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Persistent homology in TDA

Frédéric Chazal and Bertrand Michel



Persistent homology



Nested spaces

- A general mathematical framework to encode the evolution of the topology (homology) of families of nested spaces (filtered complex, sublevel sets,...).
- Formalized by H. Edelsbrunner (2002) et al and G. Carlsson et al (2005) wide development during the last decade.
- Multiscale topological information.
- Barcodes/persistence diagrams can be efficiently computed.
- Stability properties

- Nested family (filtration) of sublevel-sets $f^{-1}((-\infty, \alpha])$ for $\alpha = -\infty$ to $+\infty$.
- Track evolution of topology throughout the family.



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Persistent homology of filtered complexes

Let $\emptyset = K^0 \subset K^1 \subset \cdots \subset K^m = K$ be a filtration of a simplicial complex K s. t. $K^{i+1} = K^i \cup \sigma^{i+1}$ where σ^{i+1} is a simplex of K.

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Relation between sublevel sets filtrations and filtered simplicial complexes:

- $\forall t \leq t' \in \mathbb{R}, f^{-1}((-\infty, t]) \subseteq f^{-1}((-\infty, t']) \rightarrow \text{filtration of } X \text{ by the sublevel sets of } f.$
- If f is defined at the vertices of a simplicial complex K, the sublevel sets filtration is a filtration of the simplicial complex K.
 - For $\sigma = [v_0, \cdots, v_k] \in K$, $f(\sigma) = \max_{i=0,\cdots,k} f(v_i)$
 - The simplices of K are ordered according increasing f values (and dimension in case of equal values on different simplices).

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Algorithm to compute the Betti numbers $\beta_0, \beta_1, \cdots, \beta_d$ of K:

$$\begin{split} \beta_0 &= \beta_1 = \cdots = \beta_d = 0; \\ \text{for } i &= 1 \text{ to } m \\ k &= \dim \sigma^i - 1; \\ \text{if } \sigma^i \text{ is contained in a } (k+1)\text{-cycle in } K^i \\ \text{then } \beta_{k+1} &= \beta_{k+1} + 1; \\ \text{else } \beta_k &= \beta_k - 1; \\ \text{end if;} & \text{an homologeneration} \\ \text{end for;} & \text{plices (birton)} \\ \text{output } (\beta_0, \beta_1, \cdots, \beta_d); & \text{to negative} \end{split}$$

Goal: adapt the algorithm to keep track of an homology basis and pairs positive simplices (birth of a new homological class) to negative simplices (death of an existing homology class).

Notation: $H_k^i = H_k(K^i)$

Cycle associated to a positive simplex



Lemma: If σ^i is a positive k-cycle, then there exists a k-cycle c_σ s.t.: - c_σ is not a boundary in K^i , - c_σ contains σ^i but no other positive k-simplex. The cycle c^σ is unique.

Proof:

By induction on the order of appearence of the simplices in the filtration.

Homology basis



- At the beginning: the basis of H_k^0 is empty.
- If a basis of H_k^{i-1} has been built and σ^i is a positive k-simplex then one adds the homology class of the cycle c^i associated to σ^i to the basis of $H_k^{i-1} \Rightarrow$ basis of H_k^i .
- If a basis of H_k^{j-1} has been built and σ^j is a negative (k+1)-simplex:
 - let c^{i_1}, \cdots, c^{i_p} be the cycles associated to the positive simplices $\sigma^{i_1}, \cdots, \sigma^{i_p}$ that form a basis of H_k^{j-1}
 - $d = \partial \sigma^j = \sum_{k=1}^p \varepsilon_k c^{i_k} + b$
 - $l(j) = \max\{i_k : \varepsilon_k = 1\}$
 - Remove the homology class of $c^{l(j)}$ from the basis of $H_k^{j-1} \Rightarrow$ basis of H_k^j .

Pairing simplices

If a basis of H_k^{j-1} has been built and σ^j is a negative (k+1)-simplex:

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- Remove the homology class of $c^{l(j)}$ from the basis of $H_k^{j-1} \Rightarrow$ basis of H_k^j .

The simplices $\sigma^{l(j)}$ and σ^j are paired to form a persistent pair $(\sigma^{l(j)}, \sigma^j)$. \rightarrow The homology class created by $\sigma^{l(j)}$ in $K^{l(j)}$ is killed by σ^j in K^j . The persistence (or life-time) of this cycle is : j - l(j) - 1.

Remark: filtrations of K can be indexed by increasing sequences α_i of real numbers (useful when working with a function defined on the vertices of a simplicial complex).

The persistence algorithm: first version

Input: $\emptyset = K^0 \subset K^1 \subset \cdots \subset K^m = K$ a *d*-dimensional filtration of a simplicial complex K s. t. $K^{i+1} = K^i \cup \sigma^{i+1}$ where σ^{i+1} is a simplex of K.

$$L_0 = L_1 = \dots = L_{d-1} = \emptyset$$

For $j = 0$ to m
 $k = \dim \sigma^j - 1$;
if σ^j is a negative simplex
 $l(j) =$ highest index of the positive simplices associated to $\partial \sigma^j$;
 $L_k = L_k \cup \{(\sigma^{l(j)}, \sigma^j)\};$
end if

end for

Output: $L_0, L_1, \cdots, L_{d-1}$;

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end for
Output: $L_{0}, L_{1}, \cdots, L_{d-1}$;
How to test this condition?

