

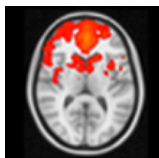
# Vector Representations of Persistence Diagrams

Oleg Kachan  
HSE University

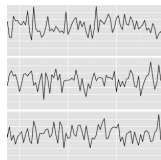
21 March 2024

## Some bits of Topological Data Analysis

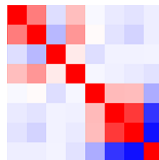
# Weighted Graphs Analysis



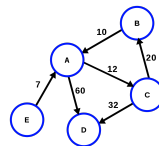
fMRI imaging



time series



correlation matrix



weighted graph

$R_{ij}$

$$r_{ij} \in [-1, 1]$$

$A_{ij}$  - adj. matrix

$$a_{ij} = 1 - |r_{ij}|$$

$$a_{ij} \in [0, 1]$$

# Clique Complex

Let  $G$  be a weighted graph, with adjacency matrix  $\mathbf{A}_{ij}$ , then *clique complex*  $K(G)$  is obtained by:

- ▶ get sparse graph by thresholding adjacency matrix  $\mathbf{A}_{ij} \leq \varepsilon$

$$\mathbf{A}'_{ij} = \begin{cases} a_{ij} & a_{ij} \leq \varepsilon \\ 0 & otherwise \end{cases}$$

- ▶ to every  $k$ -clique of graph with adjacency matrix  $\mathbf{A}'_{ij}$  associate  $(k - 1)$ -simplex in the simplicial complex  $K(G)$

Filtration is induced by weights on graph edges.

# Vietoris-Rips Complex

Consider a finite metric space (point cloud)  $X$ . A *Vietoris-Rips complex* of  $X$  at radius  $\varepsilon$  is defined:

$$VR_{\varepsilon}(X) = \{\sigma \in X \mid d(x, x') \leq 2\varepsilon, \forall (x, x') \in \sigma\}$$

That is  $k + 1$  points form a  $k$ -simplex if they are all pairwise  $2\varepsilon$ -distant.

Filtration is induced by the *distance to a set* function  $d_X(y) := d(x, y)$ , where  $x \in X$  and  $y \in \mathbb{R}^n$  for all  $x$  and  $y$ .

# Cubical Complex

Given a 2D digital image  $X$ , a pixel in an image corresponds to a 2-simplex in a cubical complex  $\text{Cube}(X)$ .

*Cubical complex*<sup>1</sup> is a simplicial complex, i.e. a family of sets closed under inclusion, consisting of simplices which are products of elementary intervals of  $\mathbb{R}$ .

Filtration is induced by a function of pixel intensity.

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1. Kaczynski, Mischaikow, and Mrozek, *Computational Homology*, 2006.

# Persistent Homology as a Mapping

Consider a pair  $(X, f)$ , where  $X$  is a *topological space* and  $f : X \rightarrow \mathbb{R}$  is a *filter function*.

*Persistent homology* is a mapping to the space of *persistence modules* (a collection of vector spaces connected by linear maps) over a field  $\mathbb{F}$ , that quantify the homology of *sublevel sets*  $X_t = \{x \in X \mid f(x) \leq t\}$  of the function  $f$  on  $X$ , where  $t$  takes values from a totally ordered *index set*  $(R, <)$ :

$$(\mathcal{X}, f) \rightarrow H_{\bullet, \mathbb{F}}^f(\mathcal{X})$$

# Decomposition of Persistence Module

A persistent module  $H_k^{f, \mathbb{F}}$  can be decomposed into a direct sum of indecomposable interval modules  $\mathbb{I}_{\mathbb{F}}[b_i, d_i]$ , where  $b_i$  is the *birth* of  $k$ -th homological class and  $d_i$  is its *death*.

$$H_k^{f, \mathbb{F}} \cong \bigoplus_{i=1}^{n=\beta_k} \mathbb{I}_{\mathbb{F}}[b_i, d_i]$$



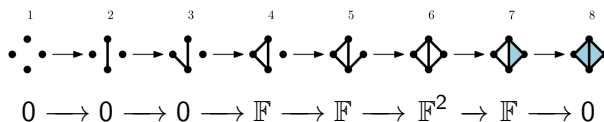
# Interval Module

A subset  $I \subseteq R$  is an *interval* if it is non-empty and  $r \leq s \leq t$  with  $r, t \in I$  implies  $s \in I$ . An *interval module*  $\mathbb{I}_{\mathbb{F}}$  is given by  $V_t = \mathbb{F}$  for  $t \in I$ ,  $V_t = 0$  for  $t \notin I$ , and  $\rho_{ts} = \text{id}$  for  $s, t \in I$  with  $s \leq t$ .

$$\begin{array}{ccccccc}
 0 & \xrightarrow{0} & \dots & \xrightarrow{0} & 0 & \xrightarrow{0} & \mathbb{F} & \xrightarrow{1} & \dots & \xrightarrow{1} & \mathbb{F} & \xrightarrow{0} & 0 & \xrightarrow{0} & \dots & \xrightarrow{0} & 0 \\
 | & & & & & & | & & & & | & & & & & & | \\
 & & & & [1, b-1] & & & & & & [b, d] & & & & & & [d+1, n]
 \end{array}$$

# Example of Decomposition

Filtration <sup>2</sup>:



Decomposition of persistence module:

