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AIH Institute of AI for Health

Geometrical–Topological Loss Terms for Shape Analysis

Bastian Rieck (@Pseudomanifold)

Shape analysis is crucial, not only for biomedical applications.

Data has shape, shape has meaning, and meaning drives understanding.
(Paraphrasing Gunnar Carlsson)

Shape analysis for meshes

Shape analysis for meshes

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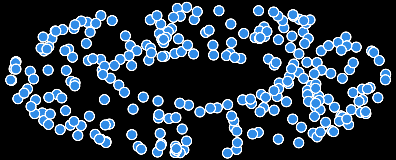
Reality is often messy...



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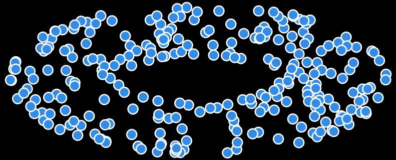
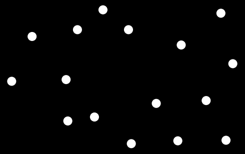


Calculating simplicial complexes from data

Vietoris–Rips complex



$$\mathcal{V}_\epsilon := \{\{x_1, x_2, \ldots\} \mid \operatorname{dist}\left(x_i, x_j\right) \leq \epsilon \text{ for all } i \neq j\}$$

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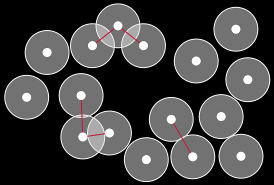

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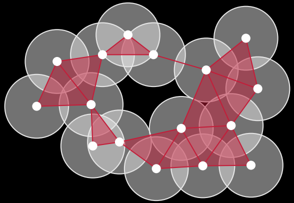

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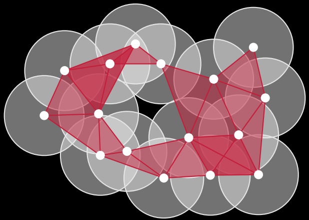

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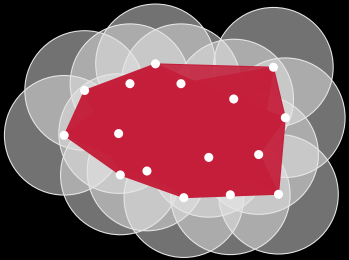

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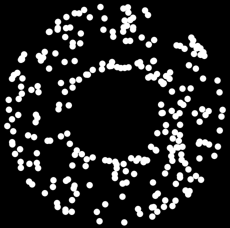
Persistent homology

Calculate simplicial complexes for *every* value of ϵ, while watching how topological features change. Assign each feature a duration, depending on ‘when’ it was created and ‘when’ it was destroyed. Store these features in a *persistence diagram*.



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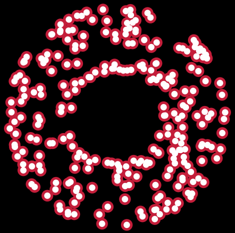

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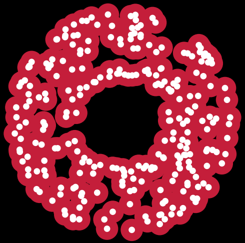

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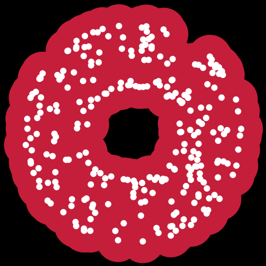

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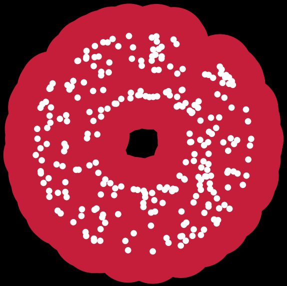

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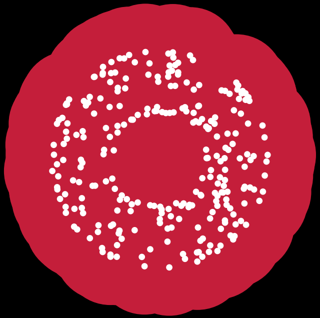

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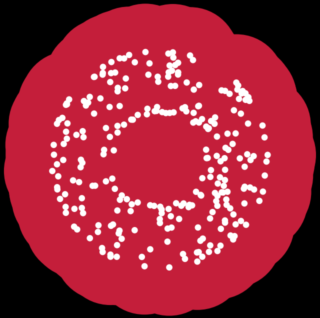

