural network (CNN) form a high-dimensional point cloud Purvine et al. [2023].

Application: deep learning



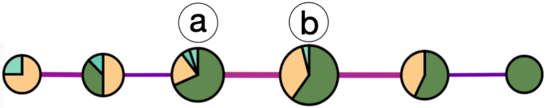
Topological summary of neuron activations using mapper graphs from a ResNet-18 model with CIFAR10 dataset, Zhou et al. [2021].

Application: topology of word embeddings



Pronoun differentiation. BERT Configuration: layer 12, Euclidean norm, 80 intervals, 30% overlap. Rathore et al. [2021].

Application: topology of word embeddings



Cost	I expected to pay for this service , but imagine my surprise when I received a bill **for** MORE than what I paid to have the original return prepared .
Cost	Also , a week after the work , Phet called me up to see how my car was running and to let me know that they had accidentally overcharged me for part of the work and wanted to give me a refund **for** that amount .
Possession	I paid 2 k cash **for** a truck with a blown motor .
Possession	Well - when you pay over $ 1000 **for** something you want it to hold up and look good !!!
Possession	$ 80 **for** a dish that has about one small lobster tail and is full of filler vegetables !
Theme	And another $ 100 **for** wrapping the furniture .
Theme	The dealer wanted $ 1300 to fix that and another $ 1500 **to** fix some other things .
Theme	Plus they will overcharge you **for** just about everything , and smile while doing it .

Capturing model confusion. BERT, Layer 9, fine-tuned on Supersense-Role during batch update 50. Rathore et al. [2023].

Theoretical Properties of Reeb Graphs and Mapper Graphs: An Incomplete Review

Theoretical questions on Reeb graphs

- **Comparison**: What is a reasonable distance or similarity measure $d(R_1, R_2)$ between a pair of Reeb graphs? With desirable properties?
  - Metric or Pseudometric
  - Discriminative
  - Computational complexity: easily implementable
  - **Stability**: w.r.t. simplification or perturbation of the underlying function?
- **Information content**: What information is encoded by the Reeb graph? How much information can we recover about the original data from the Reeb graph by solving an inverse problem?
- See Yan et al. [2021] and Bollen et al. [2022] for surveys.

Theoretical questions on mapper graphs

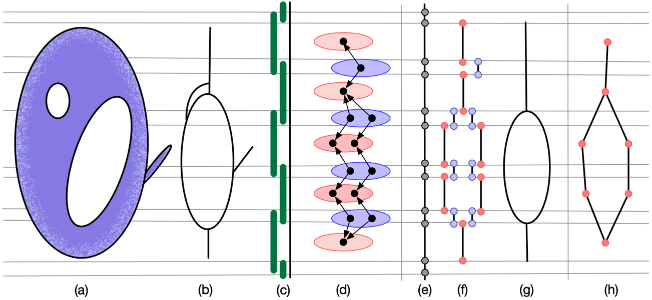
- **Information content**: What information is encoded by the mapper? How much information can we recover about the original data from the mapper by solving an inverse problem?
- **Stability:** What is the structural stability of the mapper with respect to perturbations of its function, domain and cover?
- **Convergence:** What is an appropriate metric under which the mapper converges to the Reeb graph as the number of sampled points goes to infinity and the granularity of the cover goes to zero?
- **Parameter tuning**: How to effectively and automatically tune the parameters that best capture the topology of the underlying data?
- See Brown et al. [2021] for a discussion and a number of references.

Distances between Reeb graphs

- Interleaving distance: Chazal et al. [2009], Morozov et al. [2013], De Silva et al. [2016b], Munch and Stefanou [2019].
- Labeled interleaving distance: Lan et al. [2023]
- Function distortion distance: Bauer et al. [2014, 2015]
- Edit distance: Bauer et al. [2016, 2020], Sridharamurthy et al. [2020]
- Distances based on branch decompositions and matching: Beketayev et al. [2014], Saikia et al. [2014]
- And many more, including those for merge trees and contour trees.
- Coming up: optimal transport distance by extending Li et al. [2023]

Information content

- Dey et al. [2017] studied topological information encoded by Reeb spaces, mappers and multi-scale mappers. 1-dimensional homology of the mapper was shown to be no richer than the domain itself.
- Carriére and Oudot [2018] characterized the information encoded in the mapper using the extended persistence diagram of its corresponding Reeb graph.
- Brown et al. [2021]: enhanced mapper graph reduces the information loss during summarization.



