### Learning with Persistence Diagrams

# Persistence diagrams as descriptors for data



Pros:

- strong invariance and stability:  $d_p(\operatorname{dgm} X, \operatorname{dgm} Y) \leq \operatorname{cst} d_{\operatorname{GH}}(X, Y)$
- information of a different nature
- flexible and versatile

Cons:

- slow to compare
- space of diagrams is not linear
- positive intrinsic curvature

## Persistence diagrams as descriptors for data



A solution: map diagrams to Hilbert space and use kernel trick



# Reproducing Kernel Hilbert Space

**Def:** Let  $\mathcal{H} \subset \mathbb{R}^X$  Hilbert, with inner product  $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ Then,  $\mathcal{H}$  is a **RKHS** on X if  $\exists \Phi : X \to \mathcal{H}$  s.t.:  $\forall x \in X, \forall f \in \mathcal{H}, f(x) = \langle f, \Phi(x) \rangle_{\mathcal{H}}$  reproducing property

Terminology:

- feature space  $\mathcal H_{\text{\rm J}}$  feature map  $\Phi$
- feature vector  $\Phi(x)$
- kernel  $k = \langle \Phi(\cdot), \Phi(\cdot) \rangle_{\mathcal{H}} : X \times X \to \mathbb{R}$



# **Reproducing Kernel Hilbert Space**

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**Thm:** [Moore 1950]  $k : X \times X \to \mathbb{R}$  is a kernel iff it is *positive (semi-)definite*, i.e.  $\forall n \in \mathbb{N}, \forall x_1, \dots, x_n \in X$ , the Gram matrix  $(k(x_i, x_j))_{i,j}$  is positive semi-definite.

**Examples in**  $X = (\mathbb{R}^d, \langle \cdot, \cdot \rangle)$ :

• linear:  $k(x,y) = \langle x,y \rangle$   $\mathcal{H} = (\mathbb{R}^d)^*, \ \Phi(x) = \langle x, \cdot \rangle$ 

• polynomial: 
$$k(x,y) = (1 + \langle x,y \rangle)^N = \sum_{n_1 + \dots + n_d = N} {\binom{N}{n_1,\dots,n_d} \underbrace{x_1^{n_1} \cdots x_d^{n_d}}_{\propto \Phi(x)} y_1^{n_1} \cdots y_d^{n_d}}$$

• Gaussian: 
$$k(x, y) = \exp\left(-\frac{\|x-y\|_2^2}{2\sigma^2}\right), \ \sigma > 0. \quad \mathcal{H} \subset L_2(\mathbb{R}^d)$$
 2

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**Thm:** (Representer) [Schölkopf et al 2001] Given RKHS  $\mathcal{H}$  with kernel k, any function  $f^* \in \mathcal{H}$  minimizing

 $\frac{1}{n} \sum_{i=1}^{n} L(y_i, f(x_i)) + \Omega(||f||_{\mathcal{H}})$ 

is of the form  $f^*(\cdot) = \sum_{j=1}^n \alpha_j k(x_j, \cdot)$ , where  $\alpha_1, \cdots, \alpha_n \in \mathbb{R}$ .

Three approaches:

• build kernel from kernels (algebraic operations)

- sum of kernels  $\longleftrightarrow$  concatenation of feature spaces

$$k_1(x,y) + k_2(x,y) = \left\langle \left( \begin{array}{c} \Phi_1(x) \\ \Phi_2(x) \end{array} \right), \left( \begin{array}{c} \Phi_1(y) \\ \Phi_2(y) \end{array} \right) \right\rangle$$

- product of kernels  $\longleftrightarrow$  tensor product of feature spaces

$$k_1(x,y)k_2(x,y) = \langle \Phi_1(x)\Phi_2(x)^T, \Phi_1(y)\Phi_2(y)^T \rangle$$

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- define explicit feature map  $\Phi: X \to \mathcal{H}$  (vectorization)
- define kernel from metric via radial basis function

**Thm:** [Kimeldorf, Wahba 1971] If  $d: X \times X \to \mathbb{R}_+$  symmetric is conditionally negative semidefinite, i.e.:  $\forall n \in \mathbb{N}, \ \forall x_1, \cdots, x_n \in X, \ \sum_{i=1}^n \alpha_i = 0 \Longrightarrow \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j \ d(x_i, x_j) \le 0,$ then  $k(x, y) = \exp\left(-\frac{d(x, y)}{2\sigma^2}\right)$  is positive definite for all  $\sigma > 0.$ 

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**Q:** does this apply to persistence diagrams?

