**Topological Signatures** 

**Input:** set of data points with metric or (dis-)similarity measure



Input: set of data points with metric or (dis-)similarity measure



Input: set of data points with metric or (dis-)similarity measure



Input: set of data points with metric or (dis-)similarity measure



Comparisons between geometric data sets or parts thereof occur in:

• classification (organizing large databases)





Princeton Shape Retrieval and Analysis Group Princeton Shape Benchmark

#### Shape Benchmark







Comparisons between geometric data sets or parts thereof occur in:

- classification (organizing large databases)
- retrieval (searching in databases)



Comparisons between geometric data sets or parts thereof occur in:

- classification (organizing large databases)
- retrieval (searching in databases)
- partial/global matching (finding the *best* mapping between data sets)



Comparisons between geometric data sets or parts thereof occur in:

- classification (organizing large databases)
- retrieval (searching in databases)
- partial/global matching (finding the *best* mapping between data sets)
- segmentation and labelling



Comparisons between geometric data sets or parts thereof occur in:

- classification (organizing large databases)
- retrieval (searching in databases)
- partial/global matching (finding the *best* mapping between data sets)
- segmentation and labelling

data comparison is the basic building block



• geometric data set  $\equiv$  compact metric space



• geometric data set  $\equiv$  compact metric space



- geometric data set  $\equiv$  compact metric space
- distance between data sets  $\equiv$  Gromov-Hausdorff (GH) distance



- geometric data set  $\equiv$  compact metric space
- distance between data sets  $\equiv$  Gromov-Hausdorff (GH) distance



- geometric data set  $\equiv$  compact metric space
- distance between data sets  $\equiv$  Gromov-Hausdorff (GH) distance



- geometric data set  $\equiv$  compact metric space
- distance between data sets  $\equiv$  Gromov-Hausdorff (GH) distance



- geometric data set  $\equiv$  compact metric space
- distance between data sets  $\equiv$  Gromov-Hausdorff (GH) distance
- signature  $\equiv$  persistence diagram (choose the filtration)
  - **multi-scale**  $\equiv$  reflects the structure of the shape across scales
  - global/local  $\equiv$  attached to the whole shape / to a base point(s)
  - **stable**  $\equiv$  variations with GH-distance and base point location are controlled







Some descriptors for images / 3d shapes / metric spaces:

- diameter
- curvature (mean, Gaussian, sectional)
- shape context (distribution of distances)
- heat kernel signature (heat diffusion)
- wave kernel signature (Maxwell's equations)
- spin image (local neighborhood parametrization)
- SIFT features (local distribution of gradient orientations)
- etc.

#### Outline

1. Global topological signatures

2. Local topological signatures

3. Kernels for topological signatures

#### Outline

1. Global topological signatures

2. Local topological signatures

3. Kernels for topological signatures

# **Global Topological Signatures**

Input: a compact metric space  $(X, d_X)$ 

Signature: dgm  $\mathcal{F}(X, d_X)$ , where  $\mathcal{F}(X, d_X)$  is some simplicial filtration over X derived from  $d_X$  (proxy for union of balls)



# **Global Topological Signatures**

Input: a compact metric space  $(X, d_X)$ 

Signature: dgm  $\mathcal{F}(X, d_X)$ , where  $\mathcal{F}(X, d_X)$  is some simplicial filtration over X derived from  $d_X$  (proxy for union of balls)



# **Global Topological Signatures**

Input: a compact metric space  $(X, d_X)$ 

Signature: dgm  $\mathcal{F}(X, d_X)$ , where  $\mathcal{F}(X, d_X)$  is some simplicial filtration over X derived from  $d_X$  (proxy for union of balls)



#### Examples

Signatures of some elementary shapes (approximated from finite samples):



#### Examples

Signatures of some elementary shapes (approximated from finite samples):



#### Examples

Signatures of some elementary shapes (approximated from finite samples):