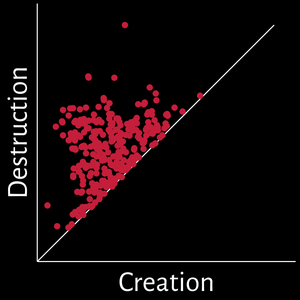

Distances between persistence diagrams

Bottleneck distance

Given two persistence diagrams $\mathscr{D}$ and $\mathscr{D}'$, their *bottleneck* distance is defined as

$$\mathrm{W}_\infty(\mathscr{D}, \mathscr{D}') := \inf_{\eta\colon \mathscr{D} \to \mathscr{D}'} \sup_{x \in \mathscr{D}} \| x - \eta(x) \|_\infty,$$

where $\eta\colon \mathscr{D} \to \mathscr{D}'$ denotes a bijection between the point sets of $\mathscr{D}$ and $\mathscr{D}'$ and $\|\cdot\|_\infty$ refers to the L_∞ distance between two points in $\mathbb{R}^2$.

Wasserstein distance

$$\mathrm{W}_p(\mathscr{D}_1, \mathscr{D}_2) := \left(\inf_{\eta\colon \mathscr{D}_1 \to \mathscr{D}_2} \sum_{x \in \mathscr{D}_1} \| x - \eta(x) \|_\infty^p \right)^{\frac{1}{p}}$$

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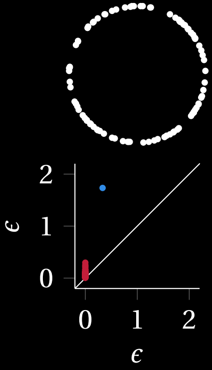
Stability theorem

Robustness to *small-scale* perturbations

Let $\mathbb{M}$ be a triangulable space with continuous tame functions $f, g\colon \mathbb{M} \to \mathbb{R}$. Then the corresponding persistence diagrams satisfy $W_\infty\left(\mathcal{D}_f, \mathcal{D}_g\right) \leq \|f - g\|_\infty$.



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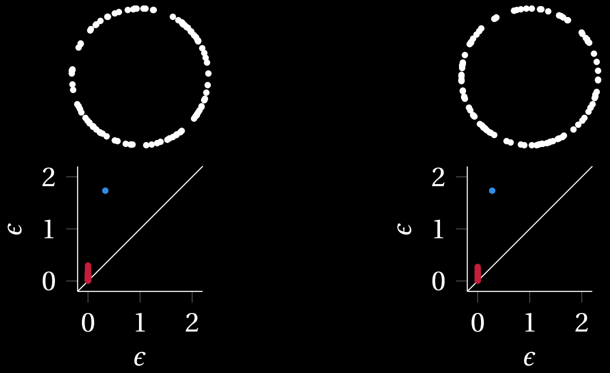

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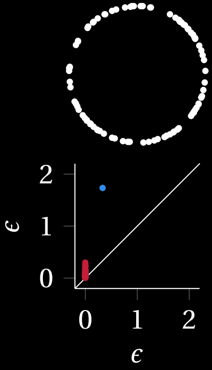

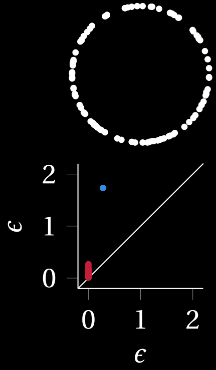

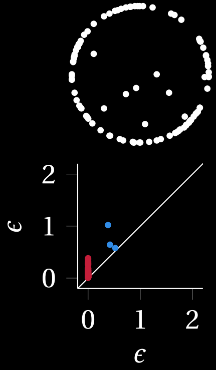

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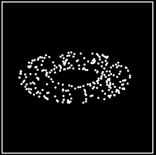
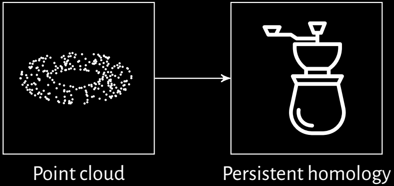
A pipeline for topological machine learning