## Space of persistence diagrams

Persistence diagram  $\equiv$  finite multiset in the open half-plane  $\Delta\times\mathbb{R}_{>0}$ 

Given a partial matching  $M: X \leftrightarrow Y$ :

cost of a matched pair  $(x, y) \in M$ :  $c_p(x, y) := ||x - y||_{\infty}^p$ 

cost of an unmatched point  $z \in X \sqcup Y$ :  $c_p(z) := ||z - \overline{z}||_{\infty}^p$ 

cost of M:

$$c_p(M) := \left(\sum_{(x, y) \text{ matched}} c_p(x, y) + \sum_{z \text{ unmatched}} c_p(z)\right)^{1/p}$$

**Def:** p-th diagram distance (extended metric):  $d_p(X, Y) := \inf_{M: X \leftrightarrow Y} c_p(M)$ 

**Def:** bottleneck distance:

 $d_{\infty}(X,Y) := \lim_{p \to \infty} d_p(X,Y)$ 



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unbalanced optimal transport  $d_p$  is **NOT** cnsd,  $\forall p \in \mathbb{R}_{>0} \cup \{\infty\}$  $\Rightarrow$  previous theorem is not applicable

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State of the Art: define  $\phi$  explicitly (vectorization) via:

- images [Adams et al. 2015]
- finite metric spaces [Carrière, O., Ovsjanikov 2015]
- polynomial roots or evaluations [Di Fabio, Ferri 2015] [Kališnik 2016]  $\{p_1, \dots, p_n\} \mapsto (P_1(p_1, \dots, p_n), \dots, P_r(p_1, \dots, p_n), \dots)$
- landscapes [Bubenik 2012] [Bubenik, Dłotko 2015]
- discrete measures:
  - $\rightarrow$  histogram [Bendich et al. 2014]
  - $\rightarrow$  convolution with fixed kernel [Chepushtanova et al. 2015]
  - ightarrow convolution with weighted kernel [Kusano, Fukumisu, Hiraoka 2016-17]
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|  |                                    | metric                             |                                   |                                     | discrete            |
|--|------------------------------------|------------------------------------|-----------------------------------|-------------------------------------|---------------------|
|  | images                             | spaces                             | polynomials                       | landscapes                          | measures            |
| ambient Hilbert space  | $(\mathbb{R}^d, \ .\ _2)$          | $(\mathbb{R}^d, \ .\ _2)$          | $\ell_2(\mathbb{R})$              | $L_2(\mathbb{N} \times \mathbb{R})$ | $L_2(\mathbb{R}^2)$ |
| positive (semi-)definiteness                                     |                                    |                                    |                                   |                                     |                     |
| $\ \phi(\cdot) - \phi(\cdot)\ _{\mathcal{H}} \le C \mathrm{d}_p$ |                                    |                                    |                                   |                                     |                     |
| $\ \phi(\cdot) - \phi(\cdot)\ _{\mathcal{H}} \ge c \mathrm{d}_p$ | ×                                  | ×                                  | ×                                 | ×                                   | ×                   |
| injectivity  | ×                                  | ×                                  |                                   |                                     |                     |
| universality   | ×                                  | ×                                  | ×                                 | ×                                   |                     |
| algorithmic cost   | f. map: $O(n^2)$<br>kernel: $O(d)$ | f. map: $O(n^2)$<br>kernel: $O(d)$ | f. map: $O(nd)$<br>kernel: $O(d)$ | $O(n^2)$                            | $O(n^2)$            |

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| positive (semi-)definiteness                                     |                                    |                                    |                                   | $\checkmark$                        | $\checkmark$         |
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|  |                                    |                                    |                                   |                                     |                      |

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| ро | ositive (semi-)definiteness                                      |                                    |                                    |                                   |                                     |                     |
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Persistence Images [Adams et al. 2017]



