Vector Representations of Persistence Diagrams

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Some bits of Topological Data Analysis

Weighted Graphs Analysis







time series



correlation matrix

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



weighted graph

$$oldsymbol{A}_{ij}$$
 - 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:

lacktriangle get sparse graph by thresholding adjacency matrix ${f A}_{ij} \leq arepsilon$

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

▶ 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 ε is defined:

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

That is k+1 points form a k-simplex if they are all pairwise 2ε -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 $\mathrm{Cube}(X)$.

Cubical complex¹ 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.

Persistent Homology as a Mapping

Consider a pair (X, f), where X is a *topological space* and $f: X \to \mathbb{R}$ 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,<):

$$(\mathcal{X},f) \to H^f_{\bullet;\mathbb{F}}(\mathcal{X})$$

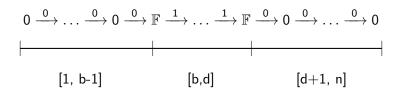
Decomposition of Persistence Module

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*.

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

Interval Module

A subset $I \subseteq R$ is an *interval* if it is non-empty and $r \le s \le t$ 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 $\rho_{ts} = \operatorname{id}$ for $s, t \in I$ with $s \le t$.



Example of Decomposition

Filtration ²:

Decomposition of persistence module:

$$0 \longrightarrow 0 \longrightarrow 0 \longrightarrow \mathbb{F} \stackrel{1}{\longrightarrow} \mathbb{F} \stackrel{1}{\longrightarrow} \mathbb{F} \stackrel{1}{\longrightarrow} \mathbb{F} \longrightarrow 0 \quad [c]$$
$$0 \longrightarrow 0 \longrightarrow 0 \longrightarrow 0 \longrightarrow 0 \longrightarrow \mathbb{F} \longrightarrow 0 \longrightarrow 0 \quad [c']$$

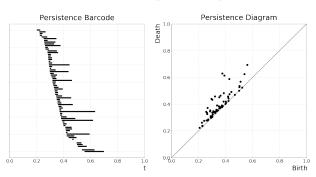
$$H_{1} \cong \bigoplus_{i=1}^{n=\beta_{1}} \mathbb{I}[b_{i}, d_{i}]$$
$$= \mathbb{I}[4, 7] \oplus \mathbb{I}[6, 6]$$

^{2.} Image courtesy of Clement Maria

Persistence Barcode and Diagram

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

A k-th persistence diagram $Dgm_k(X)$ 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 $\mathbb{\bar{R}}^2 := \{\mathbb{R}^2 \cup +\infty\}$.



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 distances³ and kernels⁴ defined on the space of persistence diagrams, we will focus on their finite vector representations.

^{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 representation⁵:

- \triangleright 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

^{5.} Adams et al., "Persistence images: A stable Vector Representation of Persistent Homology," 2017.

Software

	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, α , Cech	Yes
PHAT/DIPHA	$C{+}{+}$	H_* H^*	F_2	VR, Cub, f.comp.	No
Gudhi	$C{+}{+}$	H*	F_2	VR , α , 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 homology⁶

Algorithms: H_* - homology, H^* - cohomology, Z_* - zigzag homology Filtrations: VR - Vietoris-Rips complex, α - 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

^{6.} Otter et al., "A roadmap for the computation of persistent homology," 2017.

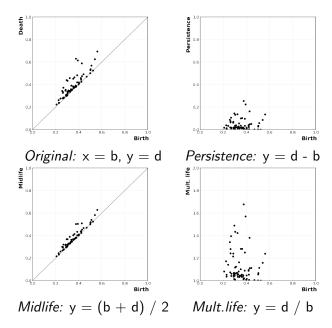
Vector Representations of Persistence Diagrams

Coordinates

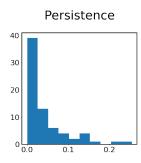
Consider an interval $(b_i, d_i)_k$ of dimension k, one can obtain a sets of quantities, summarizing different properties of interval:

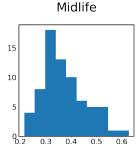
Persistence:	Midlife:	Mult. life:
$p_i = d_i - b_i$	$mI_i = (b_i + d_i)/2$	$mul_i = d_i/b_i$

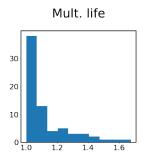
PDs in Different Coordinates



Empirical Distributions







Persistence (normalized):

$$p_i = d_i - b_i$$

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

Midlife (normalized):

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

 $\bar{m}I_i = \frac{b_i + d_i}{\sum_i (b_i + d_i)}$

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 polynomials⁷:

$$\sum_{i} b_{i}(d_{i} - b_{i})$$
 $\sum_{i} (d_{max} - d_{i})(d_{i} - b_{i})$
 $\sum_{i} b_{i}^{2}(d_{i} - b_{i})^{4}$
 $\sum_{i} (d_{max} - d_{i})^{2}(d_{i} - b_{i})^{4}$

^{7.} Adcock, Carlsson, and Carlsson, "The ring of algebraic functions on persistence bar codes," 2013.

Tropical sStatistics

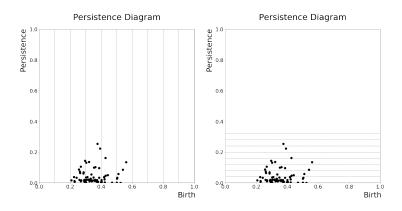
Tropical statistics

and tropical⁸ statistics:

```
\max_{i} d_i
\max_{i < j} (d_i + d_j)
\max_{i < j < k} (d_i + d_j + d_k)
\max_{i < i < k < l} (d_i + d_j + d_k + d_l)
\sum_{i} \min(28d_i, b_i)
\sum (\max_{i} (\min(28d_{i}, b_{i}) + d_{i}) - (\min(28d_{i}, b_{i}) + d_{i}))
```

^{8.} Kališnik, "Tropical coordinates on the space of persistence barcodes," 2019. 22/56

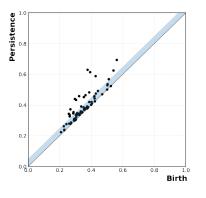
Histogram Binning

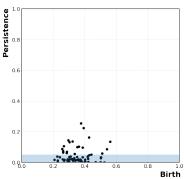


 $\phi=\,$ min, max, mean, median

ε -Robustness

Set threshold ε below which data is considered as noise:



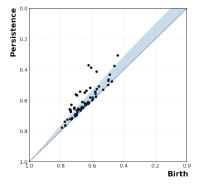


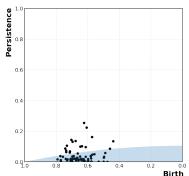
ε -Robustness as a Function of t

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

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

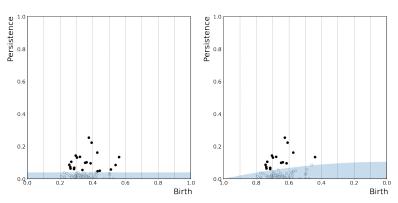
where
$$z(r) = \frac{1}{2} \ln \frac{1+r}{1-r}$$
 $r(z) = -\frac{e^z - e^{-z}}{e^z + e^{-z}}$ $z_{\alpha}(0.95) = 1.96$





ε -Robust Histogram Binning

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



Persistence Curves

Persistent curve⁹ is a function of persistent diagram at time t, given some aggregation and transform functions:

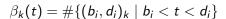
- Betti curve
- ► Euler characteristic curve
- Persistence curve
- Midlife curve
- Mult.life curve

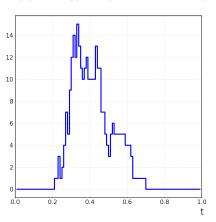
Entropy as a function of t:

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

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

Betti Curve

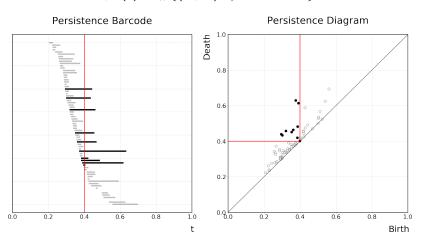




Betti Curve

Connection to Barcode and Diagram

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



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:

Midlife:

Mult. life:

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

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

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

Persistence Entropy

A persistence entropy¹⁰, a statistic measuring the homogeneity of statistics of persistence intervals of dimension k at time t.