Point cloud

A pipeline for topological machine learning



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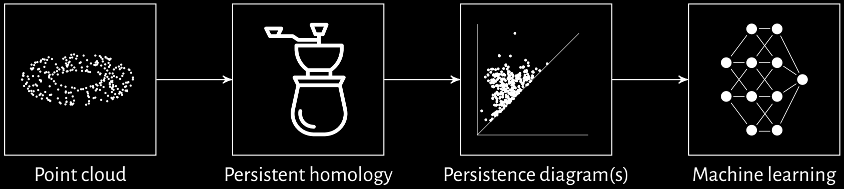

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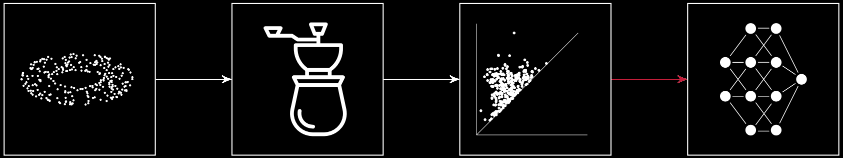
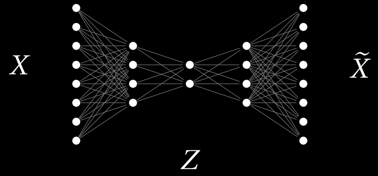


- ✩ A. Poulenard, P. Skraba and M. Ovsjanikov, 'Topological Function Optimization for Continuous Shape Matching', *Computer Graphics Forum*, 2018.
- ✩ M. Moor*, M. Horn*, **B. Rieck**† and K. Borgwardt†, 'Topological Autoencoders', *Proceedings of the 37th International Conference on Machine Learning (ICML)*, 2020, arXiv: `1906.00722 [cs.LG]`.
- ✩ M. Carrière, F. Chazal, M. Glisse, Y. Ike, H. Kannan and Y. Umeda, 'Optimizing persistent homology based functions', *Proceedings of the 38th International Conference on Machine Learning (ICML)*, 2021.

A very brief introduction to some machine learning techniques for representation learning

Autoencoders



Terminology

- $X \in \mathbb{R}^D$: input data
- $Z \in \mathbb{R}^d$: latent representation
- $\tilde{X} \in \mathbb{R}^D$: reconstructed data

Properties

- Typically, $D \gg d$.
- Use loss function $\mathcal{L}\left(X, \tilde{X}\right)$ to measure quality of reconstruction.

Why autoencoders?

- Encoder–decoder architecture (we learn the *identity* function).
- 'Middle' layer serves as *bottleneck* or *latent representation*.
- Latent representations can be used for visualisation in lower dimensions, interpolating between data, clustering, and many other tasks.

A simple autoencoder

- Encoder: linear transformation $\mathbb{R}^D \to \mathbb{R}^2$
- Decoder: linear transformation $\mathbb{R}^2 \to \mathbb{R}^D$
- Loss function: mean squared error, $\mathscr{L}\left(X, \tilde{X}\right) := \|X - \tilde{X}\|_2^2$

A simple autoencoder

Some reconstructions

0 epochs

A simple autoencoder

Some reconstructions

10 epochs

A simple autoencoder

Some reconstructions

20 epochs

A simple autoencoder

Some reconstructions

30 epochs

A simple autoencoder

Some reconstructions

40 epochs

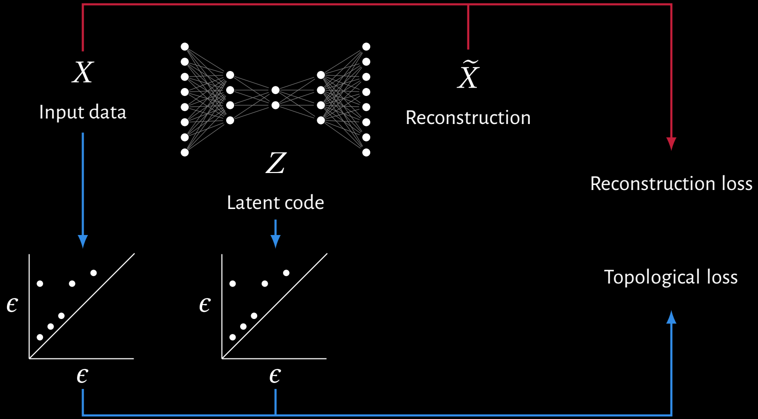
A simple autoencoder

Some reconstructions

50 epochs

Topological autoencoders

Overview



Topological autoencoders

Gradient calculation intuition

Suppose we calculate a Vietoris–Rips complex based on some distances $\mathbf{A}$:

$$\begin{bmatrix} 0 & 1 & 9 & 10 \\ 1 & 0 & 7 & 8 \\ 9 & 7 & 0 & 3 \\ 10 & 8 & 3 & 0 \end{bmatrix}$$

Every point in the persistence diagram can be mapped to *one* distance in the distance matrix! The diagram changes continuously as a function of this matrix.