**Theorem:** [Chazal, de Silva, O. 2013] For any compact metric spaces  $(X, d_X)$  and  $(Y, d_Y)$ ,  $d_B^{\infty}(\operatorname{dgm} \mathcal{R}(X, d_X), \operatorname{dgm} \mathcal{R}(Y, d_Y)) \leq 2d_{\operatorname{GH}}(X, Y).$ 

Variants and extensions:

- Čech / Nerve filtrations
- Witness complex filtrations (landmarks fixed)
- precompact metric spaces
- (dis-)similarity measures

**Theorem:** [Chazal, de Silva, O. 2013] For any compact metric spaces  $(X, d_X)$  and  $(Y, d_Y)$ ,  $d_B^{\infty}(\operatorname{dgm} \mathcal{R}(X, d_X), \operatorname{dgm} \mathcal{R}(Y, d_Y)) \leq 2d_{\operatorname{GH}}(X, Y).$ 

The bound is worst-case tight...



 $d_{\mathrm{GH}}(X,Y) = \varepsilon$  $dgm \mathcal{R}(X, d_X) = \{(0,\infty), (0,1)\}$  $dgm \mathcal{R}(Y, d_Y) = \{(0,\infty), (0,1+2\varepsilon)\}$  $\Rightarrow d_{\mathrm{B}}^{\infty}(dgm \mathcal{R}(X, d_X), dgm \mathcal{R}(Y, d_Y)) = 2\varepsilon$ 

**Theorem:** [Chazal, de Silva, O. 2013] For any compact metric spaces  $(X, d_X)$  and  $(Y, d_Y)$ ,  $d_B^{\infty}(\operatorname{dgm} \mathcal{R}(X, d_X), \operatorname{dgm} \mathcal{R}(Y, d_Y)) \leq 2d_{\operatorname{GH}}(X, Y).$ 

The bound is worst-case tight... but it is still only an upper bound



$$d_{GH}(X, Y) = \frac{1}{2}$$
  

$$dgm \mathcal{R}(X, d_X) = \{(0, \infty), (0, 1), (0.1)\}$$
  

$$dgm \mathcal{R}(Y, d_Y) = \{(0, \infty), (0, 1), (0, 1)\}$$
  

$$\Rightarrow d_B^{\infty}(dgm \mathcal{R}(X, d_X), dgm \mathcal{R}(Y, d_Y)) = 0$$

**Theorem:** [Chazal, de Silva, O. 2013] For any compact metric spaces  $(X, d_X)$  and  $(Y, d_Y)$ ,  $d_B^{\infty}(\operatorname{dgm} \mathcal{R}(X, d_X), \operatorname{dgm} \mathcal{R}(Y, d_Y)) \leq 2d_{\operatorname{GH}}(X, Y).$ 

#### **Proof outline:**

finite



# Convergence Rates

 $(X, d_X)$ : compact metric space

 $\mathcal{P}$ : proba. measures  $\mu$  on X satisfying the (a,b)-standard condition:

 $\forall x \in \operatorname{supp} \mu, \ \forall r > 0, \ \mu(B(x, r) \ge \min\{1, ar^b\}.$ 

## Convergence Rates

 $(X, d_X)$ : compact metric space

 $\mathcal{P}$ : proba. measures  $\mu$  on X satisfying the (a,b)-standard condition:

 $\forall x \in \operatorname{supp} \mu, \ \forall r > 0, \ \mu(B(x, r) \ge \min\{1, ar^b\}.$ 

Given  $\mu \in \mathcal{P}$ , let  $\hat{X}_n = \{X_1, \cdots, X_n\}$  be sampled i.i.d. according to  $\mu$ .