Convergence

- Babu [2013]: showed that the mapper converges to the Reeb graph in the bottleneck distance, using levelset zigzag persistence.
- Dey et al. [2017]: a convergence result between the mapper and the domain under a Gromov-Hausdorff metric.
- Carriére and Oudot [2018]: convergence between the (multinerve) mapper and the Reeb graph using the functional distortion distance.
- Carriére et al. [2018]:
    - Proved convergence.
    - Provided a confidence set for the mapper using a bottleneck distance on extended persistence diagrams.
    - The mapper is an optimal estimator of the Reeb graph.
    - Provided a statistical method for automatic parameter tuning using the rate of convergence.

Convergence

- Munch and Wang [2016]: characterized the mapper using constructible cosheaves. Proved the convergence between the (classic) mapper and the Reeb space in interleaving distance.
- Brown et al. [2021]: Probabilistic convergence between the mapper graph and the Reeb graph.
  - Recover (a variant of) the mapper graph using the theory of cosheaves in a probabilistic setting.
  - Assume points randomly sampled from a probability density function concentrated on the space.
  - With high probability, the distance between an enhanced mapper graph and the Reeb graph is upper bounded by the resolution of the cover as the number of samples goes to infinity.

Parameter tuning for mapper graphs

- Carriére et al. [2018]: a statistical procedure for selecting the most stable parameters for the mapper graph.
- Chalapathi et al. [2021]: adaptive covers using information criteria: multi-pass AIC and BIC. Based on X-means clustering algorithms.
- Alvarado et al. [2023]: G-Mapper. Splitting a cover repeatedly according to a statistical test for normality. Based on G-means clustering.
- Bui et al. [2020]: F-Mapper. Based on the Fuzzy C-means algorithm, a centroid-based overlapping clustering method.

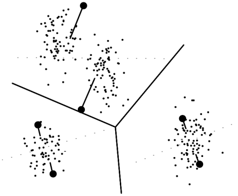


Figure 3: The first step of parallel local 2-means. The line coming out of each centroid shows where it moves to.

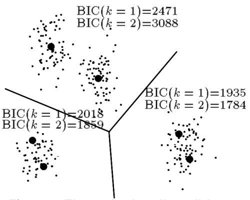


Figure 4: The result after all parallel 2-means have terminated.

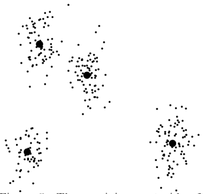


Figure 5: The surviving centroids after all the local model scoring tests.

Pelleg and Moore [2000]

Stability of mapper graphs

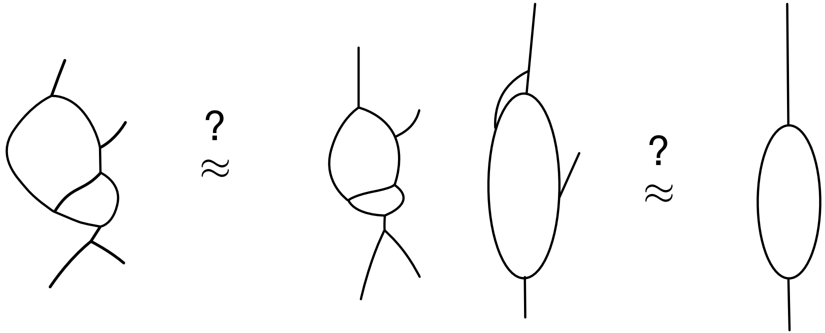
- Carriére and Oudot [2018]: stability for the mapper graph using the stability of extended persistence diagrams equipped with the bottleneck distance under Hausdorff or Wasserstein perturbations of the data.
- Brown et al. [2021]:
  - Stability for the mapper cosheaf in the interleaving distance.
  - Stability of the enhanced mapper graph with respect to perturbation of the data $(\mathbb{X}, f)$
  - The local stability depends on how the cover is positioned in relation to the critical values of f.

