Differentiable Mapper

Topological Optimization of Data Representation

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Background on Mapper Graphs

Mapper Algorithm

The Mapper was introduced in [Singh et al., 2007] as a topology based data visualization method.
Given a discrete metric space $(\mathbb{X}_n = \{X_1, \dots, X_n\}), d)$, as well as a filter function $f : \mathbb{X}_n \to \mathbb{R}$:

1. Cover the range of values $\mathbb{Y}_n = f(\mathbb{X}_n)$ with a set of consecutive intervals $I_1, \dots, I_r$ that overlap, i.e., one has $I_i \cap I_{i+1} \neq \varnothing$ for all $1 \leq i \leq r-1$.
2. Apply a clustering algorithm to each pre-image $f^{-1}(I_j)$, $j \in \{1, ..., r\}$. This defines a *pullback cover* $\mathcal{C} = \{\mathcal{C}_{1,1}, \dots, \mathcal{C}_{1,k_1}, \dots, \mathcal{C}_{r,1}, \dots, \mathcal{C}_{r,k_r}\}$ of $\mathbb{X}_n$.
3. The Mapper graph is defined as the *nerve* of $\mathcal{C}$. Each node $v_{j,k}$ of the Mapper graph corresponds to an element $\mathcal{C}_{j,k}$ of $\mathcal{C}$, and two nodes $v_{j,k}$ and $v_{j',k'}$ are connected by an edge if and only if $\mathcal{C}_{j,k} \cap \mathcal{C}_{j',k'} \neq \varnothing$.

Mapper Example

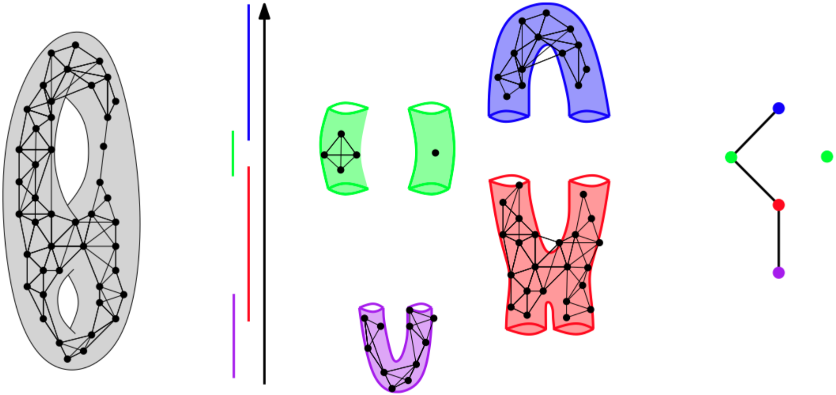

Figure: Example of a Mapper graph taken from [Carriere et al., 2018]. The clustering is specified from a neighborhood graph.

Hyperparameters

Most commonly, the intervals are chosen to have the same length, with a fixed percentage of overlap between consecutive ones.

Hyperparameters to choose

1. Number of intervals (resolution) : r,
2. Percentage of overlap (gain) : g,
3. Clustering,
4. Filter function.

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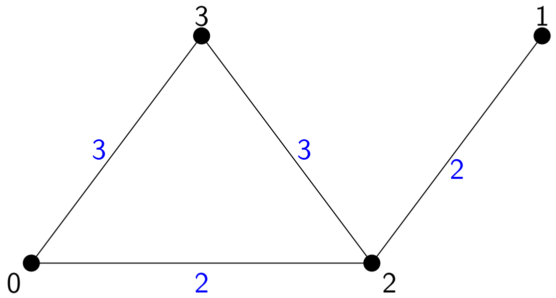
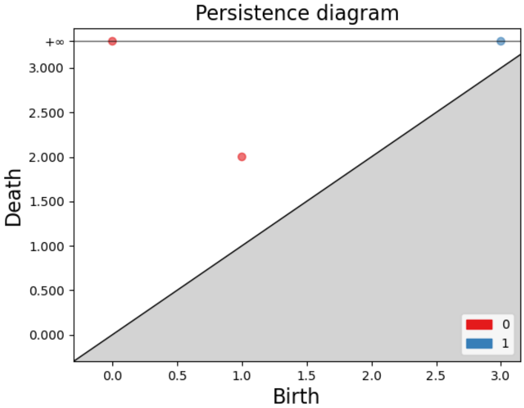
Hyperparameters to choose

