Stability of Persistence Diagrams: Continued

Edelsbrunner and Harer (2010), C.VIII
A *triangulation* of a topological space $X$ is a simplicial complex $K$ together with a homeomorphism between $X$ and $|K|$, the support of $K$.

Let $X$ be *triangulable* (i.e., if it has a triangulation) and $f : X \to \mathbb{R}$ continuous.

Define *sublevel set*

$$X_a = f^{-1}(-\infty, a],$$

for $a \in \mathbb{R}$ and for $a \leq b$

$$f_p^{a,b} : \mathbb{H}_p(X_a) \to \mathbb{H}_p(X_b).$$

The *$p$-th persistent homology group* is defined to be

$$\mathbb{H}^{a,b}_p = \text{im } f_p^{a,b}.$$

The *$p$-th persistent Betti number* is

$$\beta^{a,b}_p = \text{rank } \mathbb{H}^{i,j}_p.$$
Tame functions

- A group isomorphism is a function between two groups that sets up a one-to-one correspondence between the elements of the groups that respects the given group operations/relations among the elements.
- Greek: iso means “equal”, and morphosis means “to shape”.
- \( a \in \mathbb{R} \) is a homological critical value if there is no \( \epsilon > 0 \) for which \( f_{p}^{a-\epsilon, a+\epsilon} \) is an isomorphismism for each \( p \).
- \( f \) is tame if it has only finitely many homological critical values and all homology groups of all sub level sets have finite rank.
Let $X$ be a triangulable topological space, $f, g : X \to \mathbb{R}$ two tame functions. For each dimension $p$, the bottleneck distance between the diagrams $X = \text{Dgm}_p(f)$ and $Y = \text{Dgm}_p(g)$ is bounded from above by the $L_\infty$ distance between the functions (Edelsbrunner and Harer, 2010, Page 183), that is,

$$W_\infty(X, Y) \leq \|f - g\|_\infty.$$
Given two persistence diagrams $X$ and $Y$

The **degree-$q$ Wasserstein distance** is

$$W_q(X, Y) = \left[ \inf_{\eta: X \to Y} \sum_{x \in X} ||x - \eta(x)||_\infty^q \right]^{1/q}$$

Think about assignment problem

Hungarian algorithm: find a perfect matching (in a bipartite graph) with a minimum total cost

**Software:** [https://bitbucket.org/grey_narn/hera](https://bitbucket.org/grey_narn/hera)

Kerber et al. (2016)
Stability with Wasserstein distance

- A function $f : \mathbb{X} \to \mathbb{R}$ is **Lipschitz** if there is a constant $C$ such that
  \[ |f(x) - f(y)| \leq C||x - y|| \]
  for all points $x, y \in \mathbb{X}$.
- mesh: max distance between two points in $\sigma \in K$
- $N(r)$: minimum number of simplices whose mesh $\leq r$.
- A triangulation of $\mathbb{X}$ **grows polynomially** if there are constants $c$ and $j$ such that $N(r) \leq \frac{c}{r^j}$. 
Let $f, g : X \to \mathbb{R}$ be two tame Lipschitz functions on a metric space whose triangulations grow polynomially with constant $j$. Then there are constants $C$ and $k > j$ no smaller than 1 such that the degree-$q$ Wasserstein distance between $X = \text{Dgm}_p(f)$ and $Y = \text{Dgm}_p(g)$ is

$$W_q(X, Y) \leq C \cdot \|f - g\|_{\infty}^{1 - k/q}$$

for every $q \geq k$.
The Assignment Problem

- Given a weighted bipartite graph \( G \) with \( n + n \) vertices (\( n \) vertices on each side), find a perfect matching with minimal cost.
- A common cost function is the minimum of the sum of the \( q \)-th power of weights of the matching edges for some \( q \leq 1 \).
- The solution: \( q \)-Wasserstein distance
- Bottleneck distance computation: Hopcroft + Karp using k-d tree
- Wasserstein distance computation: Bertsekas using weighted k-d tree
Kernels for barcodes
Let $H$ be a vector space over $\mathbb{R}$

A function $\langle \cdot , \cdot \rangle_H : H \times H \to \mathbb{R}$ is an inner product on $H$ if

- Linear: $\langle \alpha_1 f_1 + \alpha_2 f_2, g \rangle_H = \alpha_1 \langle f_1, g \rangle_H + \alpha_2 \langle f_2, g \rangle_H$.
- Symmetric: $\langle f, g \rangle_H = \langle g, h \rangle_H$.
- $\langle f, f \rangle_H \geq 0$.
- $\langle f, f \rangle_H = 0$ iff $f = 0$.

Norm induced by the inner product

$$\| f \|_H := \sqrt{\langle f, f \rangle_H}.$$
Hilbert space

- Hilbert space: an inner product space that contains a Cauchy sequence.
- Wait a minute...
- A *Hilbert space* is an abstract vector space with the structure of an inner product that allows lengths and angles to be measured.
- A generalizes the notion of Euclidean space.
Given a set $X$, a function $K : X \times X \to \mathbb{R}$ is a \textit{kernel} if there exists a Hilbert space $H$ called a \textit{feature space} such that

$$K(x, y) = \langle \Phi(x), \Phi(y) \rangle_H$$

for all $x, y \in X$.

Alternatively, $K$ is a kernel if it is symmetric and positive definite.

A symmetric function $K : X \times X \to \mathbb{R}$ is \textit{positive definite} if $\forall n \geq 1$, $\forall a_1, \cdots, a_n \in \mathbb{R}^n$, $\forall x_1, \cdots, x_n \in X^n$,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j K(x_i, x_j) \geq 0.$$ 

Kernels are positive definite

Let $H$ be a Hilbert space, $X$ is a nonempty set and $\Phi : \mathbb{X} \to H$, then $K(x, y) := \langle \Phi(x), \Phi(y) \rangle_H$ is positive definite.
TDA Kernels and Vectorizations

- [link] https://github.com/MathieuCarriere/sklearn_tda
- **Kernels:**
  - Persistence scale space kernel, Reininghaus et al. (2015)
  - Persistence weighted Gaussian kernel
  - Sliced Wasserstein kernel
  - Persistence Fisher kernel
- **Vectorizations:**
  - Persistence Image, Adams et al. (2017)
  - Persistence landscape
  - Betti Curve
  - Silhouette
TDA Kernels in applications

Reininghaus et al. (2015)
Let $F, G$ be two persistence diagram (of a fixed dimension $p$).

The persistence scale space kernel is

$$K_\sigma(F, G) = \frac{1}{8\pi\sigma} \sum_{p \in F, q \in G} \left( e^{-\frac{||p-q||^2}{8\sigma}} - e^{-\frac{||p-\bar{q}||^2}{8\sigma}} \right)$$

$\bar{p}$ is $p$ mirrored at the diagonal.
Persistence scale space kernel

- $\mathcal{D}$ : set of persistence diagrams
- Parameter: $\sigma$
- $L_2(\Omega)$: set of $L_2$ functions (square integrable) on $\Omega \subset \mathbb{R}^2$
- Feature map: $\Phi_\sigma : \mathcal{D} \rightarrow L_2(\Omega)$
- $K_\sigma(F, G) = \langle \Phi_\sigma(F), \Phi_\sigma(G) \rangle_{L_2(\Omega)}$
- Stability of the persistence scale space kernel:
  \[ ||\Phi_\sigma(F) - \Phi_\sigma(G)||_{L_2(\Omega)} \leq \frac{1}{\sigma \sqrt{8\pi}} W_1(F, G) \]
- $W_1(F, G)$: degree-1 Wasserstein distance.