Stability of Reeb graphs

Theorem ([De Silva et al., 2016a, Theorem 4.4])

Let $R(\mathbb{X}, f)$ and $R(\mathbb{X}, g)$ be two Reeb graphs built from the same ambient space $\mathbb{X}$. Then the interleaving distance satisfies

$$d_I(R(\mathbb{X}, f), R(\mathbb{X}, g)) \leq \|f - g\|_\infty.$$



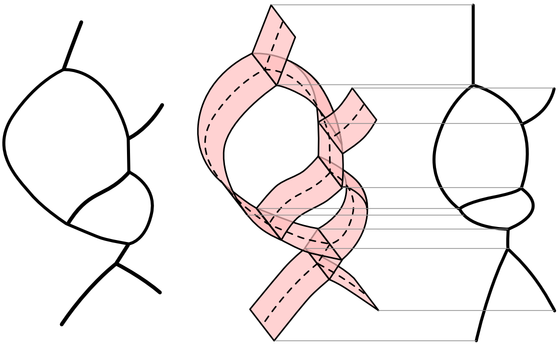
Smoothing of Reeb graph

- Given a Reeb graph G, let G_ε denote the space $G \times [-\varepsilon, \varepsilon]$ and define the ε-smoothing of G as the Reeb graph of the function

$$\begin{aligned} f_\varepsilon : \quad G_\varepsilon &\longrightarrow \mathbb{R} \\ (x, t) &\longmapsto f(x) + t. \end{aligned}$$

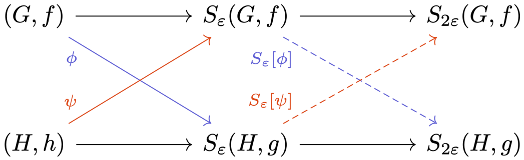
- De Silva et al. [2016a]: *ε-smoothing of a Reeb graph*

$$S_\varepsilon(G, f) := G_\varepsilon / \sim_{f_\varepsilon}$$



Interleaving distance

- For any $\epsilon > 0$, an ε-interleaving between two Reeb graphs (G, f) and (H, g) is a pair of maps, φ and ψ such that the following diagram commutes,



  $S_\varepsilon[\phi]$ is the map induced by $\Phi : G \times [-\varepsilon, \varepsilon] \to S_\varepsilon(H, g) \times [-\varepsilon, \varepsilon]$, $\Phi(x, t) = (\phi(x), t)$. See De Silva et al. [2016a] for details.

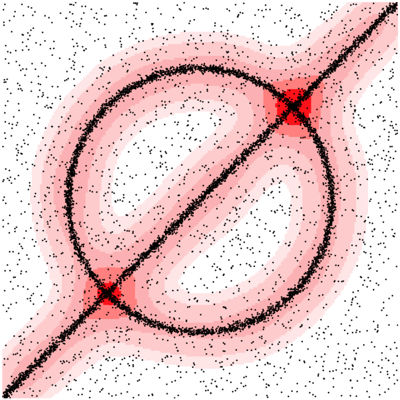
- The interleaving distance $d_I((G, f), (H, h))$ is defined as

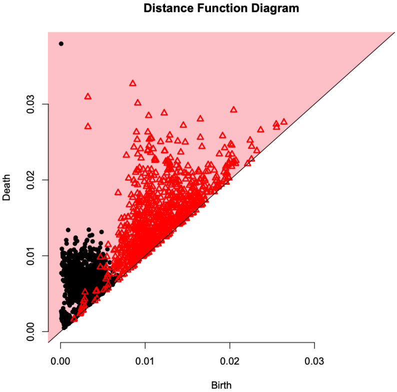
$$d_I((G, f), (H, h)) = \inf_{\varepsilon}\{\exists\ \varepsilon\text{-interleaving of } (G, f) \text{ and } (H, h)\}.$$

- **Smallest amount of thickening that gives rise to an ε-interleaving.**

Measure Theoretic Reeb Graphs

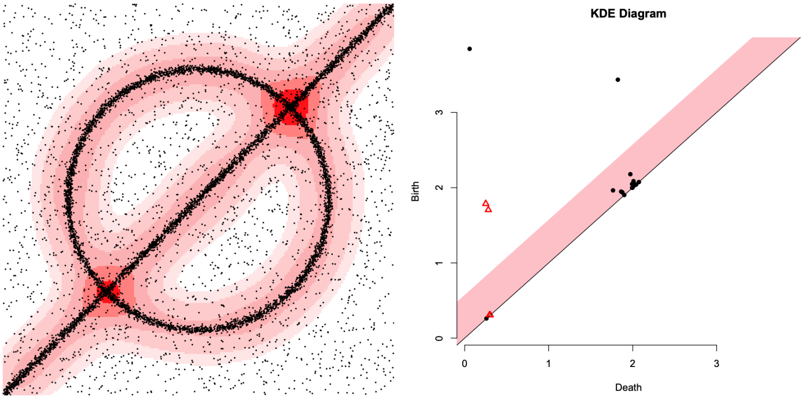
Robust topological descriptors and structural inference