The persistence algorithm: second version

The matrix of the boundary operator:



• $M = (m_{ij})_{i,j=1,\cdots,m}$ with coefficient in $\mathbb{Z}/2$ defined by

 $m_{ij} = 1$ if σ^i is a face of σ^j and $m_{ij} = 0$ otherwise

• For any column C_j , l(j) is defined by

$$(i = l(j)) \Leftrightarrow (m_{ij} = 1 \text{ and } m_{i'j} = 0 \quad \forall i' > i)$$

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Compute the matrix of the boundary operator MFor j = 0 to mWhile (there exists j' < j such that l(j') == l(j)) $C_j = C_j + C_{j'} \mod(2)$; End while End for Output the pairs (l(j), j);

Remark: The worst case complexity of the algorithm is $O(m^3)$ but much lower in most practical cases.

The persistence algorithm: second version

A simple example:



Persistence diagram



- each pair $(\sigma^{l(j)}, \sigma^j)$ is represented by (l(j), j) or $(f(\sigma^{l(j)}), f(\sigma^j)) \in \mathbb{R}^2$ when considering filtrations induced by functions, or $(\alpha_{l(j)}, \alpha_j)$ if the filtration is induced by a real valued sequence $(\alpha_i)_{i \in I}$.
- The diagonal $\{y = x\}$ is added to the persistence diagram.
- Unpaired positive simplex $\sigma^i \to (i, +\infty)$.

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Points may have multiplicity

Persistence diagram



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- Unpaired positive simplex $\sigma^i \to (i, +\infty)$.

Barcodes: an alternative (equivalent) representation where each pair (i, j) is represented by the interval [i, j]



Distance between persistence diagrams



The bottleneck distance between two diagrams D_1 and D_2 is

$$d_B(D_1, D_2) = \inf_{\gamma \in \Gamma} \sup_{p \in D_1} \|p - \gamma(p)\|_{\infty}$$

where Γ is the set of all the bijections between D_1 and D_2 and $||p - q||_{\infty} = \max(|x_p - x_q|, |y_p - y_q|).$

Stability properties



What if f is slightly perturbed?



Stability properties

Theorem (Stability): For any *tame* functions $f, g : \mathbb{X} \to \mathbb{R}$, $d_{B}^{\infty}(D_{f}, D_{g}) \leq ||f - g||_{\infty}$.

[Cohen-Steiner, Edelsbrunner, Harer 05], [C., Cohen-Steiner, Glisse, Guibas, Oudot - SoCG 09], [C., de Silva, Glisse, Oudot 12]



Persistence-based clustering

Combine a mode seeking approach with (0-dim) persistence computation.

[C.,Guibas,Oudot,Skraba - J. ACM 2013]



Input:

1. A finite set X of observations (point cloud with coordinates or pairwise distance matrix),

2. A real valued function f defined on the observations (e.g. density estimate).

Goal: Partition the data according to the basins of attraction of the peaks of f

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- 1. Build a neighborhing graph G on top of X.
- 2. Compute the (0-dim) persistence of f to identify prominent peaks \rightarrow number of clusters (union-find algorithm).
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3. Chose a threshold $\tau > 0$ and use the persistence algorithm to merge components with prominence less than τ .

Combine a mode seeking approach with (0-dim) persistence computation.

[C.,Guibas,Oudot,Skraba - J. ACM 2013]



Complexity of the algorithm: $O(n \log n)$

Theoretical guarantees:

- Stability of the number of clusters (w.r.t. perturbations of X and f).
- Partial stability of clusters: well identified stable parts in each cluster.

Application to non-rigid shape segmentation

[Skraba, Ovsjanikov, C., Guibas, NORDIA 10]



Problem: some part of clusters are unstable \rightarrow dirty segments

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Idea:

- Run the persistence based algorithm several times on random perturbations of f (size bounded by the "persistence" gap).

- Partial stability of clusters allows to establish correspondences between clusters across the different runs \rightarrow for any $x \in X$, a vector giving the probability for x to belong to each cluster.

Application to non-rigid shape segmentation

[Skraba, Ovsjanikov, C., Guibas, NORDIA 10]





Other applications: classification, object recognition

Examples:

- Hand gesture recognition [Li, Ovsjanikov, C. - CVPR'14]



- Persistence-based pooling for shape recognition [Bonis, Ovsjanikov, Oudot, C. 2015]



Persistent homology for (point cloud) data



• Challenges and goals:

 \rightarrow no direct access to topological/geometric information: need of intermediate constructions (simplicial complexes);

- \rightarrow distinguish topological "signal" from noise;
- ightarrow topological information may be multiscale; -
- \rightarrow statistical analysis of topological information.