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Concatenate all I(P) into a single vector PI(dgm)

Persistence Images [Adams et al. 2017]



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Prop: [Adams et al. 2017]

- $\|\operatorname{PI}(\operatorname{dgm}) \operatorname{PI}(\operatorname{dgm}')\|_{\infty} \leq C(w, \phi_p) \operatorname{d}_1(\operatorname{dgm}, \operatorname{dgm}')$
- $\|\operatorname{PI}(\operatorname{dgm}) \operatorname{PI}(\operatorname{dgm}')\|_2 \le \sqrt{d}C(w, \phi_p) \operatorname{d}_1(\operatorname{dgm}, \operatorname{dgm}')$

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 $\begin{bmatrix} 0 & 4 & 5 \\ b & 4 & 0 & 3 \\ c & 5 & 3 & 0 \end{bmatrix}$ 





Persistence diagrams as discrete measures:



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Pb:  $\mu_D$  is unstable (points on diagonal disappear)  $w(x) := \arctan{(c d(x, \Delta)^r)}, c, r > 0$ 



Persistence diagrams as discrete measures:



**Pb:**  $\mu_D$  is unstable (points on diagonal disappear)

$$w(x) := \arctan{(c \operatorname{d}(x, \Delta)^r)}, c, r > 0$$

**Def:**  $\phi(D)$  is the density function of  $\mu_D^w * \mathcal{N}(0, \sigma)$  w.r.t. Lebesgue measure:

$$\langle \phi(D) := \frac{1}{\sqrt{2\pi\sigma}} \sum_{x \in D} \arctan(c \operatorname{d}(x, \Delta)^r) \exp\left(-\frac{\|\cdot - x\|^2}{2\sigma^2}\right)$$
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Persistence diagrams as discrete measures:



**Pb:** convolution reduces discriminativity  $\rightarrow$  use discrete measure instead

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#### One kernel to rule them all...

Sliced Wasserstein Kernel [Carrière, Cuturi, O. 2017]

No feature map Provably stable Provably discriminative Mimicks the Gaussian kernel

View diagrams as discrete measures w/o density functions



**Pb:**  $d_p(D, D') \not \propto W_p(\mu_D, \mu_{D'})$  ( $W_p$  does not even make sense here)



 $\mu_D := \sum_{x \in D} \delta_x$ 

birth

**Pb:**  $d_p(D, D') \not \propto W_p(\mu_D, \mu_{D'})$  ( $W_p$  does not even make sense here)

$$\rightarrow \text{ given } D, D', \text{ let} \qquad \bar{\mu}_D := \sum_{x \in D} \delta_x + \sum_{y \in D'} \delta_{\pi_\Delta(y)}$$
$$\bar{\mu}_{D'} := \sum_{y \in D'} \delta_y + \sum_{x \in D} \delta_{\pi_\Delta(x)}$$

Then,  $d_p(D, D') \le W_p(\bar{\mu}_D, \bar{\mu}_{D'}) \le 2 d_p(D, D')$ 





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**Pb:**  $\bar{\mu}_D$  depends on D'



**Pb:**  $d_p(D, D') \not \propto W_p(\mu_D, \mu_{D'})$  ( $W_p$  does not even make sense here)

Solution: transfer mass negatively:

$$\tilde{\mu}_D := \mu_D - (\pi_\Delta)_* \, \mu_D = \sum_{x \in D} \delta_x - \sum_{x \in D} \delta_{\pi_\Delta(x)} \quad \in \mathcal{M}_0(\mathbb{R}^2)$$

 $\rightarrow$  signed discrete measure of total mass zero Kantorovich norm:  $\|\tilde{\mu}_D\|_K = W_1(\mu_D, (\pi_\Delta)_* \mu_D)$ 

#### A Wasserstein Gaussian kernel for PDs?

**Thm.:** [Kimeldorf, Wahba 1971] If  $d: X \times X \to \mathbb{R}_+$  symmetric is conditionally negative semidefinite, i.e.:  $\forall n \in \mathbb{N}, \ \forall x_1, \cdots, x_n \in X, \ \sum_{i=1}^n \alpha_i = 0 \Longrightarrow \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j \ d(x_i, x_j) \le 0,$ then  $k(x, y) := \exp\left(-\frac{d(x, y)}{2\sigma^2}\right)$  is positive semidefinite.