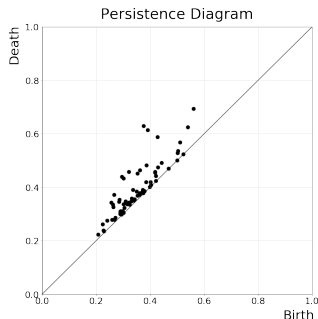
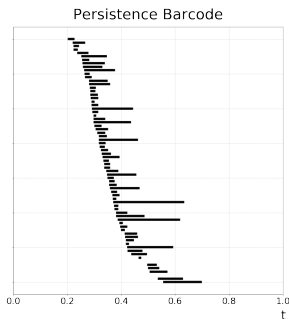
$$\begin{aligned}
 0 &\longrightarrow 0 \longrightarrow 0 \longrightarrow \mathbb{F} \xrightarrow{1} \mathbb{F} \xrightarrow{1} \mathbb{F} \xrightarrow{1} \mathbb{F} \longrightarrow 0 & [c] \\
 0 &\longrightarrow 0 \longrightarrow 0 \longrightarrow 0 \longrightarrow 0 \longrightarrow \mathbb{F} \longrightarrow 0 \longrightarrow 0 & [c']
 \end{aligned}$$

$$\begin{aligned}
 H_1 &\cong \bigoplus_{i=1}^{n=\beta_1} \mathbb{I}[b_i, d_i] \\
 &= \mathbb{I}[4, 7] \oplus \mathbb{I}[6, 6]
 \end{aligned}$$

# Persistence Barcode and Diagram

For each dimension  $k$ , a  $k$ -th *persistence barcode*  $\text{Bar}_k(X)$  is a collection of intervals  $\{\mathbb{I}[b_i, d_i]_k\}$ , describing the decomposition of a persistent module.

A  $k$ -th *persistence diagram*  $\text{Dgm}_k(X)$  is a natural bijection from a collection of intervals to a multiset of points  $\{(b_i, d_i)_k \mid i \in I\}$  on extended Euclidean plane  $\bar{\mathbb{R}}^2 := \{\mathbb{R}^2 \cup +\infty\}$ .



# Machine Learning with Topological Signatures

A persistence diagram being a multiset of points is not suited for machine learning algorithms generally expecting a vector of fixed dimension as an input. Although there are a number of distances<sup>3</sup> and kernels<sup>4</sup> defined on the space of persistence diagrams, we will focus on their finite vector representations.

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3. Edelsbrunner and Harer, *Computational Topology: An Introduction*, 2010.

4. Carriere, Cuturi, and Oudot, "Sliced wasserstein kernel for persistence diagrams," 2017; Le and Yamada, "Persistence fisher kernel: A riemannian manifold kernel for persistence diagrams," 2018.

# Machine Learning with Topological Signatures

Desired properties of representation<sup>5</sup>:

- ▶ is a vector in  $\mathbb{R}^n$ ,
- ▶ is stable with respect to input noise,
- ▶ is efficient to compute,
- ▶ maintains an interpretable connection to the original PD,
- ▶ allows one to adjust the relative importance of points in different regions of the PD

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5. Adams et al., “Persistence images: A stable Vector Representation of Persistent Homology,” 2017.

	Lang.	Algos.	Coeffs.	Filtrations	Gens.
JavaPlex	Java	$H_*$ $H^*$ $Z_*$	$Q, F_p$	VR, W	Yes
Perseus	C++	$H_*$ $Z_*$	$F_2$	VR, Cub	No
Dionysus	C++	$H_*$ $H^*$ $Z_*$	$F_2, F_p$	VR, $\alpha$ , Cech	Yes
PHAT/DIPHA	C++	$H_*$ $H^*$	$F_2$	VR, Cub, f.comp.	No
Gudhi	C++	$H^*$	$F_2$	VR, $\alpha$ , W, Cub	No
Ripser/Flagser	C++	$H^*$	$F_p$	VR, dir. flag	Yes
Eirene	Julia	$H_*$	$F_2$	VR, f.comp.	No
Simplicial.jl	Julia	$H_*$	$F_2$	VR, directed	No

**Table:** Software for computation of persistent homology<sup>6</sup>

*Algorithms:*  $H_*$  - homology,  $H^*$  - cohomology,  $Z_*$  - zigzag homology

*Filtrations:* VR - Vietoris-Rips complex,  $\alpha$  - alpha complex, Cech - Cech complex, W - witness complex, Cube - cubical complex, f.comp. - general complex with user-defined filtration, *Gens.* stands for (co)homology generators

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6. Otter et al., “A roadmap for the computation of persistent homology,” 2017.

# Vector Representations of Persistence Diagrams

# Coordinates

Consider an interval  $(b_i, d_i)_k$  of dimension  $k$ , one can obtain a sets of quantities, summarizing different properties of interval:

*Persistence:*

$$p_i = d_i - b_i$$

*Midlife:*

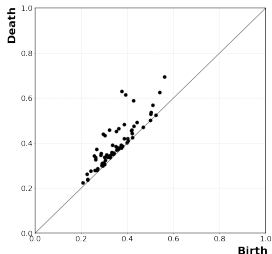
$$ml_i = (b_i + d_i)/2$$

*Mult. life:*

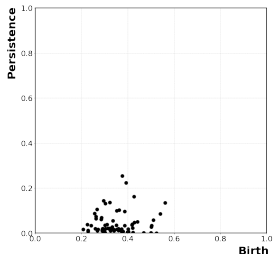
$$mul_i = d_i/b_i$$



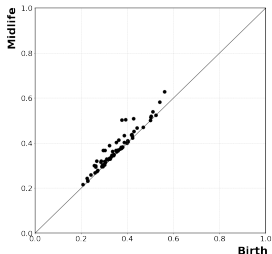
# PDs in Different Coordinates



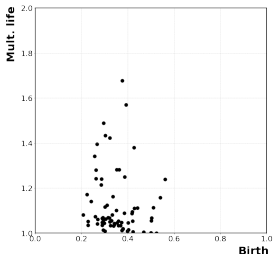
*Original:*  $x = b$ ,  $y = d$



*Persistence:*  $y = d - b$



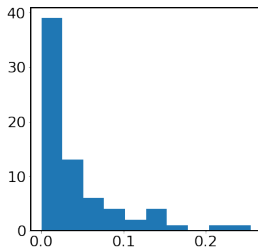
*Midlife:*  $y = (b + d) / 2$



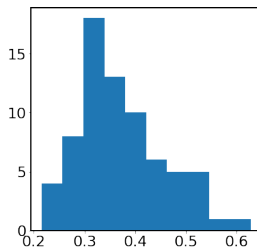
*Mult.life:*  $y = d / b$

# Empirical Distributions

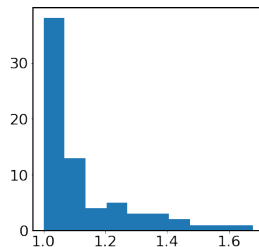
Persistence



Midlife



Mult. life



Persistence (normalized):

$$p_i = d_i - b_i$$
$$\bar{p}_i = \frac{d_i - b_i}{\sum_i (d_i - b_i)}$$

Midlife (normalized):

$$ml_i = (b_i + d_i)/2$$
$$\bar{ml}_i = \frac{b_i + d_i}{\sum_i (b_i + d_i)}$$

Mult. life (normalized):

$$mul_i = d_i/b_i$$
$$\bar{mul}_i = \frac{d_i/b_i}{\sum_i (d_i/b_i)}$$

# Statistics

One can fix a quantity and consider a vector of statistics of its empirical distribution:

- ▶ min, max
- ▶ sum
- ▶ mean
- ▶ standard deviation, skewness, kurtosis
- ▶ median
- ▶ mean absolute deviation, 25-th and 75-th percentiles, interquartile range range
- ▶ entropy

# Statistics

## Entropy

Entropy is highest when the distribution is uniform, and lowest (exactly 0) when it is the Dirac delta function.

$$E_k(\mathbf{x}) = - \sum_{i=1}^n \mathbf{x}_i \log \mathbf{x}_i$$

# PolynomialStatistics

## Polynomials

Different authors consider polynomials<sup>7</sup>:

$$\sum_i b_i(d_i - b_i)$$

$$\sum_i (d_{\max} - d_i)(d_i - b_i)$$

$$\sum_i b_i^2(d_i - b_i)^4$$

$$\sum_i (d_{\max} - d_i)^2(d_i - b_i)^4$$

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7. Adcock, Carlsson, and Carlsson, “The ring of algebraic functions on persistence bar codes,” 2013.

# Tropical sStatistics

## Tropical statistics

and tropical<sup>8</sup> statistics:

$$\max_i d_i$$

$$\max_{i < j} (d_i + d_j)$$

$$\max_{i < j < k} (d_i + d_j + d_k)$$

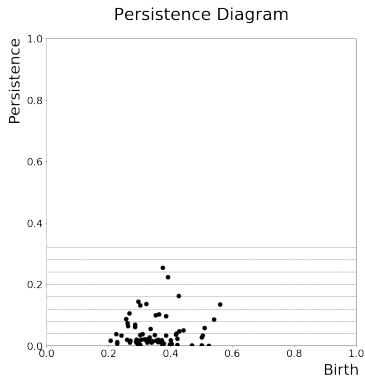
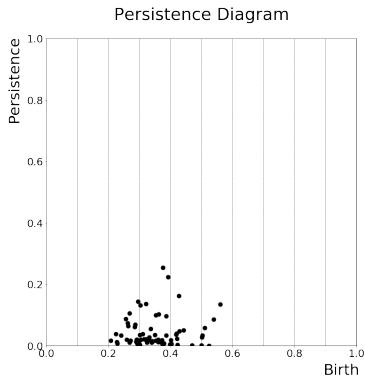
$$\max_{i < j < k < l} (d_i + d_j + d_k + d_l)$$

$$\sum_i d_i$$

$$\sum_i \min(28d_i, b_i)$$

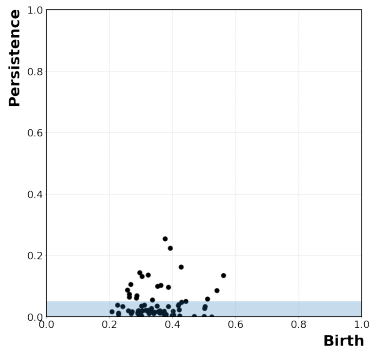
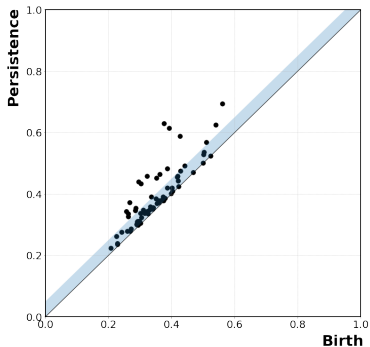
$$\sum_i (\max_i (\min(28d_i, b_i) + d_i) - (\min(28d_i, b_i) + d_i))$$