Persistent homology for (point cloud) data



- Build a geometric filtered simplicial complex on top of $\widehat{\mathbb{X}}_m \to$ multiscale topol. structure.
- Compute the persistent homology of the complex \rightarrow multiscale topol. signature.
- Compare the signatures of "close" data sets \rightarrow robustness and stability results.
- Statistical properties of signatures

Filtered complexes and filtrations



A filtered simplicial complex S built on top of a set X is a family $(S_a \mid a \in \mathbf{R})$ of subcomplexes of some fixed simplicial complex \overline{S} with vertex set X s. t. $S_a \subseteq S_b$ for any $a \leq b$.

A filtration \mathbb{F} of a space \mathbb{X} is a nested family $(\mathbb{F}_a \mid a \in \mathbb{R})$ of subspaces of \mathbb{X} such that $\mathbb{F}_a \subseteq \mathbb{F}_b$ for any $a \leq b$.

► Example: If $f : \mathbb{X} \to \mathbf{R}$ is a function, then the sublevelsets of f, $\mathbb{F}_a = f^{-1}((-\infty, a])$ define the sublevel set filtration associated to f.

Example: Rips and Cech filtrations



- An efficient way to encode the evolution of the topology (homology) of families of nested spaces (filtered complex, sublevel sets,...).
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Persistence diagram

Stability properties

"Stability theorem": Close spaces/data sets have close persistence diagrams! [C., de Silva, Oudot - Geom. Dedicata 2013].

If $\mathbb X$ and $\mathbb Y$ are pre-compact metric spaces, then



Rem: This result also holds for other families of filtrations (particular case of a more general theorem).

Application: non rigid shape classification

[C., Cohen-Steiner, Guibas, Mémoli, Oudot - SGP '09]



- Non rigid shapes in a same class are almost isometric, but computing Gromov-Hausdorff distance between shapes is extremely expensive.
- Compare diagrams of sampled shapes instead of shapes themselves.

Definition: A persistence module \mathbb{V} is an indexed family of vector spaces $(V_a \mid a \in \mathbb{R})$ and a doubly-indexed family of linear maps $(v_a^b : V_a \to V_b \mid a \leq b)$ which satisfy the composition law $v_b^c \circ v_a^b = v_a^c$ whenever $a \leq b \leq c$, and where v_a^a is the identity map on V_a .

Examples:

- Let S be a filtered simplicial complex. If V_a = H(S_a) and v^b_a : H(S_a) → H(S_b) is the linear map induced by the inclusion S_a → S_b then (H(S_a) | a ∈ R) is a persistence module.
- Given a metric space (X, d_X) , H(Rips(X)) is a persistence module.
- If f : X → R is a function, then the filtration defined by the sublevel sets of f, F_a = f⁻¹((-∞, a]), induces a persistence module at homology level.

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Definition: A persistence module \mathbb{V} is q-tame if for any a < b, v_a^b has a finite rank.

Theorem: [C., Cohen-Steiner, Glisse, Guibas, Oudot - SoCG'09], [C., de Silva, Glisse, Oudot 12]

q-tame persistence modules have well-defined persistence diagrams.

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An idea about the definition of persistence diagrams:



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Exercise: Let X be a precompact metric space. Then H(Rips(X)) and H(Cech(X)) are q-tame.

Recall that a metric space (X, ρ) is precompact if for any $\epsilon > 0$ there exists a finite subset $F_{\epsilon} \subset X$ such that $d_{H}(X, F_{\epsilon}) < \epsilon$ (i.e. $\forall x \in X, \exists p \in F_{\epsilon} \text{ s.t. } \rho(x, p) < \epsilon$).

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A homomorphism of degree ϵ between two persistence modules $\mathbb U$ and $\mathbb V$ is a collection Φ of linear maps

$$(\phi_a: U_a \to V_{a+\epsilon} \mid a \in \mathbf{R})$$

such that $v_{a+\epsilon}^{b+\epsilon} \circ \phi_a = \phi_b \circ u_a^b$ for all $a \leq b$.



An ε -interleaving between \mathbb{U} and \mathbb{V} is specified by two homomorphisms of degree ϵ $\Phi : \mathbb{U} \to \mathbb{V}$ and $\Psi : \mathbb{V} \to \mathbb{U}$ s.t. $\Phi \circ \Psi$ and $\Psi \circ \Phi$ are the "shifts" of degree 2ϵ between \mathbb{U} and \mathbb{V} .



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Stability Thm: [C., Cohen-Steiner, Glisse, Guibas, Oudot - SoCG '09], [C., de Silva, Glisse Oudot 12] If U and V are q-tame and ϵ -interleaved for some $\epsilon \geq 0$ then

 $d_B(\mathsf{dgm}(\mathbb{U}),\mathsf{dgm}(\mathbb{V})) \leq \epsilon$

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Exercise: Show the stability theorem for (tame) functions :

let X be a topological space and let $f, g : X \to \mathbb{R}$ be two *tame* functions. Then

$$\mathsf{d}_{\mathrm{B}}(\mathrm{D}_f,\mathrm{D}_g) \le \|f-g\|_{\infty}.$$

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Stability Thm: [C., Cohen-Steiner, Glisse, Guibas, Oudot - SoCG '09], [C., de Silva, Glisse Oudot 12]

If $\mathbb U$ and $\mathbb V$ are q-tame and $\epsilon\text{-interleaved}$ for some $\epsilon\geq 0$ then

 $d_B(\mathsf{dgm}(\mathbb{U}),\mathsf{dgm}(\mathbb{V})) \leq \epsilon$

Strategy: build filtrations that induce **q-tame** homology persistence modules and that turn out to be ϵ -interleaved when the considered spaces/functions are $O(\epsilon)$ -close.