Examine superlevel sets of kernel density estimate (sublevel sets of the kernel distance) for robust topological inference. Phillips et al. [2015]

Robust topological descriptors and structural inference

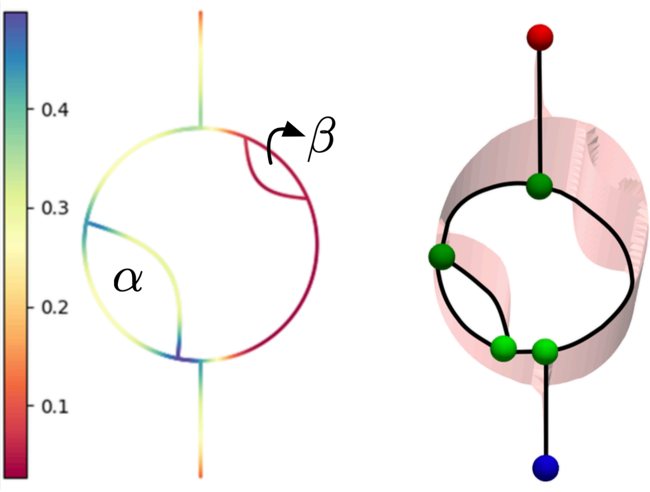


Examine superlevel sets of kernel density estimate (sublevel sets of the kernel distance) for robust topological inference. Phillips et al. [2015]

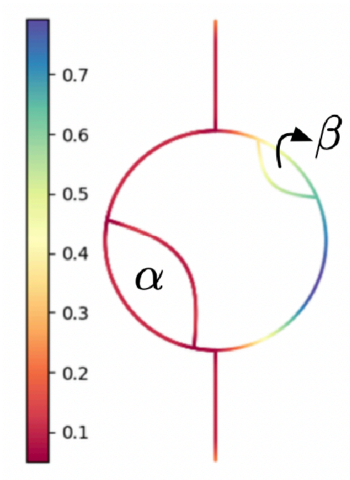
Robust topological descriptors

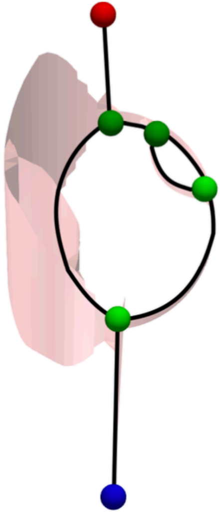
- Data science applications: associate weights to data points, which represent how much we trust these data points, or how important their corresponding features are.
- Conventional Reeb graphs do not take into consideration the data distributions and (possibly) non-uniform importance of data points, leading to discrepancies between the represented and actual topologies of the data.
- E.g., a significant loop in the Reeb graph might be caused by a sparse set of data points or lies in regions of low importance in function values.
- **Capture robust topology in data**.

An illustrative example

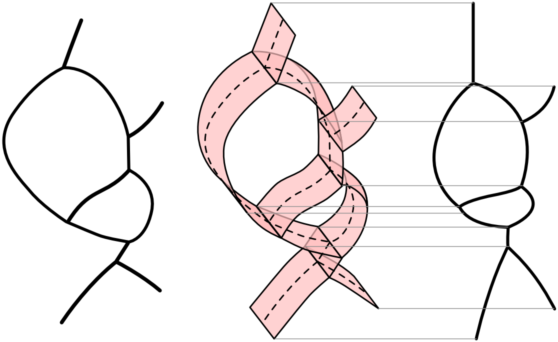


An illustrative example





Locally smoothed Reeb graph



What if we vary the thickening parameter?