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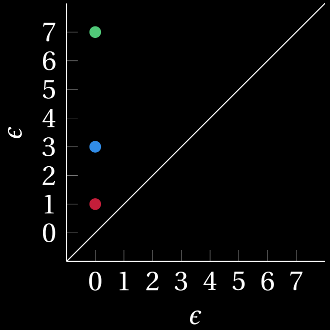

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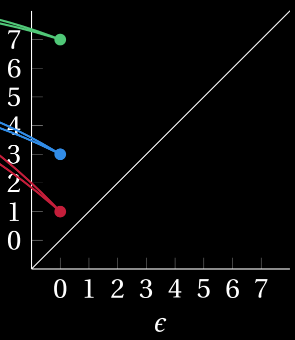

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Topological autoencoders

Loss term

$$\mathscr{L}_t := \mathscr{L}_{\mathscr{X}\to\mathscr{Z}} + \mathscr{L}_{\mathscr{Z}\to\mathscr{X}}$$

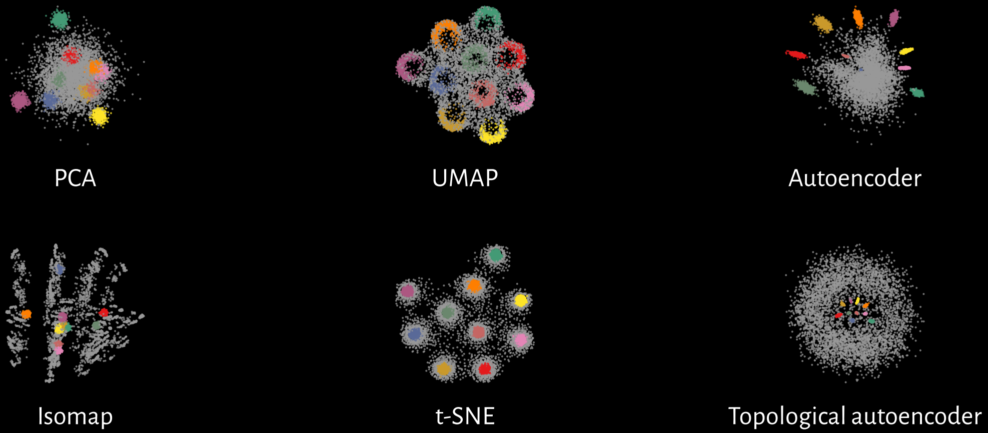
$$\mathscr{L}_{\mathscr{X}\to\mathscr{Z}} := \frac{1}{2}\left\|\mathbf{A}^X\left[\pi^X\right] - \mathbf{A}^Z\left[\pi^X\right]\right\|^2 \qquad \mathscr{L}_{\mathscr{Z}\to\mathscr{X}} := \frac{1}{2}\left\|\mathbf{A}^Z\left[\pi^Z\right] - \mathbf{A}^X\left[\pi^Z\right]\right\|^2$$

- $\mathscr{X}$: input space
- $\mathscr{Z}$: latent space
- $\mathbf{A}^X$: distances in input mini-batch
- $\mathbf{A}^Z$: distances in latent mini-batch
- π^X: persistence pairing of input mini-batch
- π^Z: persistence pairing of latent mini-batch

The loss is *bi-directional*!

Qualitative evaluation

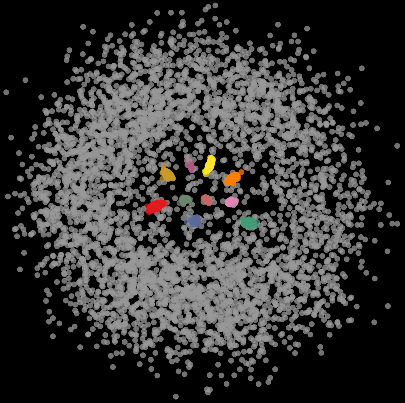
'Spheres' data set



Qualitative evaluation

'Spheres' data set; zooming in...