Theorem. [Chazal, Glisse, Labruère, Michel 2014]

$$\sup_{\mu \in \mathcal{P}} \mathbb{E} \left[ d_{B} \left( \operatorname{dgm} \mathcal{R}(\hat{X}_{n}), \operatorname{dgm} \mathcal{R}(\operatorname{supp} \mu) \right) \right] \leq C \left( \frac{\log n}{n} \right)^{1/b},$$

where C depends only on a, b. Moreover, the estimator  $\operatorname{dgm} \mathcal{R}(\hat{X}_n)$  is minimax optimal on the space  $\mathcal{P}$  up to a  $\log n$  factor.

# Convergence Rates

 $(X, d_X)$ : compact metric space

 $\mathcal{P}$ : proba. measures  $\mu$  on X satisfying the (a,b)-standard condition:

 $\forall x \in \operatorname{supp} \mu, \ \forall r > 0, \ \mu(B(x, r) \ge \min\{1, ar^b\}.$ 

Given  $\mu \in \mathcal{P}$ , let  $\hat{X}_n = \{X_1, \cdots, X_n\}$  be sampled i.i.d. according to  $\mu$ .

Theorem. [Chazal, Glisse, Labruère, Michel 2014]

$$\sup_{\mu \in \mathcal{P}} \mathbb{E} \left[ d_{\mathrm{B}} \left( \operatorname{dgm} \mathcal{R}(\hat{X}_{n}), \ \operatorname{dgm} \mathcal{R}(\operatorname{supp} \mu) \right) \right] \leq C \left( \frac{\log n}{n} \right)^{1/b},$$

where C depends only on a, b. Moreover, the estimator  $\operatorname{dgm} \mathcal{R}(\hat{X}_n)$  is minimax optimal on the space  $\mathcal{P}$  up to a  $\log n$  factor.

**Proof:** 

- upper bound: Hausdorff estimation of  $\operatorname{supp} \mu$  + stability
- lower bound: Le Cam's lemma
## Application: Unsupervised Classification



# Application: Unsupervised Classification



# Application: Unsupervised Classification



### Outline

1. Global topological signatures

2. Local topological signatures

3. Kernels for topological signatures

# Local Topological Signatures



# Local Topological Signatures



# Local Topological Signatures

Input: a compact Riemannian manifold  $(X, d_X)$ , a basepoint  $x \in X$ 

Construction: filtration of the sublevel sets of  $d_{x_0}(\cdot) = d_X(x_0, \cdot)$ 

Signature: the persistence diagram of the filtration, denoted  $\operatorname{dgm} \operatorname{d}_{x_0}$ 



# Stability



# Stability

**Theorem:** [Carrière, O., Ovsjanikov 2015] Let  $(X, d_X)$  and  $(Y, d_Y)$  be compact Riemannian manifolds. Let  $x_0 \in X$ and  $y_0 \in Y$ . If  $d_{GH}((X, x_0), (Y, y_0)) \leq \frac{1}{20} \min\{\varrho(X), \varrho(Y)\}$ , then  $d_B^{\infty}(\operatorname{dgm} d_{x_0}, \operatorname{dgm} d_{y_0}) \leq 20 d_{GH}((X, x_0), (Y, y_0))$ .

Prerequisite:  $d_{GH}(X, Y) < \frac{1}{20} \min\{\varrho(X), \varrho(Y)\}$ 



 $d_{\rm GH}(X,Y) < \infty = \varrho(Y)$ 

 $\mathrm{d}^\infty_\mathrm{B}(\mathrm{dgm}\,f,\mathrm{dgm}\,g)=\infty$ 

- input: shapes from the TOSCA database, in mesh form
- select a few base points by hand on each shape
- approximate geodesic distances to base points using the 1-skeleton graph
- use the PDs of the PL interpolations over the meshes as signatures













### Outline

1. Global topological signatures

2. Local topological signatures

3. Kernels for topological signatures

# Persistence Diagrams as Signatures



- topological signatures carry complementary information
- stability properties, e.g.  $d^{\infty}_{B}(\mathcal{R}(X), \mathcal{R}(Y)) \leq 2d_{GH}(X, Y)$