Locally smoothed Reeb graph

- Smoothing with variable thickness.
- Let $\mathbb{X}$ be a topological space and $f : \mathbb{X} \to \mathbb{R}$ be a function on $\mathbb{X}$.
- Let $r : \mathbb{X} \to \mathbb{R}$ be a bounded positive function on $\mathbb{X}$ with

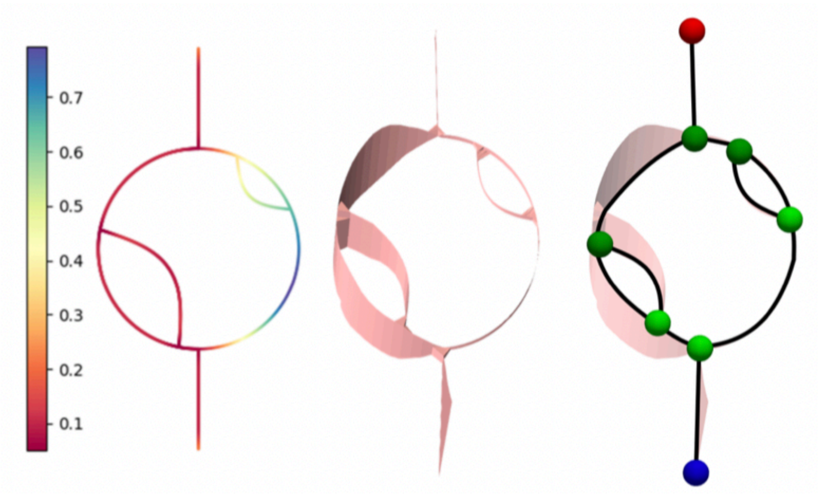
$$M := \sup_{x \in \mathbb{X}} r(x).$$

- The function r is viewed as a local smoothing factor.
- Let $\mathbb{X}_r$ denote the space

$$\mathbb{X}_r = \{(x, t) \in \mathbb{X} \times [-M, M] \mid |t| \leq r(x)\}.$$

- Then the function f naturally extends to a function f_r on $\mathbb{X}_r$ by $f_r(x, t) = f(x) + t$.
- The r-*smoothed Reeb graph* of $(\mathbb{X}, f)$ is the Reeb graph $R(\mathbb{X}_r, f_r)$.

Locally smoothed Reeb graph



Stability of locally smoothed Reeb graph

Lemma (Stability of locally smoothed Reeb graph)

Let $\mathbb{X}$ be a topological space and f be a function on $\mathbb{X}$. Additionally, let r_1 and r_2 be two bounded positive function on $\mathbb{X}$ with

$$\varepsilon := \sup_{x \in \mathbb{X}} |r_1(x) - r_2(x)|.$$

Then the r_1-smoothed Reeb graph $R(\mathbb{X}_{r_1}, f_{r_1})$ and the r_2-smoothed Reeb graph $R(\mathbb{X}_{r_2}, f_{r_2})$ are ε-interleaved.

Metric measure spaces

- A *metric measure space* is a triple $(\mathbb{X}, d_{\mathbb{X}}, \mu)$ where $(\mathbb{X}, d_{\mathbb{X}})$ is a metric space and μ is a probability measure on (the Borel σ-algebra of) $\mathbb{X}$.
- What measure do we use to model the data importance?
- Use distance to a measure $d_{\mu,m}$ or Kernel distance to a measure $D_{\mu,K}$ as local smoothing parameters:
  - Distance to a measure: $d_{\mu,m}$, Buchet et al. [2016]
  - Kernel distance to a measure: $D_{\mu,K}$ Phillips et al. [2015]

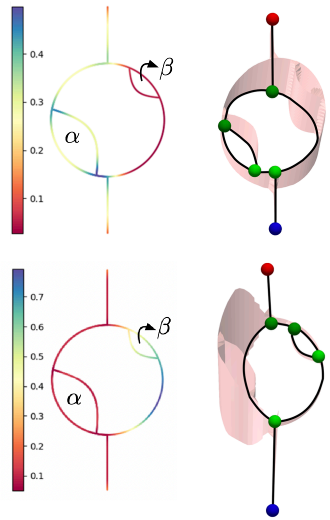
Distance between measures

- Let $(\mathbb{X}, d_{\mathbb{X}})$ be a metric space and μ, ν be two probability measures on $\mathbb{X}$. The 2-Wasserstein distance between μ and ν is defined as

$$W_2(\mu,\nu) = \inf_{\pi \in \Pi(\mu,\nu)} \left(\int_{\mathbb{X}\times\mathbb{X}} d_{\mathbb{X}}(x,y)^2 d\pi(x,y) \right)^{1/2},$$

  where $\Pi(\mu,\nu)$ is the set of all probability measures on $\mathbb{X} \times \mathbb{X}$ with marginals μ and ν.

Locally smoothed Reeb graphs



Locally smoothed Reeb graphs based on distance to a measure (top) and kernel distance to a measure (bottom).