1. Number of intervals (resolution) : r, $\leftarrow$ Grid search, Look for stability, Infer it from the inherent manifold structure of the data.
2. Percentage of overlap (gain) : g, $\leftarrow$ Same as resolution.
3. Clustering, $\leftarrow$ Depends on the nature of the dataset.
4. Filter function. $\leftarrow$?

Topological Signatures on Mapper graphs

Persistence Diagram





Filtering a Mapper graph

Fix a dataset (discrete metric space) $\mathbb{X}_n$, a integer r and a clustering function Clus.
Let $\mathbb{K}$ be the set of simplicial complexes of dimension less or equal to 1 (i.e., graphs) and such that their sets of vertices (i.e., their $0-$skeletons) are subsets of the power set $\mathcal{P}(\mathbb{X}_n)$.

Filtration values

For a function $F \in \mathcal{F}(\mathbb{X}_n, \mathbb{R})$, we associate a filtration ϕ to some $K \in \mathbb{K}$ with:

$$\forall \sigma \in K \ : \ \phi(\sigma) = \max_{c \in \sigma} \frac{\sum_{x \in c} F(x)}{\mathrm{card}(c)}.$$

Persistence loss

Denoting PD as the set of subsets of $\mathbb{R}^2$ consisting of a finite number of points outside the diagonal $\Delta = \{(x,x) : x \in \mathbb{R}\}$, we also consider a loss function : $\ell \colon PD \longrightarrow \mathbb{R}$.
For example :

$$\{(u_i, v_i)\}_{1 \leq i \leq n} \longmapsto -\sum_{i=1}^{n} |u_i - v_i|.$$

Soft Mapper

Formal definition of the Mapper

Cover assignment

We call any binary matrix $e \in \{0,1\}^{n \times r}$ an *r-latent cover assignment* of $\mathbb{X}_n$, where $e_{i,j} = 1$ must be understood as point x_i belonging to the j-th element of a *latent cover* of the data.

Mapper complex generating function

Define

$$\mathrm{MapComp} \colon \{0,1\}^{n \times r} \longrightarrow \mathbb{K},$$

to be the function that takes a cover assignment and associates its corresponding Mapper complex. It uses the same algorithm for Mapper but replaces $f^{-1}(I_j)$ by $\{x_i \,:\, e_{i,j} = 1\}$.

Soft Mapper

We use this formalism to define distributions on Mapper graphs.

Cover assignment scheme

A *cover assignment scheme* is a double indexed sequence of random variables

$$A = (A_{i,j})_{\substack{1 \leq i \leq n \\ 1 \leq j \leq r}}$$

such that each $A_{i,j}$ is a Bernoulli random variable conditionally to $\mathbb{X}_n$.
Let $p_{i,j}(\mathbb{X}_n)$ be the parameter of the Bernoulli distribution of $(A_{i,j}|\mathbb{X}_n)$, which is thus a function of the point cloud $\mathbb{X}_n$.

Soft Mapper

Let A be a cover assignment scheme. The *Soft Mapper* of A is defined as the associated distribution of Mapper complexes, which corresponds to the push forward measure of the distribution of A by the map MapComp.