# Persistence Diagrams as Signatures



- topological signatures carry complementary information
- stability properties, e.g.  $d^{\infty}_{B}(\mathcal{R}(X), \mathcal{R}(Y)) \leq 2d_{GH}(X, Y)$

Cons:

- the space of persistence diagrams is not a Hilbert space
- signatures are slow to compute and (more importantly) to compare

# Persistence Diagrams as Signatures



- topological signatures carry complementary information
- stability properties, e.g.  $d^{\infty}_{B}(\mathcal{R}(X), \mathcal{R}(Y)) \leq 2d_{GH}(X, Y)$

Cons:

• the space of persistence diagrams is not a Hilbert space

 $\rightarrow$  define kernels on the space of diagrams

• signatures are slow to compute and (more importantly) to compare

 $\rightarrow$  explicit mapping to feature space

 $\mathcal{X}:$  be a space in which we want to compare/classify elements

- feature map  $\phi: \mathcal{X} \to \mathcal{H}$  equipped with inner product  $< \cdot, \cdot >_{\mathcal{H}}$
- $\bullet$  lift training/testing data to  ${\mathcal H}$  through  $\phi$  then solve learning problem

 $\mathcal{X}$ : be a space in which we want to compare/classify elements

- feature map  $\phi: \mathcal{X} \to \mathcal{H}$  equipped with inner product  $< \cdot, \cdot >_{\mathcal{H}}$
- $\bullet$  lift training/testing data to  ${\mathcal H}$  through  $\phi$  then solve learning problem
- observation: many learning methods use only inner product  $\rightarrow$  do not lift the data, instead compute the  $k(x,y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}}$

 $\mathcal{X}$ : be a space in which we want to compare/classify elements

- feature map  $\phi: \mathcal{X} \to \mathcal{H}$  equipped with inner product  $< \cdot, \cdot >_{\mathcal{H}}$
- $\bullet$  lift training/testing data to  ${\mathcal H}$  through  $\phi$  then solve learning problem
- observation: many learning methods use only inner product  $\rightarrow$  do not lift the data, instead compute the  $k(x,y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}}$
- **Def.:** A reproducing kernel is a map  $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$  such that  $k(\cdot, \cdot) = \langle \phi(\cdot), \phi(\cdot) \rangle_{\mathcal{H}}$  for some pair  $(\phi, \mathcal{H})$ .

**Thm.:** [Moore, Aronszajn] A pair  $(\phi, \mathcal{H})$  exists whenever k is *positive semidefinite*, i.e.  $\sum_{i,j=1}^{n} c_i c_j k(x_i, x_j) \ge 0$  for all  $n \in \mathbb{N}, c_1, \cdots, c_n \in \mathbb{R}$ , and  $x_1, \cdots, x_n \in \mathcal{X}$ .





## Kernels for Persistence Diagrams

View persistence diagrams as:

- landscapes [Bubenik 2012] [Bubenik, Dłotko 2015]
- empirical measures:
  - $\rightarrow$  histogram [Bendich et al. 2014]
  - $\rightarrow$  density estimator [Chepushtanova et al. 2015]
  - $\rightarrow$  heat diffusion [Bauer et al. 2015]
- metric spaces [Carrière, O., Ovsjanikov 2015]
- roots of polynomials [Di Fabio, Ferri 2015]

## Side-by-side Comparison

landscapes

[Bubenik 2012]

feature space:  $L^2(\mathbb{N} imes \mathbb{R}) o L^2(\mathbb{R}^2)$ 

feature map: explicit (comb. construction)

complexity on n-points diagrams:

kernel(s): linear, Gaussian, etc.