# Histogram Binning



$$\phi = \min, \max, \text{mean}, \text{median}$$

Set threshold  $\varepsilon$  below which data is considered as noise:



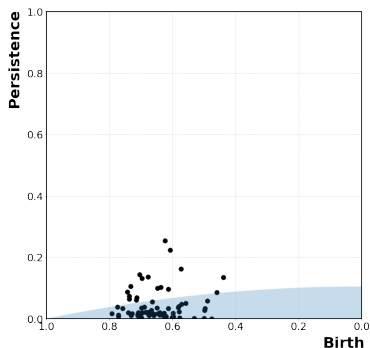
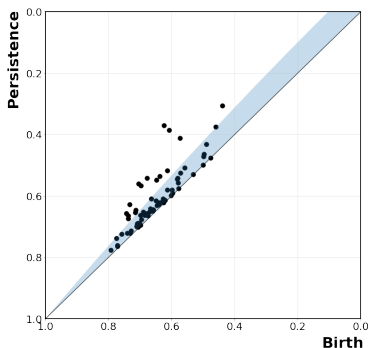


## $\varepsilon$ -Robustness as a Function of $t$

$\varepsilon$ -Robustness can be generalized to depend on  $t$ . For example the error of correlation coefficient  $r$  does depend on its value:

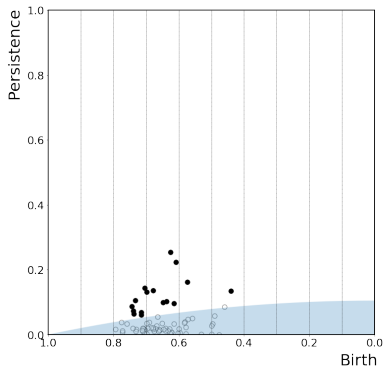
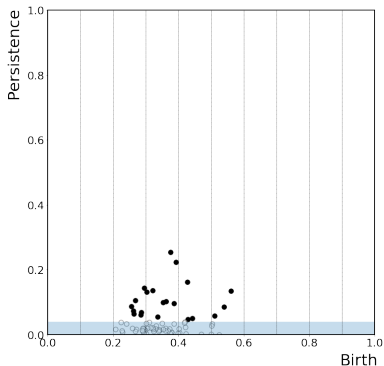
$$\text{error}_r = \frac{r(z(r) + \frac{z_\alpha}{\sqrt{n-3}}) - r(z(r) - \frac{z_\alpha}{\sqrt{n-3}})}{2},$$

$$\text{where } z(r) = \frac{1}{2} \ln \frac{1+r}{1-r} \quad r(z) = -\frac{e^z - e^{-z}}{e^z + e^{-z}} \quad z_\alpha(0.95) = 1.96$$



## $\varepsilon$ -Robust Histogram Binning

For histogram binning, one would consider only statistics of bins of intervals with persistence greater than  $\varepsilon$ :



# Persistence Curves

*Persistent curve*<sup>9</sup> is a function of persistent diagram at time  $t$ , given some aggregation and transform functions:

- ▶ Betti curve
- ▶ Euler characteristic curve
- ▶ Persistence curve
- ▶ Midlife curve
- ▶ Mult.life curve

Entropy as a function of  $t$ :

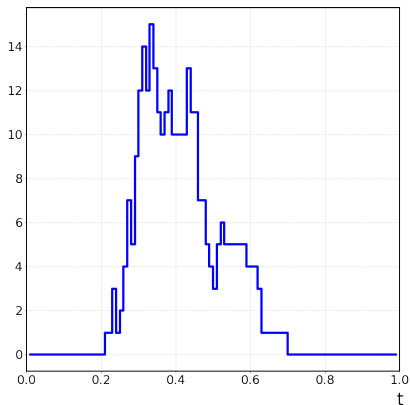
- ▶ Persistence entropy curve
- ▶ Midlife entropy
- ▶ Mult.life entropy

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9. Chung and Lawson, "Persistence Curves: A canonical framework for summarizing persistence diagrams," 2019.

# Betti Curve

$$\beta_k(t) = \#\{(b_i, d_i)_k \mid b_i < t < d_i\}$$

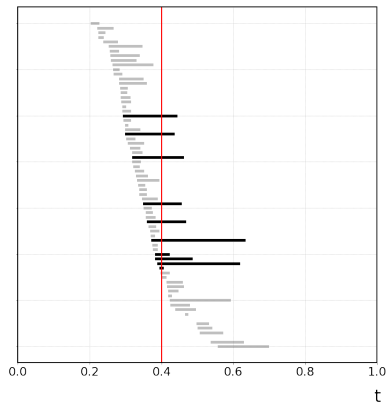


# Betti Curve

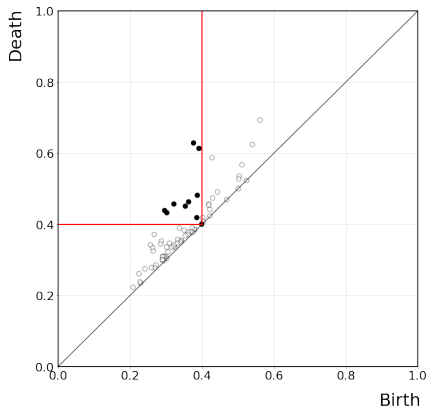
## Connection to Barcode and Diagram

$$\beta_k(t) = \#\{(b_i, d_i)_k \mid b_i < t < d_i\}$$

Persistence Barcode



Persistence Diagram



# Euler Characteristic Curve

$$\chi(t) = \sum_{k=0}^{+\infty} (-1)^k \beta_k(t)$$

# Persistence Curves

## Other persistent curves

$$PC_k^\phi(t) = \left\{ \sum_i \phi(b_i, d_i)_k \mid b_i < t < d_i \right\}$$

Persistence:

$$\phi_P = \frac{d_i - b_i}{\sum_i^n (d_i - b_i)}$$

Midlife:

$$\phi_{P^+} = \frac{b_i + d_i}{\sum_i^n (b_i + d_i)}$$

Mult. life:

$$\phi_{P^*} = \frac{d_i / b_i}{\sum_i^n (d_i / b_i)}$$

# Persistence Entropy

A *persistence entropy*<sup>10</sup>, a statistic measuring the homogeneity of statistics of persistence intervals of dimension  $k$  at time  $t$ .

$$E_k(\mathbf{x})(t) = - \sum_{i=1}^n \mathbf{x}_i \log \mathbf{x}_i$$

$$\mathbf{x}_i(t) = \{ \phi(b_i, d_i)_k \mid b_i \leq t \leq d_i \}$$

Persistence:

$$\phi_p = \frac{d_i - b_i}{\sum_i^n (d_i - b_i)}$$

Midlife:

$$\phi_{p^+} = \frac{b_i + d_i}{\sum_i^n (b_i + d_i)}$$

Mult. life:

$$\phi_{p^*} = \frac{d_i / b_i}{\sum_i^n (d_i / b_i)}$$

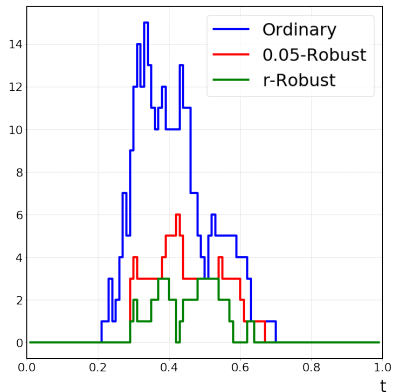
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10. Atienza, Gonzalez-Diaz, and Soriano-Trigueros, "On the Stability of Persistent Entropy and New Summary Functions for TDA," 2019.