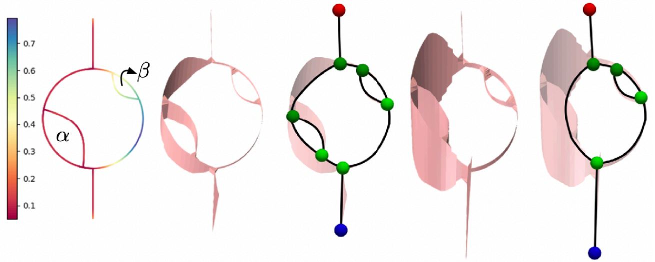
Stability of measure theoretic Reeb graphs

Theorem (Stability of $d_{\mu,m}$-smoothed Reeb graph)

Let $(\mathbb{X}, d_{\mathbb{X}}, \mu)$ *and* $(\mathbb{X}, d_{\mathbb{X}}, \nu)$ *be two metric measure spaces and* $f, g : \mathbb{X} \to \mathbb{R}$ *be two continuous functions. Let* $m \in (0, 1]$ *be a mass parameter. Then we have*

$$d_I(R(\mathbb{X}_{d_{\mu,m}}, f_{d_{\mu,m}}), R(\mathbb{X}_{d_{\nu,m}}, g_{d_{\nu,m}})) \le \|f - g\|_\infty + \frac{1}{\sqrt{m}} W_2(\mu, \nu).$$

Stability w.r.t. perturbations of the function and the measure.



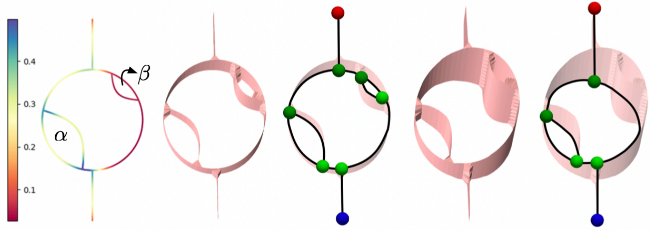
Stability of measure theoretic Reeb graphs

Theorem (Stability of $D_{\mu,K}$-smoothed Reeb graph)

Let $\mathbb{X}$ be a topological space. Let μ and ν be two probability measures on $\mathbb{X}$. Let K be an integrally strictly positive definite kernel function on $\mathbb{X}$. Consider two continuous functions $f, g : \mathbb{X} \to \mathbb{R}$. Then we have

$$d_I(R(\mathbb{X}_{D_{\mu,K}}, f_{D_{\mu,K}}), R(\mathbb{X}_{D_{\nu,K}}, g_{D_{\nu,K}})) \leq \|f - g\|_\infty + D_K(\mu, \nu).$$

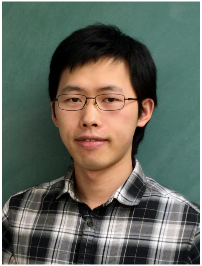
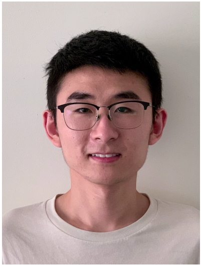
Stability w.r.t. perturbations of the function and the measure.



Discussion: robust topological descriptors

- What is the robust topology of data?
- Data importance captured by a measure.
- Our stability results hold for Reeb spaces, $R(\mathbb{X}, f), f : \mathbb{X} \to \mathbb{R}^d$, multivariate data analysis.
- Our findings demonstrate the stability of both Reeb graph and Reeb space constructions against perturbations of the function and the measure, thereby offering robust improvements for these topological descriptors.
- More: range-integrated reeb graphs, with a measure on the range of a function. Stability results.
- Ongoing: applications in topological data analysis and visualization.

Acknowledgement

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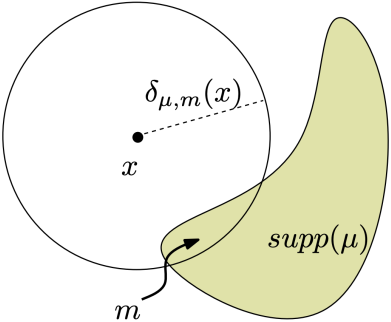
Extra

Distance to a measure: pointwise importance or robustness

- $(\mathbb{X}, \mu)$: a metric measure space; $m \in (0, 1]$: a mass parameter.
- Define $\delta_{\mu,s}$ as $\delta_{\mu,s} : x \in \mathbb{X} \mapsto \inf\{r > 0 \mid \mu(\bar{B}(x, r)) > s\}$.
- $\bar{B}(x, r)$ denotes the closed ball of radius r centered at x.
- $\delta_{\mu,s}$: smallest distance needed to capture a mass of at least s.