Multivalued maps and correspondencesCX C^T

 \mathbb{X}

Y

A multivalued map $C : \mathbb{X} \rightrightarrows \mathbb{Y}$ from a set \mathbb{X} to a set \mathbb{Y} is a subset of $\mathbb{X} \times \mathbb{Y}$, also denoted C, that projects surjectively onto \mathbb{X} through the canonical projection $\pi_{\mathbb{X}} : \mathbb{X} \times \mathbb{Y} \to \mathbb{X}$. The image $C(\sigma)$ of a subset σ of \mathbb{X} is the canonical projection onto \mathbb{Y} of the preimage of σ through $\pi_{\mathbb{X}}$.

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The transpose of C, denoted C^T , is the image of C through the symmetry map $(x, y) \mapsto (y, x)$.

A multivalued map $C : \mathbb{X} \rightrightarrows \mathbb{Y}$ is a correspondence if C^T is also a multivalued map.

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Example: *c*-correspondence and Gromov-Hausdorff distance.

Let $(\mathbb{X}, \rho_{\mathbb{X}})$ and $(\mathbb{Y}, \rho_{\mathbb{Y}})$ be compact metric spaces. A correspondence $C : \mathbb{X} \rightrightarrows \mathbb{Y}$ is an ϵ -correspondence if $\forall (x, y), (x', y') \in C$, $|\rho_{\mathbb{X}}(x, x') - \rho_{\mathbb{Y}}(y, y')| \leq \varepsilon$.

 $(x,y), (x',y') \in C, |\rho_{\mathbb{X}}(x,x') - \rho_{\mathbb{Y}}(y,y')| \leq \varepsilon.$ $y = \frac{1}{2} \inf\{\varepsilon \geq 0 : \text{there exists an } \varepsilon\text{-correspondence between } \mathbb{X} \text{ and } \mathbb{Y}\}$

 \boldsymbol{y}



Let \mathbb{S} and \mathbb{T} be two filtered simplicial complexes with vertex sets \mathbb{X} and \mathbb{Y} respectively. A multivalued map $C : \mathbb{X} \rightrightarrows \mathbb{Y}$ is ε -simplicial from \mathbb{S} to \mathbb{T} if for any $a \in \mathbb{R}$ and any simplex $\sigma \in \mathbb{S}_a$, every finite subset of $C(\sigma)$ is a simplex of $\mathbb{T}_{a+\varepsilon}$.



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Proposition: Let \mathbb{S} , \mathbb{T} be filtered complexes with vertex sets \mathbb{X} , \mathbb{Y} respectively. If $C : \mathbb{X} \rightrightarrows \mathbb{Y}$ is a correspondence such that C and C^T are both ε -simplicial, then together they induce a canonical ε -interleaving between $H(\mathbb{S})$ and $H(\mathbb{T})$.

The example of the Rips and Čech filtrations

Proposition: Let $(\mathbb{X}, \rho_{\mathbb{X}})$, $(\mathbb{Y}, \rho_{\mathbb{Y}})$ be metric spaces. For any $\epsilon > 2d_{\mathrm{GH}}(\mathbb{X}, \mathbb{Y})$ the persistence modules $\mathrm{H}(\mathrm{Rips}(\mathbb{X}))$ and $\mathrm{H}(\mathrm{Rips}(\mathbb{Y}))$ are ϵ -interleaved.

The example of the Rips and Čech filtrations

Proposition: Let (X, ρ_X) , (Y, ρ_Y) be metric spaces. For any $\epsilon > 2d_{GH}(X, Y)$ the persistence modules H(Rips(X)) and H(Rips(Y)) are ϵ -interleaved.

Proof: Let $C : \mathbb{X} \rightrightarrows \mathbb{Y}$ be a correspondence with distortion at most ϵ . If $\sigma \in \operatorname{Rips}(\mathbb{X}, a)$ then $\rho_{\mathbb{X}}(x, x') \leq a$ for all $x, x' \in \sigma$. Let $\tau \subseteq C(\sigma)$ be any finite subset. For any $y, y' \in \tau$ there exist $x, x' \in \sigma$ s. t. $y \in C(x)$, $y' \in C(x')$ so

 $\rho_{\mathbb{Y}}(y, y') \le \rho_{\mathbb{X}}(x, x') + \epsilon \le a + \epsilon \text{ and } \tau \in \operatorname{Rips}(\mathbb{Y}, a + \epsilon)$

 $\Rightarrow C \text{ is } \epsilon \text{-simplicial from } \operatorname{Rips}(\mathbb{X}) \text{ to } \operatorname{Rips}(\mathbb{Y}).$ Symetrically, C^T is $\epsilon \text{-simplicial from } \operatorname{Rips}(\mathbb{Y}) \text{ to } \operatorname{Rips}(\mathbb{X}).$

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Proposition: Let $(\mathbb{X}, \rho_{\mathbb{X}}), (\mathbb{Y}, \rho_{\mathbb{Y}})$ be metric spaces. For any $\epsilon > 2d_{GH}(\mathbb{X}, \mathbb{Y})$ the persistence modules $H(\operatorname{\check{Cech}}(\mathbb{X}))$ and $H(\operatorname{\check{Cech}}(\mathbb{Y}))$ are ϵ -interleaved.
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Proposition: Let (X, ρ_X) , (Y, ρ_Y) be metric spaces. For any $\epsilon > 2d_{GH}(X, Y)$ the persistence modules H(Rips(X)) and H(Rips(Y)) are ϵ -interleaved.