**Pb:**  $W_1$  is not cnsd, neither is  $d_1$ 

Solutions:

- relax the measures (e.g. convolution)
- relax the metric (e.g. regularization, slicing)

**Special case:**  $X = \mathbb{R}$ ,  $\mu, \nu$  discrete measures of same mass m

$$\mu := \sum_{i=1}^m \delta_{x_i}$$
,  $\nu := \sum_{i=1}^m \delta_{y_i}$ 

Sort the atoms of  $\mu, \nu$  along the real line:  $x_i \leq x_{i+1}$  and  $y_i \leq y_{i+1}$  for all i

Then: 
$$W_1(\mu,\nu) = \sum_{i=1}^m |x_i - y_i| = ||(x_1,\cdots,x_m) - (y_1,\cdots,y_m)||_1$$



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 $\rightarrow W_1$  is considered and easy to compute (same with  $\|\cdot\|_K$  for signed measures)

Def (sliced Wasserstein distance): for  $\mu, \nu \in \mathcal{M}_+(\mathbb{R}^2)$ ,

$$SW_1(\mu,\nu) := \frac{1}{2\pi} \int_{\theta \in S^1} W_1((\pi_\theta)_* \mu, \, (\pi_\theta)_* \nu) \, d\theta$$

where  $\pi_{\theta}$  = orthogonal projection onto line passing through origin with angle  $\theta$ .



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$$SW_1(\mu,\nu) := \frac{1}{2\pi} \int_{\theta \in \mathbb{S}^1} W_1((\pi_\theta)_* \mu, (\pi_\theta)_* \nu) d\theta$$

where  $\pi_{\theta}$  = orthogonal projection onto line passing through origin with angle  $\theta$ .

**Props:** (inherited from  $W_1$  over  $\mathbb{R}$ ) [Rabin, Peyré, Delon, Bernot 2011]

- satisfies the axioms of a metric
- well-defined barycenters, fast to compute via stochastic gradient descent, etc.
- conditionally negative semidefinite

## Sliced Wasserstein kernel

**Def:** Given 
$$\sigma > 0$$
, for any  $\mu, \nu \in \mathcal{M}_+(\mathbb{R}^2)$ :  
 $k_{SW}(\mu, \nu) := \exp\left(-\frac{SW_1(\mu, \nu)}{2\sigma^2}\right)$ 

**Corollary:** [Kolouri, Zou, Rohde]  $k_{SW}$  is positive semidefinite.

## Sliced Wasserstein kernel

**Def:** Given 
$$\sigma > 0$$
, for any  $\mu, \nu \in \mathcal{M}_+(\mathbb{R}^2)$ :  
 $k_{SW}(\mu, \nu) := \exp\left(-\frac{SW_1(\mu, \nu)}{2\sigma^2}\right)$ 

**Corollary:** [Kolouri, Zou, Rohde]  $k_{SW}$  is positive semidefinite.

**Thm.:** [Carrière, Cuturi, O. 2017] The metrics  $d_1$  and  $SW_1$  on the space  $\mathcal{D}_N$  of persistence diagrams of size bounded by N are strongly equivalent, namely: for  $D, D' \in \mathcal{D}_N$ ,

$$\frac{1}{2+4N(2N-1)} d_1(D,D') \leq SW_1(D,D') \leq 2\sqrt{2} d_1(D,D')$$

**Corollary:** the feature map  $\phi$  associated with  $k_{SW}$  is weakly metric-preserving:  $\exists g, h$  nonzero except at 0 such that  $g \circ d_1 \leq \|\phi(\cdot) - \phi(\cdot)\|_{\mathcal{H}} \leq h \circ d_1$ .