Chazal 2010[1]

[1] https://atmcs4.appliedtopology.org/talks/Chazal/geomInference.pdf

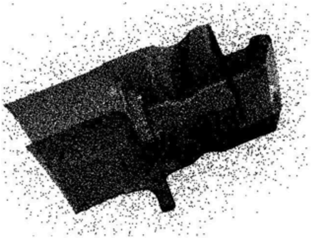
Distance to a measure $d_{\mu,m}$

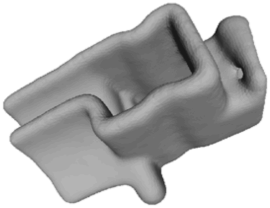
Definition ([Buchet et al., 2016, Definition 1.1])

Let $(\mathbb{X}, \mu)$ be a metric measure space and let $m \in (0, 1]$ be a mass parameter. We define the *distance to a measure* function $d_{\mu,m} : \mathbb{X} \to \mathbb{R}$ as

$$d_{\mu,m} : x \in \mathbb{X} \mapsto \sqrt{\frac{1}{m} \int_0^m \delta_{\mu,s}^2(x) ds},$$

where $\delta_{\mu,s} : x \in \mathbb{X} \mapsto \inf\{r > 0 \mid \mu(\bar{B}(x, r)) > s\}$. $\bar{B}(x, r)$ denotes the closed ball of radius r centered at x.





Stability of distance to a measure $d_{\mu,m}$

Theorem ([Buchet et al., 2016, Theorem 3.3] for $\mathbb{R}^n$; [Buchet, 2014, Proposition 3.14] for general metric spaces)

Let μ and ν be two probability measures on a metric space $(\mathbb{X}, d_{\mathbb{X}})$ and let $m \in (0, 1]$ be a mass parameter. Then:

$$\|d_{\mu,m} - d_{\nu,m}\|_\infty \leq \frac{1}{\sqrt{m}} W_2(\mu, \nu),$$

where $W_2(\mu, \nu)$ is the 2-Wasserstein distance between μ and ν.

Integrally strictly positive definite kernel function

Definition (Sriperumbudur et al. [2010])

Let $\mathbb{X}$ be topological space. A (Borel) measurable function $K : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ is called an *integrally strictly positive definite* kernel function if for all finite signed Borel measures μ on $\mathbb{X}$, there is

$$\int_{\mathbb{X}\times\mathbb{X}} K(x, x')d\mu(x)d\mu(x') > 0.$$

E.g. a Gaussian kernel function

Kernel distance

Definition (Sriperumbudur et al. [2010], Phillips et al. [2015])

Let $\mathbb{X}$ be a topological space. Let μ and ν be two probability measures on $\mathbb{X}$. Let K be an integrally strictly positive definite kernel function. Then the kernel distance D_K between μ and ν is defined as

$$D_K(\mu, \nu) := \sqrt{\kappa(\mu, \mu) + \kappa(\nu, \nu) - 2\kappa(\mu, \nu)},$$

where $\kappa(\mu, \nu)$ is defined as $\kappa(\mu, \nu) := \int_{\mathbb{X}\times\mathbb{X}} K(x, x')d\mu(x)d\nu(x')$.

Kernel distance to a measure $D_{\mu,K}$

Definition (Phillips et al. [2015])

Let μ be a probability measure on a topological space $\mathbb{X}$. Let K be an integrally strictly positive definite kernel function. Then the kernel distance $D_{\mu,K}$ with respect to μ is a function $D_{\mu,K} : \mathbb{X} \to \mathbb{R}$ defined as

$$D_{\mu,K}(x) = D_K(\mu, \delta_x),$$

where δ_x is the Dirac delta measure at x.

Stability of a kernel distance to a measure

Theorem (Phillips et al. [2015])

Let μ and ν be two probability measures on a topological space $\mathbb{X}$. Let K be an integrally strictly positive definite kernel function. Then

$$\|D_{\mu,K} - D_{\nu,K}\|_{\infty} \leq D_K(\mu, \nu),$$

where $D_K(\mu, \nu)$ is the kernel distance between μ and ν.