Autoencoder



Topological autoencoder

A new evaluation metric

Use *distance to a measure* density estimator, i.e.

$$f_\sigma^{\mathscr{X}}(x) := \sum_{y \in \mathscr{X}} \exp\left(-\sigma^{-1} \operatorname{dist}(x, y)^2\right),$$

where dist denotes a metric such as the Euclidean distance. This is well-defined on mini-batches and on the full input data set.

Given σ, we evaluate $\mathrm{KL}_\sigma := \mathrm{KL}\left(f_\sigma^X \parallel f_\sigma^Z\right)$, which measures the similarity between the two density distributions.

Quantitative evaluation

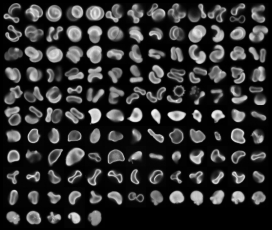
Method	$\mathrm{KL}_{0.01}$	$\mathrm{KL}_{0.1}$	KL_{1}	ℓ-MRRE	ℓ-Cont	ℓ-Trust	ℓ-RMSE	MSE (data)
Isomap	0.181	*0.420*	*0.008 81*	*0.246*	*0.790*	*0.676*	10.4	
PCA	0.332	0.651	0.015 30	0.294	0.747	0.626	11.8	0.9610
t-SNE	*0.152*	0.527	0.012 71	**0.217**	0.773	**0.679**	**8.1**	
UMAP	0.157	0.613	0.016 58	0.250	0.752	0.635	*9.3*	
AE	0.566	0.746	0.016 64	0.349	0.607	0.588	13.3	**0.8155**
TopoAE	**0.085**	**0.326**	**0.006 94**	0.272	**0.822**	0.658	13.5	*0.8681*

Application: Predicting the Shape of Cells

Cell shape prediction

- Use confocal fluorescence microscopy to obtain images of cells.
- What is the 3D shape of a cell?
- Morphological analysis is crucial for certain pathologies!

  When used properly, RBC [red blood cell] morphology can be a ***key tool*** *for laboratory hematology professionals to recommend appropriate clinical and laboratory follow-up and to select the best tests for definitive diagnosis.* *(J. Ford, 'Red blood cell morphology', International Journal of Laboratory Hematology, 2013.)*



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SHAPR

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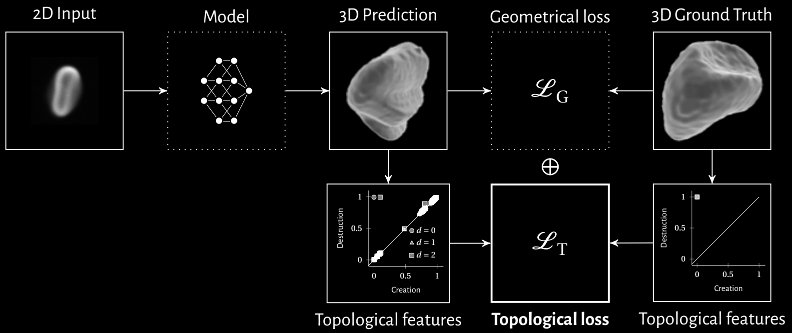
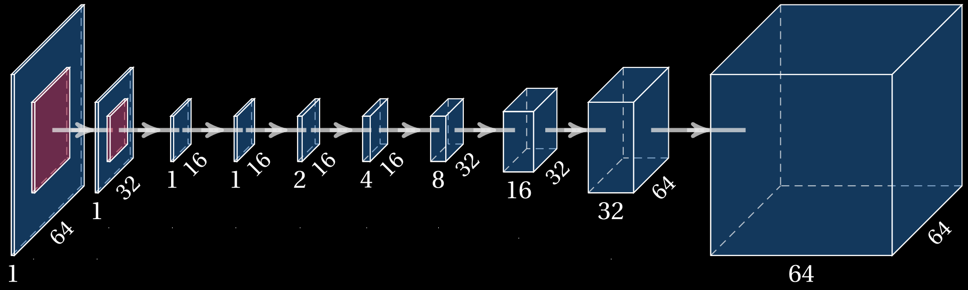


We are trying to solve a complicated *inverse problem*, going from 2D to 3D. This is an ill-defined problem with a large number of potential solutions.