Proof: Let $C : \mathbb{X} \rightrightarrows \mathbb{Y}$ be a correspondence with distortion at most ϵ . If $\sigma \in \operatorname{Rips}(\mathbb{X}, a)$ then $\rho_{\mathbb{X}}(x, x') \leq a$ for all $x, x' \in \sigma$. Let $\tau \subseteq C(\sigma)$ be any finite subset. For any $y, y' \in \tau$ there exist $x, x' \in \sigma$ s. t. $y \in C(x), y' \in C(x')$ so

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Remark: Similar results for witness complexes (fixed landmarks)

Tameness of the Rips and Čech filtrations

Theorem: Let X be a compact metric space. Then H(Rips(X)) and H(Cech(X)) are q-tame.

As a consequence dgm(H(Rips(X))) and dgm($H(\check{Cech}(X))$) are well-defined!

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Proof: show that I_a^b : $H(Rips(X, a)) \to H(Rips(X, b))$ has finite rank whenever a < b.

Let $\epsilon = (b-a)/2$ and let $F \subset X$ be finite s. t. $d_H(X,F) \leq \epsilon/2$.

Then $C = \{(x, f) \in X \times F | d(x, f) \le \epsilon/2\}$ is an ϵ -correspondence.

Using the interleaving map, I_a^b factorizes as

 $\mathbf{H}\operatorname{Rips}(X, a) \to \mathbf{H}\operatorname{Rips}(F, a + \varepsilon) \to \mathbf{H}\operatorname{Rips}(X, a + 2\varepsilon) = \mathbf{H}\operatorname{Rips}(X, b)$ finite dimensional



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As a consequence dgm(H(Rips(X))) and dgm(H(Čech(X))) are well-defined!

Theorem: Let \mathbb{X}, \mathbb{Y} be compact metric spaces. Then

 $d_{\mathrm{b}}(\mathsf{dgm}(\mathrm{H}(\check{\mathrm{Cech}}(\mathbb{X}))),\mathsf{dgm}(\mathrm{H}(\check{\mathrm{Cech}}(\mathbb{Y})))) \leq 2d_{\mathrm{GH}}(\mathbb{X},\mathbb{Y}),$

 $d_{b}(\mathsf{dgm}(H(\operatorname{Rips}(\mathbb{X}))),\mathsf{dgm}(H(\operatorname{Rips}(\mathbb{Y})))) \leq 2d_{\operatorname{GH}}(\mathbb{X},\mathbb{Y}).$

Remark: The proofs never use the triangle inequality! The previous approch and results easily extend to other settings like, e.g. spaces endowed with a similarity measure.

Why persistence

• Even when X is compact, $H_p(Rips(X, a))$, $p \ge 1$, might be infinite dimensional for some value of a:

X a

It is also possible to build such an example with the open Rips t_{t} complex:

 $[x_0, x_1, \cdots, x_k] \in \operatorname{Rips}(X, a^-) \Leftrightarrow d_X(x_i, x_j) < a, \text{ for all } i, j$

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• For any $\alpha, \beta \in \mathbf{R}$ such that $0 < \alpha \leq \beta$ and any integer k there exists a compact metric space X such that for any $a \in [\alpha, \beta]$, $H_k(\operatorname{Rips}(X, a))$ has a non countable infinite dimension (can be embedded in \mathbf{R}^4 [Droz 2013]).

Why persistence

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- If X is compact, then dim H₁(Čech(X, a)) < +∞ for all a ([Smale-Smale, C.-de Silva]).
- If X is geodesic, then $\dim H_1(\operatorname{Rips}(X, a)) < +\infty$ for all a > 0 and $\operatorname{Dgm}(H_1(\operatorname{Rips}(X)))$ is contained in the vertical line x = 0.
- If X is a geodesic δ -hyperbolic space then $Dgm(H_2(Rips(X)))$ is contained in a vertical band of width $O(\delta)$.

Some weaknesses

If \mathbb{X} and \mathbb{Y} are pre-compact metric spaces, then

 $d_{\mathrm{b}}(\mathsf{dgm}(\operatorname{Rips}(\mathbb{X})), \mathsf{dgm}(\operatorname{Rips}(\mathbb{Y}))) \leq d_{GH}(\mathbb{X}, \mathbb{Y}).$

 \rightarrow Vietoris-Rips (or Cech, witness) filtrations quickly become prohibitively large as the size of the data increases ($O(|X|^d)$), making the computation of persistence practically almost impossible.

 \rightarrow Persistence diagrams of Rips-Vietoris (and Cěch, witness,..) filtrations and Gromov-Hausdorff distance are very sensitive to noise and outliers.