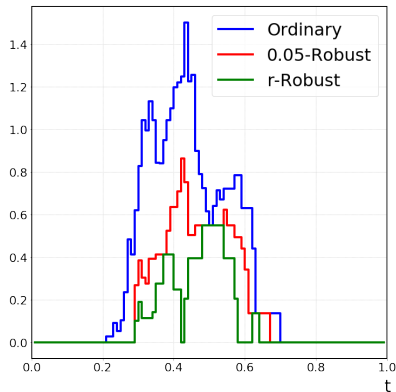


# $\varepsilon$ -Robust Persistence Curves

Betti Curve



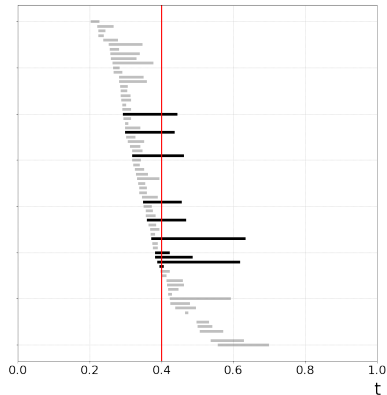
Entropy Curve



# $\varepsilon$ -Robust Persistence Curves

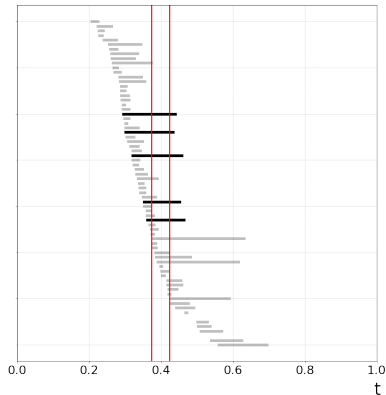
## Connection to Barcodes

Persistence Barcode



$$t = 0.4, \varepsilon = 0$$

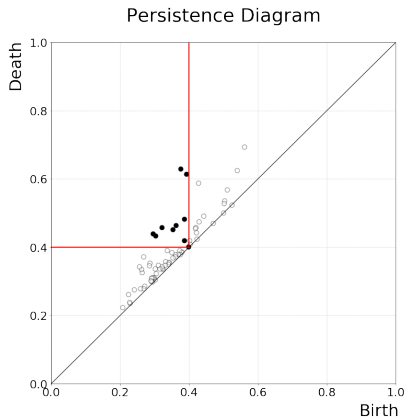
Persistence Barcode



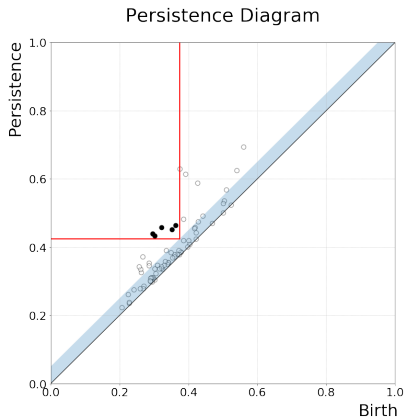
$$t = 0.4, \varepsilon = 0.05$$

# $\varepsilon$ -Robust Persistence Curves

## Connection to Diagrams



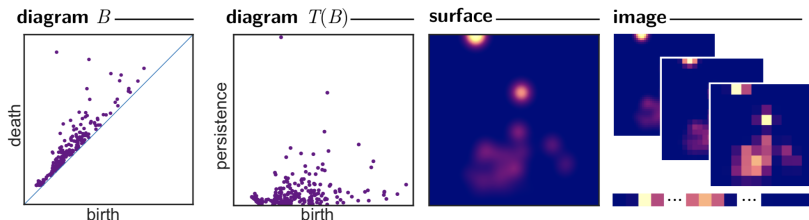
$$t = 0.4, \varepsilon = 0$$



$$t = 0.4, \varepsilon = 0.05$$

# Persistence Image

A *persistence image*<sup>11</sup> views a persistence diagram as a 2-dimensional probability distribution and discretize its kernel density estimation by Gaussian kernel.



That is, at first, PD is transformed by  $T : \mathbb{R}^2 \rightarrow \mathbb{R}^2$  to birth-persistence coordinates:  $T(b, d) = (b, d - b)$ .

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11. Adams et al., "Persistence images: A stable Vector Representation of Persistent Homology," 2017.

## Persistence Image

Second, a smooth persistence surface  $\rho_{PD_k} : \mathbb{R}^2 \rightarrow \mathbb{R}_+$  of  $T(PD_k)$  defined as:

$$\rho(PD_k) = \sum_{u \in T(PD_k)} f(u) g_u(z)$$

is computed, where  $f(u) : \mathbb{R} \rightarrow \mathbb{R}$  is a *weighting function*, weighting points with small persistence less:

$$w_b(t) = \begin{cases} 0, & \text{if } t \leq 0, \\ t/p_{max}, & \text{if } 0 < t < p_{max}, \\ 1, & \text{if } t \geq p_{max} \end{cases}$$

## Persistence Image

$$g_u(z) = \frac{1}{2\pi\sigma} \exp -[(z_x - \mu_x)^2 + (z_y - \mu_y)^2]/2\sigma^2$$

is a Gaussian kernel. Third, a discretization over a grid of desired size is obtained by integration:

$$I(\rho_{PD_k}) = \int \int \rho_{PD_k}(z_x, z_y) dz_x dz_y.$$

# Persistence Landscape

A persistence landscape<sup>11</sup> is an embedding of a persistence diagram in a space of continuous functions  $L^2$ . That is, for each birth-death point  $p = b_i, d_i \in PD_k$ , a continuous piecewise linear basis function  $\Lambda_p(\varepsilon)$  is:

$$\Lambda_p(t) = \begin{cases} t - b, & t \in [b, \frac{b+d}{2}] \\ d - t, & t \in (\frac{b+d}{2}, d] \\ 0, & \text{otherwise} \end{cases}$$

Given a set of basis functions of a points, a *persistence landscape* is defined  $\lambda_{PD_k}(t) = \text{kmax}_{p \in PD_k} \Lambda_p(t)$ , where  $t \in [0, T]$ ,  $k \in \mathbb{N}$  and kmax is the  $k$ -th largest value in the set.

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11. Bubenik and Dłotko, "A Persistence Landscapes Toolbox for Topological Statistics," 2017.

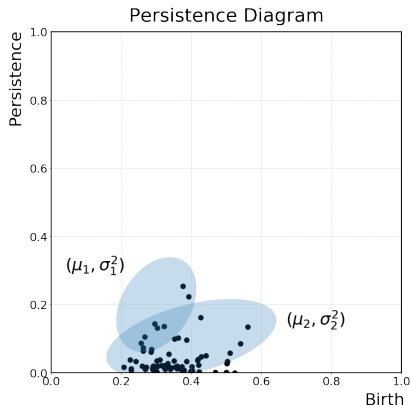
Learning task-specific vector representations



# Learning with Topological Signatures

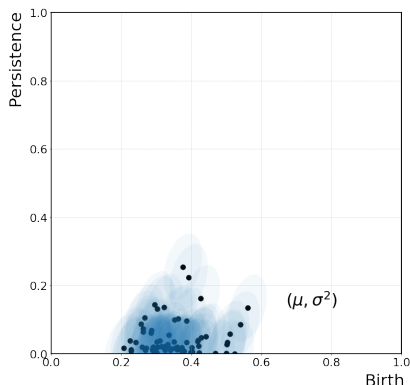
The first approach to learn vector representation of persistence diagram<sup>12</sup> evaluates the points against mixture of Gaussians with parameters  $(\mu, \sigma)$  that are learned:

$$s_{\mu, \sigma^2} = \exp \sigma_b^2(-b - \mu_b) - \sigma_d^2(-d - \mu_d)$$



# Learning Representations of Persistence Barcodes

In a recent work authors<sup>13</sup> further suggest three possible functions  $\phi : \mathbb{R}^2 \rightarrow \mathbb{R}$ , which roughly correspond to *Gaussian*, *spike* and *cone* functions centered on the diagram points.



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13. Hofer, Kwitt, and Niethammer, “Learning representations of persistence barcodes,” 2019.