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

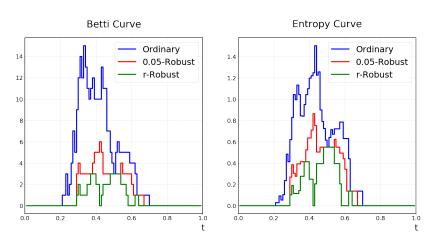
$$\mathbf{x}_i(t) = \big\{ \phi(b_i, d_i)_k \mid b_i \leq t \leq d_i \big\}$$

Persistence: Midlife: Mult. life:

$$\phi_p = \frac{d_i - b_i}{\sum_{i=1}^{n} (d_i - b_i)}$$
 $\phi_{p^+} = \frac{b_i + d_i}{\sum_{i=1}^{n} (b_i + d_i)}$ $\phi_{p^*} = \frac{d_i / b_i}{\sum_{i=1}^{n} (d_i / b_i)}$

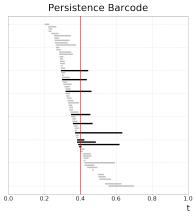
^{10.} Atienza, Gonzalez-Diaz, and Soriano-Trigueros, "On the Stability of Persistent Entropy and New Summary Functions for TDA," 2019.

ε -Robust Persistence Curves

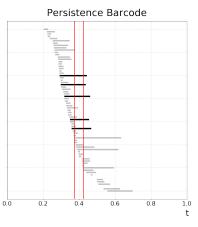


ε -Robust Persistence Curves

Connection to Barcodes

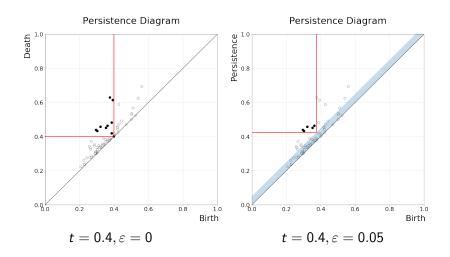


t = 0.4, ε = 0



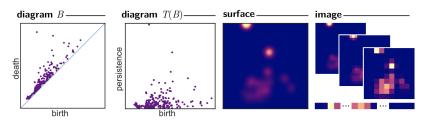
ε -Robust Persistence Curves

Connection to Diagrams



Persistence Image

A persistence image¹¹ 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 $T : \mathbb{R}^2 \to \mathbb{R}^2$ to birth-persistence coordinates: T(b,d) = (b,d-b).

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

Persistence Image

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

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

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

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

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 landscape¹¹ 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:

$$\Lambda_p(t) = egin{cases} t-b, & t \in [b,rac{b+d}{2}] \ d-t, & t \in (rac{b+d}{2},d] \ 0, & ext{otherwise} \end{cases}$$

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

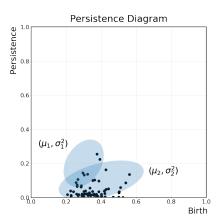
^{11.} Bubenik and Dłotko, "A Persistence Landscapes Toolbox for Topological Statistics," 2017.

Learning task-specific vector representations

Learning with Topological Signatures

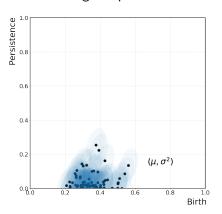
The first approach to learn vector representation of persistence diagram¹² evaluates the points against mixture of Gaussians with parameters (μ, σ) that are learned:

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



Learning Represenations of Persistence Barcodes

In a recent work authors¹³ further suggest three possible functions $\phi: \mathbb{R}^2 \to \mathbb{R}$, which roughly correspond to *Gaussian*, *spike* and *cone* functions centered on the diagram points.