Statistical setting

 (\mathbb{M},ρ) metric space

 μ a probability measure with compact support $\mathbb{X}_{\mu}.$

Sample m points according to μ .

Examples:

- $\operatorname{Filt}(\widehat{\mathbb{X}}_m) = \operatorname{Rips}_{\alpha}(\widehat{\mathbb{X}}_m)$
- $\operatorname{Filt}(\widehat{\mathbb{X}}_m) = \operatorname{\check{C}ech}_{\alpha}(\widehat{\mathbb{X}}_m)$

- $\operatorname{Filt}(\widehat{\mathbb{X}}_m) = \operatorname{sublevelset} \operatorname{filtration} \operatorname{of} \rho(., \mathbb{X}_\mu).$



Questions:

• Statistical properties of dgm(Filt($\widehat{\mathbb{X}}_m$)) ? dgm(Filt($\widehat{\mathbb{X}}_m$)) \rightarrow ? as $m \rightarrow +\infty$?

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 $\mathsf{dgm}(\mathrm{Filt}(\widehat{\mathbb{X}}$

0



 $\widehat{\mathbb{X}}_m$

- Statistical properties of dgm(Filt($\widehat{\mathbb{X}}_m$)) ? dgm(Filt($\widehat{\mathbb{X}}_m$)) \rightarrow ? as $m \rightarrow +\infty$?
- Can we do more statistics with persistence diagrams?

Statistical setting



0

Stability thm: $d_b(dgm(Filt(\mathbb{X}_{\mu})), dgm(Filt(\widehat{\mathbb{X}}_m))) \leq 2d_{GH}(\mathbb{X}_{\mu}, \widehat{\mathbb{X}}_m)$

So, for any $\varepsilon > 0$, $\mathbb{P}\left(\mathrm{d}_{\mathrm{b}}\left(\mathsf{dgm}(\mathrm{Filt}(\mathbb{X}_{\mu})), \mathsf{dgm}(\mathrm{Filt}(\widehat{\mathbb{X}}_{m}))\right) > \varepsilon\right) \leq \mathbb{P}\left(d_{GH}(\mathbb{X}_{\mu}, \widehat{\mathbb{X}}_{m}) > \frac{\varepsilon}{2}\right)$

Deviation inequality



For a, b > 0, μ satisfies the (a, b)-standard assumption if for any $x \in \mathbb{X}_{\mu}$ and any r > 0, we have $\mu(B(x, r)) \ge \min(ar^{b}, 1)$.

Deviation inequality



For a, b > 0, μ satisfies the (a, b)-standard assumption if for any $x \in X_{\mu}$ and any r > 0, we have $\mu(B(x, r)) \ge \min(ar^{b}, 1)$.

Theorem: If μ satisfies the (a, b)-standard assumption, then for any $\varepsilon > 0$:

$$\mathbb{P}\left(\mathrm{d}_{\mathrm{b}}\left(\mathsf{dgm}(\mathrm{Filt}(\mathbb{X}_{\mu})), \mathsf{dgm}(\mathrm{Filt}(\widehat{\mathbb{X}}_{m}))\right) > \varepsilon\right) \le \min(\frac{8^{b}}{a\varepsilon^{b}}\exp(-ma\varepsilon^{b}), 1).$$

Moreover
$$\lim_{n \to \infty} \mathbb{P}\left(\mathrm{d}_{\mathrm{b}}\left(\mathsf{dgm}(\mathrm{Filt}(\mathbb{X}_{\mu})), \mathsf{dgm}(\mathrm{Filt}(\widehat{\mathbb{X}}_{m})) \right) \leq C_{1}\left(\frac{\log m}{m} \right)^{1/b} \right) = 1.$$

where C_1 is a constant only depending on a and b.

Deviation inequality



For a, b > 0, μ satisfies the (a, b)-standard assumption if for any $x \in \mathbb{X}_{\mu}$ and any r > 0, we have $\mu(B(x, r)) \ge \min(ar^{b}, 1)$.

Sketch of proof:

- 1. Upperbound $\mathbb{P}\left(d_H(\mathbb{X}_{\mu}, \widehat{\mathbb{X}}_m) > \frac{\varepsilon}{2}\right)$.
- 2. (a, b) standard assumption \Rightarrow an explicit upperbound for the covering number of \mathbb{X}_{μ} (by balls of radius $\varepsilon/2$).
- 3. Apply "union bound" argument.