- feature map:  $O(n^2)$ - kernel:  $O(n^2)$ 

stability:  $\| \cdot \|_{\infty} \leq O(\mathbf{d}_{\mathbf{B}}^{\infty})$  $\| \cdot \|_{p} \leq O(\text{Pers } \mathbf{d}_{\mathbf{B}}^{\infty}(\cdot))$ 

injective feature map

 $\rightarrow$  pd kernel?

kernels on diagrams are not additive

#### empirical measures

[Bauer et al. 2015]

feature space:  $L^2(\mathbb{R}^2)$ 

feature map: explicit (closed form solution)

kernel(s):  $k_{\sigma}$ 

complexity on n-points diagrams: - feature map: N/A (or discretize...) - kernel:  $O(n^2)$ 

stability:  $\|\cdot\|_2 \leq O(\mathrm{d}^1_\mathrm{B}(\cdot))$ 

injective feature map  $\rightarrow$  pd kernel? kernel is additive

#### metric spaces

[Carrière, O. , Ovsjanikov 2015]

feature space:  $\ell^p \to (\mathbb{R}^D, \ell^p)$ 

feature map: explicit (comb. construction)

kernel(s): linear Gaussian, etc.

complexity on n-points diagrams:

- feature map:  $O(n^2)$ - kernel: O(D)

stability:  $\| \cdot \|_{\infty} \leq O(\mathbf{d}_{\mathbf{B}}^{\infty})$  $\| \cdot \|_{p} \leq O(D^{1/p} \mathbf{d}_{\mathbf{B}}^{\infty}(\cdot))$ 

non-injective feature map  $\rightarrow$  psd kernel kernels on diagrams are not additive

## Side-by-side Comparison

landscapes

[Bubenik 2012]

feature space:  $L^2(\mathbb{N} imes \mathbb{R}) o L^2(\mathbb{R}^2)$ 

feature map: explicit (comb. construction) kernel(s): linear, Gaussian, etc.

complexity on n-points diagrams:

- feature map:  $O(n^2)$ - kernel:  $O(n^2)$ 

stability:  $\| \cdot \|_{\infty} \leq O(\mathbf{d}_{\mathbf{B}}^{\infty})$  $\| \cdot \|_{p} \leq O(\operatorname{Pers} \mathbf{d}_{\mathbf{B}}^{\infty}(\cdot))$ 

injective feature map

 $\rightarrow$  pd kernel?

kernels on diagrams are not additive

#### empirical measures

[Bauer et al. 2015]

feature space:  $L^2(\mathbb{R}^2)$ 

feature map: explicit (closed form solution)

kernel(s):  $k_{\sigma}$ 

complexity on n-points diagrams: - feature map: N/A (or discretize...) - kernel:  $O(n^2)$ 

stability:  $\|\cdot\|_2 \leq O(\mathrm{d}^1_\mathrm{B}(\cdot))$ 

injective feature map  $\rightarrow$  pd kernel? kernel is additive

#### metric spaces

[Carrière, O. , Ovsjanikov 2015]

feature space:  $\ell^p \to (\mathbb{R}^D, \ell^p)$ 

feature map: explicit (comb. construction)

kernel(s): linear Gaussian, etc.

complexity on n-points diagrams:

- feature map:  $O(n^2)$ - kernel: O(D)

stability:  $\| \cdot \|_{\infty} \leq O(\mathbf{d}_{\mathbf{B}}^{\infty})$  $\| \cdot \|_{p} \leq O(D^{1/p} \mathbf{d}_{\mathbf{B}}^{\infty}(\cdot))$ 

non-injective feature map → psd kernel kernels on diagrams are not additive

finite metric space



#### finite metric space







 $\Phi = \phi_4 \circ \phi_3 \circ \phi_2 \circ \phi_1$ 



## **Stability Properties** $\Phi = \phi_4 \circ \phi_3 \circ \phi_2 \circ \phi_1$



## **Stability Properties** $\Phi = \phi_4 \circ \phi_3 \circ \phi_2 \circ \phi_1$



## **Stability Properties** $\Phi = \phi_4 \circ \phi_3 \circ \phi_2 \circ \phi_1$



# Adding the diagonal



# Adding the diagonal


## Adding the diagonal



$$\mathbf{d}_{\mathbf{B}}^{\infty} = \inf_{m:X\leftrightarrow Y} \max\left\{\sup_{p \text{ matched}} \|p - m(p)\|_{\infty}, \sup_{p \text{ unmatched}} \|p - \bar{p}\|_{\infty}\right\}$$