Example 1 : The regular case

let $f : \mathbb{X}_n \to \mathbb{R}$ be a filter function and let $(I_j)_{1 \leq j \leq r}$ be a finite cover of the image $f(\mathbb{X}_n)$ of f. The standard Mapper graph is then defined as MapComp(e^*), where for every $1 \leq i \leq n$ and $1 \leq j \leq r$:

$$e^*_{i,j} = 1 \text{ if } f(x_i) \in I_j.$$

The cover assignment scheme A^*, in this case, is degenerate at e^*.

$$\mathbb{P}(A^* = e|\mathbb{X}_n) = \begin{cases} 1 & \text{if } e = e^*, \\ 0 & \text{otherwise.} \end{cases}$$

Example 2 : Smooth relaxation of the regular case

Let $\delta > 0$. Using the same notations as before, and denoting each element of the cover with $I_j = [a_j, b_j]$, consider, for each $j \in \{1, ..., r\}$, the function $q_j : \mathbb{X}_n \longrightarrow [0, 1]$ defined with:

$$x \mapsto \begin{cases} 1, & \text{if } f(x) \in [a_j, b_j] \\ \exp(1 - 1/(1 - (\frac{a_j - f(x)}{\delta})^2)), & \text{if } f(x) \in [a_j - \delta, a_j] \\ \exp(1 - 1/(1 - (\frac{f(x) - b_j}{\delta})^2)), & \text{if } f(x) \in [b_j, b_j + \delta] \\ 0, & \text{otherwise} \end{cases}$$

Now, define $A_\delta = (A_{\delta,i,j})_{\substack{1 \le i \le n \\ 1 \le j \le r}}$ to be the random variable in $\{0, 1\}^{n \times r}$ such that for every $(i, j) \in \{1, ..., n\} \times \{1, ..., r\}$:

$$A_{\delta,i,j} \mid \mathbb{X}_n \sim \mathcal{B}(q_j(x_i)).$$

Comparison between A^* and A_δ

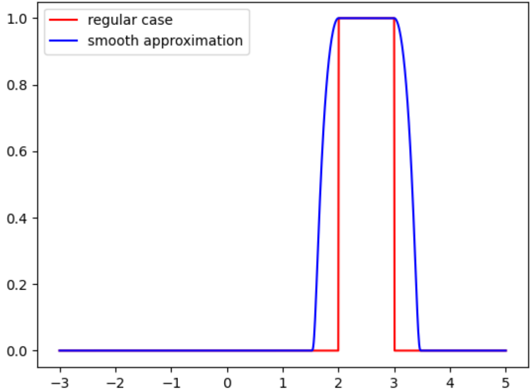
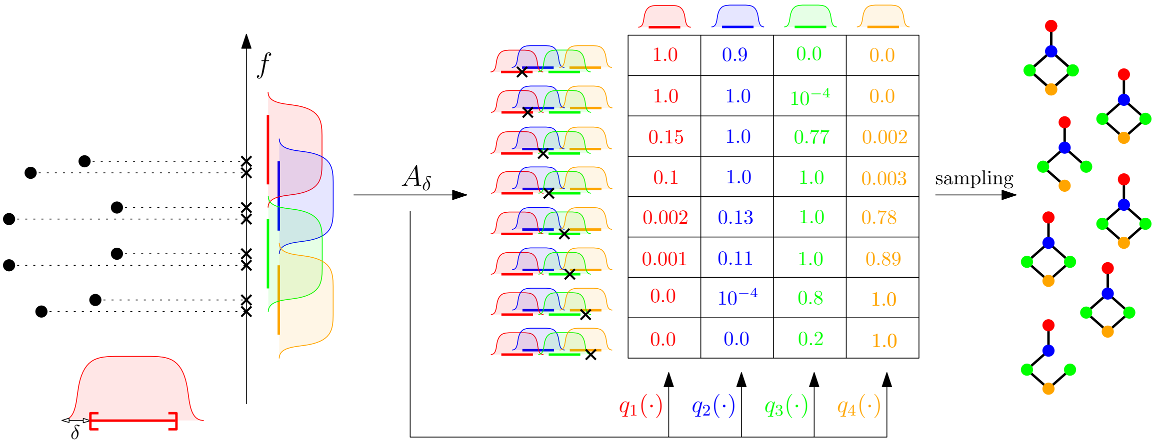


Figure: Assignment probability $p_{i,j}(\mathbb{X}_n)$ of a point x_i to an interval $I_j = [2, 3]$ for A^* and A_δ, plotted against $f(x_i)$.