Minimax rate of convergence

[C., Glisse, Labruère, Michel ICML'14 - JMLR'15]

Let $\mathcal{P}(a, b, \mathbb{M})$ be the set of all the probability measures on the metric space (\mathbb{M}, ρ) satisfying the (a, b)-standard assumption on \mathbb{M} :

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Theorem: Let $\mathcal{P}(a, b, \mathbb{M})$ be the set of (a, b)-standard proba measures on \mathbb{M} . Then:

$$\sup_{\mu \in \mathcal{P}(a,b,\mathbb{M})} \mathbb{E}\left[\mathrm{d}_{\mathrm{b}}(\mathsf{dgm}(\mathrm{Filt}(\mathbb{X}_{\mu})), \mathsf{dgm}(\mathrm{Filt}(\widehat{\mathbb{X}}_{m})))\right] \leq C\left(\frac{\ln m}{m}\right)^{1/b}$$

where the constant C only depends on a and b (not on $\mathbb{M}!$). Assume moreover that there exists a non isolated point x in \mathbb{M} and let x_m be a sequence in $\mathbb{M} \setminus \{x\}$ such that $\rho(x, x_m) \leq (am)^{-1/b}$. Then for any estimator $\widehat{\operatorname{dgm}}_m$ of $\operatorname{dgm}(\operatorname{Filt}(\mathbb{X}_\mu))$:

$$\liminf_{m \to \infty} \rho(x, x_m)^{-1} \sup_{\mu \in \mathcal{P}(a, b, \mathbb{M})} \mathbb{E}\left[\mathrm{d}_{\mathrm{b}}(\mathsf{dgm}(\mathrm{Filt}(\mathbb{X}_{\mu})), \widehat{\mathsf{dgm}}_m) \right] \ge C'$$

where C' is an absolute constant.

Remark: we can obtain slightly better bounds if \mathbb{X}_{μ} is a submanifold of \mathbb{R}^{D} - see [Genovese, Perone-Pacifico, Verdinelli, Wasserman 2011, 2012]

Numerical illustrations



- μ : unif. measure on Lissajous curve \mathbb{X}_{μ} . - Filt: distance to \mathbb{X}_{μ} in \mathbb{R}^2 .

- sample k = 300 sets of m points for m = [2100:100:3000].

- compute

$$\widehat{\mathbb{E}}_m = \widehat{\mathbb{E}}[d_B(\mathsf{dgm}(\mathrm{Filt}(\mathbb{X}_\mu)), \mathsf{dgm}(\mathrm{Filt}(\widehat{\mathbb{X}_n})))].$$

- plot $\log(\widehat{\mathbb{E}}_m)$ as a function of $\log(\log(m)/m)$.



Numerical illustrations







Persistence landscapes



Persistence landscape [Bubenik 2012]:

$$\lambda_D(k,t) = \underset{p \in \mathsf{dgm}}{\mathsf{kmax}} \Lambda_p(t), \quad t \in \mathbb{R}, k \in \mathbb{N},$$

where kmax is the kth largest value in the set.

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Properties

- For any $t \in \mathbb{R}$ and any $k \in \mathbb{N}$, $0 \leq \lambda_D(k, t) \leq \lambda_D(k+1, t)$.
- For any $t \in \mathbb{R}$ and any $k \in \mathbb{N}$, $|\lambda_D(k,t) \lambda_{D'}(k,t)| \leq d_B(D,D')$ where $d_B(D,D')$ denotes the bottleneck distance between D and D'.

stability properties of persistence landscapes

Persistence landscapes



- Persistence encoded as an element of a functional space (vector space!).
- Expectation of distribution of landscapes is well-defined and can be approximated from average of sampled landscapes.
- process point of view: convergence results and convergence rates → confidence intervals can be computed using bootstrap.

[C., Fasy, Lecci, Rinaldo, Wasserman SoCG 2014]

Weak convergence of landscapes

Let \mathcal{L}_T be the space of landscapes with support contained in [0, T].

Let P be a probability distribution on \mathcal{L}_T , and let $\lambda_1, \ldots, \lambda_n \sim P$. Let μ be the mean landscape:

$$\mu(t) = \mathbb{E}[\lambda_i(t)], \quad t \in [0, T].$$

We estimate μ with the sample average

$$\overline{\lambda}_n(t) = \frac{1}{n} \sum_{i=1}^n \lambda_i(t), \quad t \in [0, T].$$

Since $\mathbb{E}(\overline{\lambda}_n(t)) = \mu(t)$, $\overline{\lambda}_n$ is a point-wise unbiased estimator of μ .

For fixed t: pointwise convergence of $\lambda_n(t)$ to $\mu(t) + CLT$

Here, convergence of the process

$$\left\{\sqrt{n}\left(\overline{\lambda}_n(t) - \mu(t)\right)\right\}_{t \in [0,T]}$$

Weak convergence of landscapes

Let

 $\mathcal{F} = \{f_t\}_{0 \le t \le T}$

where $f_t : \mathcal{L}_T \to \mathbb{R}$ is defined by $f_t(\lambda) = \lambda(t)$. Empirical process indexed by $f_t \in \mathcal{F}$:

$$\mathbb{G}_n(t) = \mathbb{G}_n(f_t) := \sqrt{n} \left(\overline{\lambda}_n(t) - \mu(t)\right) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \left(f_t(\lambda_i) - \mu(t)\right) = \sqrt{n} (P_n - P)(f_t)$$

Theorem [Weak convergence of landscapes]. Let \mathbb{G} be a Brownian bridge with covariance function $\kappa(t,s) = \int f_t(\lambda) f_s(\lambda) dP(\lambda) - \int f_t(\lambda) dP(\lambda) \int f_s(\lambda) dP(\lambda)$, for $t,s \in [0,T]$. Then $\mathbb{G}_n \rightsquigarrow \mathbb{G}$.