# PersLay: A Neural Network Layer for Persistence Diagrams

$$\text{PersLay}(Dg) := \text{op}(\{w(p) \cdot \phi(p)\}_{p \in Dg})$$

where:

- ▶  $\text{op}$  is any *permutation invariant operation* (such as minimum, maximum, sum,  $k$ -th largest value),
- ▶  $w : \mathbb{R}^2 \rightarrow \mathbb{R}$  is a *weight function* for the persistence diagram points (can be linear, Gaussian mixture and grid), and
- ▶  $\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^n$  is a *point transformation function*, mapping each point  $(b_i, d_i)$  of a persistence diagram to a vector.

$W_{\theta_1}$  and  $\phi_{\theta_2}$  are chosen from a class of differentiable functions, and parameters  $\theta_1, \theta_2$  are optimized by backpropagation.<sup>14</sup>

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14. Carriere et al., “PersLay: A Neural Network Layer for Persistence Diagrams and New Graph Topological Signatures,” 2019.

The *triangle point transformation*  $\phi_{\Lambda} : \mathbb{R}^2 \rightarrow \mathbb{R}^n$ ,  
 $p \mapsto [\Lambda_p(t_1), \dots, \Lambda_p(t_n)]^T$ , where the triangle function  $\Lambda_p$   
 associated to a point  $p = (x, y) \in \mathbb{R}^2$  is  
 $\Lambda_p : t \mapsto \max\{0, y - |t - x|\}$ , with  $q \in \mathbb{N}$  and  $t_1, \dots, t_n \in \mathbb{R}$ .

The *indicator transformation*  $\phi_{\mathbb{I}} : \mathbb{R}^2 \rightarrow \mathbb{R}^n$ ,  
 $p \mapsto [\mathbb{I}_p(t_1), \dots, \mathbb{I}_p(t_n)]^T$ , where the indicator function  $\mathbb{I}_p$   
 associated to a point  $p = (x, y) \in \mathbb{R}^2$  is  $\mathbb{I}_p : t \mapsto \mathbb{I}\{x < t < y\}$ ,  
 with  $q \in \mathbb{N}$  and  $t_1, \dots, t_n \in \mathbb{R}$ .

The *Gaussian point transformation*  $\phi_{\Gamma} : \mathbb{R}^2 \rightarrow \mathbb{R}^n$ ,  
 $p \mapsto [\Gamma_p(t_1), \dots, \Gamma_p(t_n)]^T$ , where the Gaussian function  $\Gamma_p$   
 associated to a point  $p = (x, y) \in \mathbb{R}^2$  is  
 $\Gamma_p : t \mapsto \exp(-\|p - t\|_2^2 / 2\sigma^2)$  for a given  $\sigma > 0$ ,  $q \in \mathbb{N}$  and  
 $t_1, \dots, t_n \in \mathbb{R}^2$ .

The *persistence landscape*:  $\phi = \phi_\Lambda$  with samples  $t_1, \dots, t_n \in \mathbb{R}$ ,  $\text{op} = k\text{-th largest value}$ ,  $w = 1$  (a constant weight function).

The *Betti curve*:  $\phi = \phi_{\mathbb{I}}$  with samples  $t_1, \dots, t_n \in \mathbb{R}$ ,  $\text{op} = \text{sum}$ ,  $w = 1$  (a constant weight function).

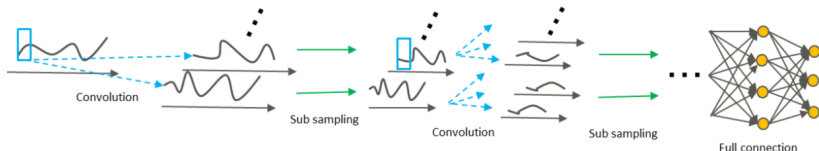
The *persistence image*:  $\phi = \phi_\Gamma$  with samples  $t_1, \dots, t_n \in \mathbb{R}^2$ ,  $\text{op} = \text{sum}$ , arbitrary weight function  $w$ .

	PD	PERSLAY
REDDIT5K	55.0	55.6( $\pm 0.3$ )
REDDIT12K	44.2	47.7( $\pm 0.2$ )
COLLAB	71.6	76.4( $\pm 0.4$ )
IMDB-B	68.8	71.2( $\pm 0.7$ )
IMDB-M	48.2	48.8( $\pm 0.6$ )
COX2 *	81.5	80.9( $\pm 1.0$ )
DHFR *	78.2	80.3( $\pm 0.8$ )
MUTAG *	85.1	89.8( $\pm 0.9$ )
PROTEINS *	72.2	74.8( $\pm 0.3$ )
NCI1 *	72.3	73.5( $\pm 0.3$ )
NCI109 *	67.0	69.5( $\pm 0.3$ )

**Table:** Classification performance

# 1-dimensional CNN

Umeda<sup>15</sup> considers 1-d CNN on Betti curves:



Datasets	Gyro sensor	EEG dataset	EMG dataset
	Accuracy		
method\validation	Leave one subject out [%]	10-fold[%]	Leave one subject out[%]
SVM+Betti sequence	$63.5 \pm 11.3$	$66.7 \pm 5.6$	$49.6 \pm 18.2$
connected input 1-CNN+Betti sequence	$79.8 \pm 5.0$	$75.38 \pm 5.7$	$74.4 \pm 10.6$
parallel 1-CNN+Betti sequence	$86.1 \pm 7.2$	-	$76.4 \pm 7.2$

Table: Classification performance

# Deep Sets

Deep Sets<sup>16</sup> model  $f : (\mathbb{R}^3)^N \rightarrow \mathbb{R}^d$  consists of

$$f(\{x_1, \dots, x_N\}) = \rho \left( \sum_{i=1}^n \phi_{\theta}(x_i) \right), \quad (1)$$

- ▶ a MLP encoder  $\phi_{\theta} : \mathbb{R}^3 \rightarrow \mathbb{R}^D$  mapping each diagram point  $x_i = (b_i, d_i, h_i)$ , with parameters  $\theta$  shared between points,
- ▶ a permutation invariant pooling operation  $(\cdot) : (\mathbb{R}^D)^N \rightarrow \mathbb{R}^D$  to obtain a representation of a diagram at whole (particularly for Deep Sets - sum pooling), and
- ▶ a decoder  $\rho : \mathbb{R}^D \rightarrow \mathbb{R}^d$  which further transforms the diagram representation.