^{13.} Hofer, Kwitt, and Niethammer, "Learning representations of persistence barcodes," 2019.

PersLay: A Neural Network Layer for Persistence Diagrams

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

where:

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

 W_{θ_1} and ϕ_{θ_2} are chosen from a class of differentiable functions, and parameters θ_1 , θ_2 are optimized by backpropagation.¹⁴

^{14.} Carriere et al., "PersLay: A Neural Network Layer for Persistence Diagrams and New Graph Topological Signatures," 2019.

PersLay

Implemented point transformation functions

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

PersLay

Connections to popular vectorizations

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

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

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

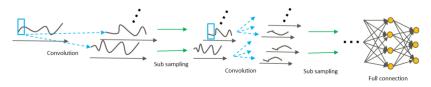
PersLay Results

	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

Umeda¹⁵ 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 ± 11.3	66.7 ± 5.6	49.6 ± 18.2	
connected input 1-CNN+Betti sequence	79.8 ± 5.0	75.38 ± 5.7	74.4 ± 10.6	
parallel 1-CNN+Betti sequence	86.1 ± 7.2	-	76.4 ± 7.2	

Table: Classification performance

Deep Sets

Deep Sets¹⁶ model $f:(\mathbb{R}^3)^N \to \mathbb{R}^d$ consists of

$$f(\lbrace x_1,\ldots,x_N\rbrace) = \rho\left(\sum_{i=1}^n \phi_\theta(x_i)\right), \qquad (1)$$

- ▶ a MLP encoder $\phi_{\theta} : \mathbb{R}^3 \to \mathbb{R}^D$ mapping each diagram point $x_i = (b_i, d_i, h_i)$, with parameters θ shared between points,
- ▶ a permutation invariant pooling operation (\cdot) : $(\mathbb{R}^D)^N \to \mathbb{R}^D$ to obtain a representation of a diagram at whole (particularly for Deep Sets sum pooling), and
- ▶ a decoder $\rho: \mathbb{R}^D \to \mathbb{R}^d$ 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 transformer¹⁷ makes each point \mathbf{x}_i a nonlinear weighted combination of every point in the diagram

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

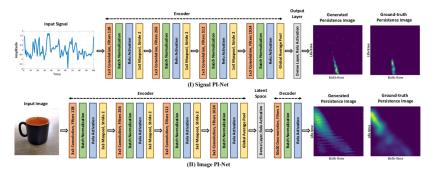
where $\Phi_{ATTN}: (\mathbb{R}^3)^N \to (\mathbb{R}^D)^N$.

^{17.} Reinauer, Caorsi, and Berkouk, "Persformer: A transformer architecture for topological machine learning," 2021.

Learning the persistent homology map

PI-Net

PI-Net¹⁸ 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	
Wiethou	Mean±SD	p-Value	Mean±SD	p-Value
Alexnet	80.49±0.30	-	93.08±0.17	-
Alexnet + PI	80.52±0.38	0.8932	93.72±0.10	0.0001
Alexnet + Image PI-Net	81.25±0.49	0.0182	93.83±0.11	< 0.0001
Alexnet + Image PI-Net FA	81.23±0.42	0.0125	93.92±0.13	< 0.0001
Alexnet + Image PI-Net FS	81.80±0.24	0.0001	93.94±0.13	< 0.0001
NIN	84.93±0.13	-	95.83±0.07	-
NIN + PI	85.29 ± 0.30	0.0392	95.75±0.08	0.1309
NIN + Image PI-Net	86.61±0.19	< 0.0001	96.04±0.04	0.0004
NIN + Image PI-Net FA	86.62±0.39	< 0.0001	95.97±0.05	0.0066
NIN + Image PI-Net FS	86.61±0.40	< 0.0001	96.06±0.04	0.0002

Table: Classification performance

PI-Net

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

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

Table: Computation speed

Another paper on learning the persistent homology map ¹⁹.

^{19.} Montúfar, Otter, and Wang, "Can neural networks learn persistent homology features?," 2020.

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