Weak convergence of landscapes

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For $t \in [0,T]$, let $\sigma(t)$ be the standard deviation of $\sqrt{n}\,\overline{\lambda}_n(t)$, i.e. $\sigma(t) = \sqrt{N \operatorname{Var}(\overline{\lambda}_n(t))} = \sqrt{\operatorname{Var}(f_t(\lambda_1))}.$

Theorem [Uniform CLT]. Suppose that $\sigma(t) > c > 0$ in an interval $[t_*, t^*] \subset [0, T]$, for some constant c. Then there exists a random variable $W \stackrel{d}{=} \sup_{t \in [t_*, t^*]} |\mathbb{G}(f_t)|$ such that

$$\sup_{z \in \mathbb{R}} \left| \mathbb{P}\left(\sup_{t \in [t_*, t^*]} \left| \mathbb{G}_n(t) \right| \le z \right) - \mathbb{P}\left(W \le z \right) \right| = O\left(\frac{(\log n)^{7/8}}{n^{1/8}} \right).$$

Some consequences

Bootstrap for landscapes \rightarrow confidence bands for landscapes.

Theorem. Suppose that $\sigma(t) > c > 0$ in an interval $[t_*, t^*] \subset [0, T]$, for some constant c. Then, given a confidence level $1 - \alpha$, one can construct confidence functions $\ell_n(t)$ and $u_n(t)$ such that

$$\mathbb{P}\Big(\ell_n(t) \le \mu(t) \le u_n(t) \text{ for all } t \in [t_*, t^*]\Big) \ge 1 - \alpha - O\left(\frac{(\log n)^{7/8}}{n^{1/8}}\right)$$



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To summarize



Wasserstein distance

Let (\mathbb{M}, ρ) be a metric space and let μ , ν be probability measures on \mathbb{M} with finite p-moments ($p \ge 1$).

"The" Wasserstein distance $W_p(\mu, \nu)$ quantifies the optimal cost of pushing μ onto ν , the cost of moving a small mass dx from x to y being $\rho(x, y)^p dx$.



- Transport plan: Π a proba measure on $M \times M$ such that $\Pi(A \times \mathbb{R}^d) = \mu(A)$ and $\Pi(\mathbb{R}^d \times B) = \nu(B)$ for any borelian sets $A, B \subset M$.
- Cost of a transport plan:

$$C(\Pi) = \left(\int_{M \times M} \rho(x, y)^p d\Pi(x, y)\right)^{\frac{1}{p}}$$

• $W_p(\mu,\nu) = \inf_{\Pi} C(\Pi)$

(Sub)sampling and stability of expected landscapes

[C., Fasy, Lecci, Michel, Rinaldo, Wasserman ICML 2015]



Theorem: Let (\mathbb{M}, ρ) be a metric space and let μ , ν be probal measures on \mathbb{M} with compact supports. We have

$$\|\Lambda_{\mu,m} - \Lambda_{\nu,m}\|_{\infty} \le m^{\frac{1}{p}} W_p(\mu,\nu)$$

where W_p denotes the Wasserstein distance with cost function $\rho(x, y)^p$.

Remarks:

- similar results by Blumberg et al (2014) in the (Gromov-)Prokhorov metric (for distributions, not for expectations) ;

- also work with "Gromov-Wasserstein" metric;

- $m^{\overline{p}}$ cannot be replaced by a constant.

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where W_p denotes the Wasserstein distance with cost function $\rho(x, y)^p$.

Consequences:

- Subsampling: efficient and easy to parallelize algorithm to infer topol. information from huge data sets.
- Robustness to outliers.
- R package TDA +Gudhi library: https://project.inria.fr/gudhi/software/

(Sub)sampling and stability of expected landscapes

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$$\|\Lambda_{\mu,m} - \Lambda_{\nu,m}\|_{\infty} \le m^{\frac{1}{p}} W_p(\mu,\nu)$$

where W_p denotes the Wasserstein distance with cost function $\rho(x, y)^p$. **Proof:**

1.
$$W_p(\mu^{\otimes m}, \nu^{\otimes m}) \leq m^{\frac{1}{p}} W_p(\mu, \nu)$$

- 2. $W_p(P_{\mu}, P_{\nu}) \leq W_p(\mu^{\otimes m}, \nu^{\otimes m})$ (stability of persistence!)
- 3. $\|\Lambda_{\mu,m} \Lambda_{\nu,m}\|_{\infty} \leq W_p(P_\mu, P_\nu)$ (Jensen's inequality)

(Sub)sampling and stability of expected landscapes [C., Fasy, Lecci, Michel, Rinaldo, Wasserman ICML 2015]

Example: Circle with one outlier.



(Sub)sampling and stability of expected landscapes [C., Fasy, Lecci, Michel, Rinaldo, Wasserman ICML 2015]

Example: 3D shapes



From n = 100 subsamples of size m = 300

(Sub)sampling and stability of expected landscapes [C., Fasy, Lecci, Michel, Rinaldo, Wasserman ICML 2015]

(Toy) Example: Accelerometer data from smartphone.



spatial time series (accelerometer data from the smarphone of users).
no registration/calibration preprocessing step needed to compare!

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Software:

- The Gudhi library (C++): https://project.inria.fr/gudhi/software/
- R package TDA