# Transformers

Deep sets transforms individual points  $\mathbf{x}_i$  in the diagram  $\mathbf{X}$  independently via MLP. Self-attention transformer<sup>17</sup> makes each point  $\mathbf{x}_i$  a nonlinear weighted combination of every point in the diagram

$$\Phi_{\mathbf{W}_q, \mathbf{W}_k, \mathbf{W}_v}^{ATTN}(\{x_1, \dots, x_n\}) = \sigma \left( \frac{(\mathbf{W}_q \mathbf{X})(\mathbf{W}_k \mathbf{X})^T}{\sqrt{D}} \right) \mathbf{W}_v \mathbf{X}, \quad (2)$$

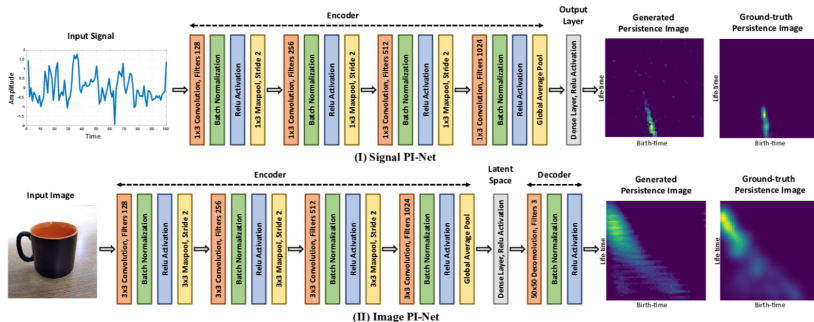
where  $\Phi_{ATTN} : (\mathbb{R}^3)^N \rightarrow (\mathbb{R}^D)^N$ .

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17. Reiauer, Caorsi, and Berkouk, "Persformer: A transformer architecture for topological machine learning," 2021.

## Learning the persistent homology map

PI-Net<sup>18</sup> learns persistence images directly from data, either 2D images or multivariate time series, after being trained on ground-truth persistence images of PDs extracted by the persistent homology algorithm.



18. Som et al., “PI-Net: A Deep Learning Approach to Extract Topological Persistence Images,” 2019.

## PI-Net

Concatenating features obtained from AlexNet and Network in Network with ground-truth and learned topological features results an improvement in image classification on CIFAR10 and SVHN datasets.

Method	CIFAR10		SVHN	
	Mean $\pm$ SD	p-Value	Mean $\pm$ SD	p-Value
Alexnet	80.49 $\pm$ 0.30	-	93.08 $\pm$ 0.17	-
Alexnet + PI	80.52 $\pm$ 0.38	0.8932	93.72 $\pm$ 0.10	0.0001
<b>Alexnet + Image PI-Net</b>	<b>81.25<math>\pm</math>0.49</b>	0.0182	<b>93.83<math>\pm</math>0.11</b>	<0.0001
<b>Alexnet + Image PI-Net FA</b>	<b>81.23<math>\pm</math>0.42</b>	0.0125	<b>93.92<math>\pm</math>0.13</b>	<0.0001
<b>Alexnet + Image PI-Net FS</b>	<b>81.80<math>\pm</math>0.24</b>	0.0001	<b>93.94<math>\pm</math>0.13</b>	<0.0001
NIN	84.93 $\pm$ 0.13	-	95.83 $\pm$ 0.07	-
NIN + PI	85.29 $\pm$ 0.30	0.0392	95.75 $\pm$ 0.08	0.1309
<b>NIN + Image PI-Net</b>	<b>86.61<math>\pm</math>0.19</b>	<0.0001	<b>96.04<math>\pm</math>0.04</b>	0.0004
<b>NIN + Image PI-Net FA</b>	<b>86.62<math>\pm</math>0.39</b>	<0.0001	<b>95.97<math>\pm</math>0.05</b>	0.0066
<b>NIN + Image PI-Net FS</b>	<b>86.61<math>\pm</math>0.40</b>	<0.0001	<b>96.06<math>\pm</math>0.04</b>	0.0002

Table: Classification performance

Authors report a decrease up of two orders of magnitude in the computation time and conclude that it makes real-time TDA applications possible.

Method	Mean $\pm$ SD ( $10^{-3}$ seconds)	
	CIFAR10 (50,000 images)	SVHN (73,257 images)
Conventional TDA - CPU	146.50 $\pm$ 3.83	105.03 $\pm$ 3.57
<b>Image PI-Net - GPU</b>	<b>2.52<math>\pm</math>0.02</b>	<b>2.19<math>\pm</math>0.02</b>

Table: Computation speed

Another paper on learning the persistent homology map<sup>19</sup>.

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19. Montúfar, Otter, and Wang, “Can neural networks learn persistent homology features?,” 2020.

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