### Metric distortion in practice



# Application to supervised shape segmentation

**Goal**: segment 3d shapes based on examples Approach:

- train a (multiclass) classifier on PDs extracted from the training shapes
- apply classifier to PDs extracted from query shape



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(training data)



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**Goal**: segment 3d shapes based on examples Approach:

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- apply classifier to PDs extracted from query shape

| Accuracies | (%) | using | TDA | descriptors | (kernels | on | barcodes | ): |
|------------|-----|-------|-----|-------------|----------|----|----------|----|
|------------|-----|-------|-----|-------------|----------|----|----------|----|

|          | TDA  | geometry | TDA + geometry |
|----------|------|----------|----------------|
| Human    | 74.0 | 78.7     | 88.7           |
| Airplane | 72.6 | 81.3     | 90.7           |
| Ant      | 92.3 | 90.3     | 98.5           |
| FourLeg  | 73.0 | 74.4     | <b>84.2</b>    |
| Octopus  | 85.2 | 94.5     | 96.6           |
| Bird     | 72.0 | 75.2     | <b>86.5</b>    |
| Fish     | 79.6 | 79.1     | 92.3           |

Approach: use framework of *functional maps* [Ovsjanikov et al. 2012]

Given a point-to-point map  $m: X \to Y$  (seen as measured spaces), consider the linear map  $m^*: L^2(Y) \to L^2(X)$  induced by composition with m

- compute an optimal linear map that best preserves a set of signatures (vectors)
- derive a point-to-point correspondence from this map (via indicator functions)
- evaluate the quality of the correspondence
- reduce the dimensionality by taking the first k eigenfunctions of the Laplace-Beltrami operator



Approach: use framework of *functional maps* [Ovsjanikov et al. 2012]



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correspondences in flat regions are improved by topological signatures





 $f:\mathbb{N}\to\mathbb{R}$ 

| ð   | signal                        | embedded data                                      |
|---|-------------------------------|--|
| $\mathrm{TD}_{m,\tau}(f) := \begin{bmatrix} f(t) \\ f(t+\tau) \\ \vdots \\ \vdots \\ f(t+\tau) \end{bmatrix}$ | periodicity                   | circularity  |
| $\int f(t+m	au) \int$<br>au: step / delay   | # prominent harmonics ( $N$ ) | min. ambient dimension $(m \ge 2N)$                |
| m	au: window size   | # non-commensurate freq.      | intrinsic dimension                                |
| m+1: embedding dimension  |                               | $(\mathbb{S}^1 \times \cdots \times \mathbb{S}^1)$ |

[J. Perea et al.:"SW1PerS: Sliding windows and 1-persistence scoring", 2015]



#### **Contributions of TDA**:

inference of:

- periodicity
- harmonics
- non-commensurate freq.
- underlying state space .....
- no Fourier transform needed





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Dynamical system:

**Thm:** [Nash, Takens] Given a Riemannian manifold X of dimension  $\frac{m}{2}$ , it is a **generic property** of  $\phi \in \text{Diff}_2(X)$ and  $\alpha \in C^2(X, \mathbb{R})$  that

$$X \to \mathbb{R}^{m+1}$$
$$x \mapsto (\alpha(x), \alpha \circ \phi(x), \cdots, \alpha \circ \phi^m(x)$$

is an embedding.



| method / dataset               | Gyro sensor           | EEG dataset            | EMG dataset            |
|--------------------------------|-----------------------|------------------------|------------------------|
| SVM + statistical features     | $67.6 \pm 4.7$        | $44.4 \pm 19.8$        | $15.0 \pm 10.0$        |
| SVM + Betti sequence           | $63.5 \pm 11.3$       | $66.7 \pm 5.6$         | $49.6 \pm 18.2$        |
| 1-d CNN + dynamic time warping | $6.4 \pm 5.1$         | $72.4 \pm 6.1$         | $15.0 \pm 10.0$        |
| imaging CNN                    | $18.9 \pm 5.2$        | $48.9 \pm 4.2$         | $10.0 \pm 0.0$         |
| 1-d CNN + Betti sequence       | <b>79.8</b> $\pm$ 5.0 | <b>75.38</b> $\pm$ 5.7 | <b>74.4</b> $\pm$ 10.6 |

[Y. Umeda:" Time Series Classification via Topological Data Analysis", 2017]

# Wrap'up



- kernels for persistence diagrams:
  - stable
  - discriminative
  - easy to compute (closed-form expr., finite-dim. vectors)
  - additive, universal, etc.
- other topic: integration of TDA into learning methods (clustering, NNs, etc.)