### Adding the diagonal



$$d_{B}^{\infty} = \inf_{m:X\leftrightarrow Y} \max\left\{\sup_{p \text{ matched}} \|p - m(p)\|_{\infty}, \sup_{p \text{ unmatched}} \|p - \bar{p}\|_{\infty}\right\}$$

Problem: generates instability in distance matrix ( $d_B^{\infty} \ll W_{\infty}$ ) Solution: change the metric Adding the diagonal  $\Phi = \phi_4 \circ \phi_3 \circ \phi_2 \circ \phi_1$ 



## Stability

**Theorem:** [Carrière et al. 2015] For any persistence diagrams X, Y, for any feature space dimension D,  $\|\Phi(X) - \Phi(Y)\|_{\infty} \leq 2d_{B}^{\infty}(X, Y)$ 

## Stability

**Theorem:** [Carrière et al. 2015] For any persistence diagrams X, Y, for any feature space dimension D,  $\|\Phi(X) - \Phi(Y)\|_{\infty} \leq 2d_{B}^{\infty}(X,Y)$  $\forall p \geq 1$ ,  $\|\Phi(X) - \Phi(Y)\|_{p} \leq 2D^{1/p}d_{B}^{\infty}(X,Y)$ 

## Stability

**Theorem:** [Carrière et al. 2015] For any persistence diagrams X, Y, for any feature space dimension D,  $\|\Phi(X) - \Phi(Y)\|_{\infty} \leq 2d_{B}^{\infty}(X,Y)$  $\forall p \geq 1$ ,  $\|\Phi(X) - \Phi(Y)\|_{p} \leq 2D^{1/p}d_{B}^{\infty}(X,Y)$ 

• case  $p = \infty$  useful for retrieval and NN-classifiers (fast proximity queries)

• case p = 2 useful for linear / kernel-based classifiers (scalar product)

### Application: supervised segmentation

Approach 1: use k-NN classifier in feature space  $(\mathbb{R}^D, \ell^{\infty})$ 



#### Application: supervised segmentation

Approach 1: use k-NN classifier in feature space  $(\mathbb{R}^D, \ell^{\infty})$ 

Approach 2: use linear classifier (SVM) in feature space  $(\mathbb{R}^D, \ell^2)$ 

+ graph cut [Kalogerakis et al. 2010]



#### Application: supervised segmentation

Approach 1: use k-NN classifier in feature space  $(\mathbb{R}^D, \ell^{\infty})$ 

Approach 2: use linear classifier (SVM) in feature space  $(\mathbb{R}^D, \ell^2)$ 

+ graph cut [Kalogerakis et al. 2010]

	SB5	SB5+PDs
Human	21.3	11.3
Cup	10.6	10.1
Glasses	21.8	25.0
Airplane	18.7	9.3
Ant	9.7	1.5
Chair	15.1	7.3
Octopus	5.5	3.4
Table	7.4	2.5
Teddy	6.0	3.5
Hand	21.1	12.0

	SB5	SB5+PDs
Plier	12.3	9.2
Fish	20.9	7.7
Bird	24.8	13.5
Armadillo	18.4	8.3
Bust	35.4	22.0
Mech	22.7	17.0
Bearing	25.0	11.2
Vase	26.4	17.8
FourLeg	25.6	15.8

percentage of mislabelling (100-rand index)

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

- 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



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



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



correspondences in flat regions are improved by topological signatures



# Wrap-Up



• topological descriptors are **provably stable** 

feature vector

- they provide **complementary information**
- they can be computed and mapped to feature spaces efficiently