D. J. E. Waibel, S. Atwell, M. Meier, C. Marr and **B. Rieck**, 'Capturing Shape Information with Multi-Scale Topological Loss Terms for 3D Reconstruction', *Medical Image Computing and Computer Assisted Intervention (MICCAI)*, 2022, arXiv: `2203.01703 [cs.CV]`, in press.

SHAPR

Architecture



We are learning a *likelihood function* $f\colon \mathbb{R}^3 \to \mathbb{R}$. Formally, f 'lives' on a voxel grid, assigning each voxel x a value that indicates the likelihood of x being part of the 'true' volume.

SHAPR

Loss function

$$\mathcal{L}_{\mathrm{G}}(f,f') := \frac{2\,\mathcal{L}_{\mathrm{Dice}}(f,f') + \mathcal{L}_{\mathrm{BCE}(f,f')}}{2}$$

$$\mathcal{L}_{\mathrm{Dice}}(f,f') := \frac{2\left|\mathrm{Vol}_f \cap \mathrm{Vol}_{f'}\right|}{\left|\mathrm{Vol}_f\right| + \left|\mathrm{Vol}_{f'}\right|} = \frac{2\mathrm{TP}}{2\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$

Intuition

Compare *geometry* of the resulting volumes on a per-voxel basis. Is the reconstructed volume well-aligned with the ground truth one?

SHAPR goes topological

$$\mathscr{L}_{\mathsf{T}}(f, f', q) := \sum_{i=0}^{d} \mathrm{W}_q\left(\mathscr{D}_f^{(i)}, \mathscr{D}_{f'}^{(i)}\right) + \mathrm{pers}\left(\mathscr{D}_{f'}^{(i)}\right)$$

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Loss components

- Aligning the ground truth likelihood f and the predicted likelihood function f'.
- Reducing the geometrical–topological variation of the predicted likelihood function f'.

SHAPR goes topological

$$\mathcal{L}_{\mathsf{T}}(f, f', q) := \sum_{i=0}^{d} \mathrm{W}_q\left(\mathcal{D}_f^{(i)}, \mathcal{D}_{f'}^{(i)}\right) + \mathrm{pers}\left(\mathcal{D}_{f'}^{(i)}\right)$$

Loss components

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We obtain a *combined loss* by choosing $\lambda \in \mathbb{R}_{>0}$ and calculating:

$$\mathcal{L} := \mathcal{L}_{\mathsf{G}} + \lambda \mathcal{L}_{\mathsf{T}}$$

Quantitative results

		Red blood cell ($n = 825$)		Nuclei ($n = 887$)	
Metric	$\mathscr{L}_T$	Median	$\mu \pm \sigma$	Median	$\mu \pm \sigma$
1-IoU	✗	0.48	0.49 ± 0.12	0.62	0.62 ± 0.11
	✓	**0.46**	**0.47 ± 0.10**	**0.61**	**0.61 ± 0.11**
Volume	✗	0.31	0.35 ± 0.31	0.34	0.48 ± 0.47
	✓	**0.21**	**0.25 ± 0.24**	**0.32**	**0.43 ± 0.42**
Surface area	✗	0.20	0.24 ± 0.20	0.21	0.27 ± 0.25
	✓	**0.13**	**0.18 ± 0.16**	**0.18**	**0.25 ± 0.24**
Surface roughness	✗	0.35	0.36 ± 0.24	**0.17**	**0.18 ± 0.12**
	✓	**0.24**	**0.29 ± 0.22**	0.18	0.19 ± 0.13

Summary

- Topology can provide useful inductive biases for shape reconstruction tasks.
- Persistence diagrams encode geometrical *and* topological properties of data.
- Integration into 'standard' machine learning models is possible!

Publications

- F. Hensel, M. Moor and **B. Rieck**, 'A Survey of Topological Machine Learning Methods', *Frontiers in Artificial Intelligence*, 2021.
- M. Moor*, M. Horn*, **B. Rieck**† and K. Borgwardt†, 'Topological Autoencoders', *Proceedings of the 37th International Conference on Machine Learning (ICML)*, 2020, arXiv: `1906.00722 [cs.LG]`.
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Software

`https://github.com/aidos-lab/pytorch-topological`

❤ Acknowledgements

My co-authors, in particular Carsten, Dominik, Felix, Karsten, Max, and Michael.