Illustration of the smooth assignment scheme A_δ



1.0	0.9	0.0	0.0
1.0	1.0	10^{-4}	0.0
0.15	1.0	0.77	0.002
0.1	1.0	1.0	0.003
0.002	0.13	1.0	0.78
0.001	0.11	1.0	0.89
0.0	10^{-4}	0.8	1.0
0.0	0.0	0.2	1.0

Risk of a Soft Mapper

We define the risk of a Soft Mapper MapComp(A) by integrating the loss according to the distribution of the Soft Mapper :

$$\mathbb{E}\left(\mathcal{L}(A, F)|\mathbb{X}_n\right) = \sum_{e \in \{0,1\}^{n \times r}} \mathcal{L}(e, F) \cdot \mathbb{P}(A = e|\mathbb{X}_n).$$

Filter Optimization

Problem setting

Let us introduce a parameterized family of functions $\{f_\theta : \mathbb{X}_n \to \mathbb{R},\ \theta \in \mathbb{R}^s\}$. Let A be a cover assignment scheme whose joint distribution $\mathbb{P}_\theta$ depends on the filter function f_θ. Denoting

$$\begin{aligned} \mathsf{L} \colon \mathbb{R}^s &\longrightarrow \mathbb{R} \\ \theta &\longmapsto \mathbb{E}_\theta(\mathcal{L}(A, f_\theta)|\mathbb{X}_n), \end{aligned} \tag{1}$$

our aim is to find a minimizer of L.

Main result

[Oulhaj et al., 2024]

Suppose that there exists an o-minimal structure $\mathcal{S}$ such that:

- for every $x \in \mathbb{X}_n$, the function $\theta \mapsto f_\theta(x)$ is definable in $\mathcal{S}$ and is locally Lipschitz,
- for every $m \in \mathbb{N}$, the restriction of ℓ to the set of (extended) persistence diagrams of size m is definable in $\mathcal{S}$ and is locally Lipschitz,
- for every $e \in \{0, 1\}^{n \times r}$, the function $\theta \mapsto \mathbb{P}_\theta(A = e|\mathbb{X}_n)$ is definable in $\mathcal{S}$ and is locally Lipschitz.

Then L is definable in $\mathcal{S}$ and is locally Lipschitz.

Main result

[Oulhaj et al., 2024]

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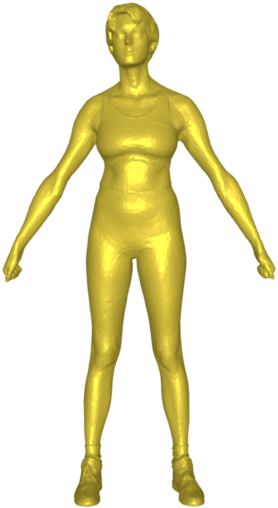
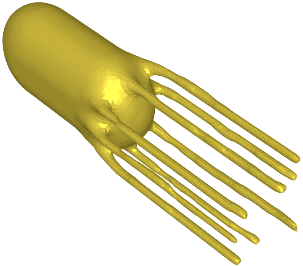
- for every $m \in \mathbb{N}$, the restriction of ℓ to the set of (extended) persistence diagrams of size m is definable in $\mathcal{S}$ and is locally Lipschitz,
- for every $e \in \{0,1\}^{n \times r}$, the function $\theta \mapsto \mathbb{P}_\theta(A = e|\mathbb{X}_n)$ is definable in $\mathcal{S}$ and is locally Lipschitz. $\leftarrow$ Doesn't work in the regular (degenerate) case

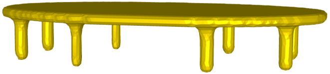
Then L is definable in $\mathcal{S}$ and is locally Lipschitz.

Experiments

3D shapes







We wish to optimize a linear parametric family of functions, i.e., equal to $\{f_\theta : x \mapsto \langle x, \theta \rangle, \theta \in \mathbb{R}^3\}$, and the cover assignment scheme A_δ is the smooth relaxation of the standard case, with $\delta = 10^{-2} \cdot (\max_{x \in \mathbb{X}_n} f_\theta(x) - \min_{x \in \mathbb{X}_n} f_\theta(x))$.

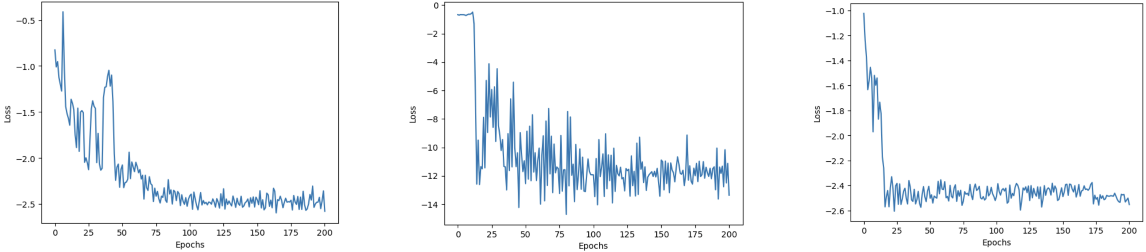
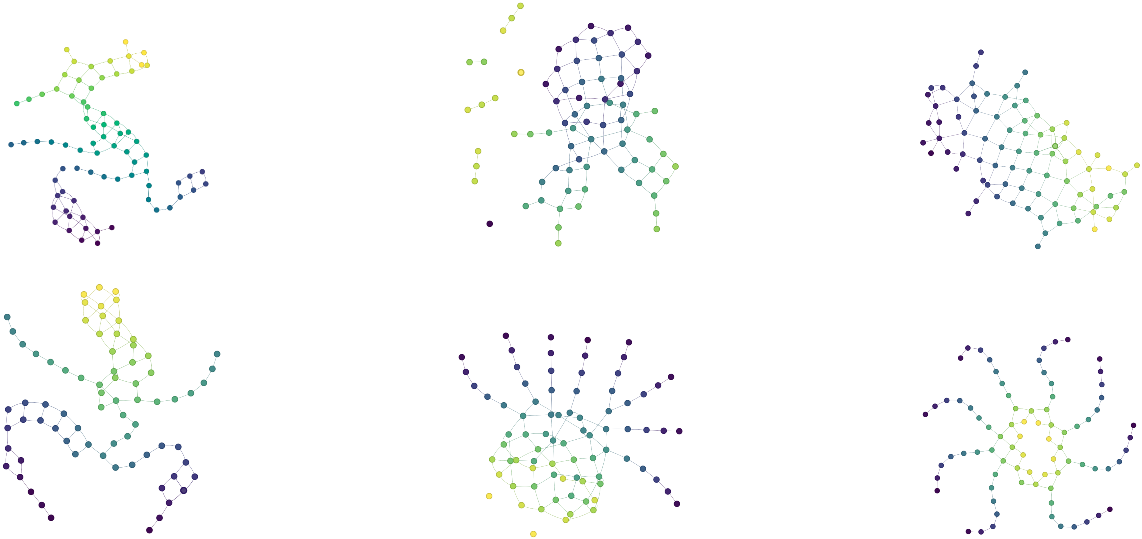


Figure: Learning curves for the 3-dimensional shapes corresponding, from left to right, to: the human, the octopus and the table.

Before - After



Thank you for listening !

Check out the poster at Hall C 4-9 #1113

Guarantees on stochastic gradient descent

[Davis et al., 2020]

Under technical conditions on the stochastic gradient descent algorithm and under the following assumptions :

- L is definable in an o-minimal structure,
- L is locally Lipschitz,

then $(\mathrm{L}(x_k))_k$ converges almost surely to a critical value and the limit points of $(x_k)_k$ are critical points of L.

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The Journal of Machine Learning Research, 19(1):478–516.

Davis, D., Drusvyatskiy, D., Kakade, S., and Lee, J. D. (2020).
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