# A Stable Multi-Scale Kernel for Topological Machine Learning

Jan Reininghaus[1], Stefan Huber[1], Ulrich Bauer[1,2], Roland Kwitt[3]
[1]IST Austria. [2]TU München. [3]University of Salzburg, Austria.

*Topological data analysis* offers a rich source of valuable information to study vision problems. Yet, so far we lack a theoretically sound connection to popular kernel-based learning techniques, such as kernel SVMs or kernel PCA. In this work, we establish such a connection by designing a multi-scale kernel for persistence diagrams (see Fig. 1), a stable summary representation of topological features in data. We show that this kernel is positive definite and prove its stability with respect to the 1-Wasserstein distance. Experiments on two benchmark datasets for 3D shape classification/retrieval and texture recognition show considerable performance gains of the proposed method compared to an alternative approach that is based on the recently introduced persistence landscapes.

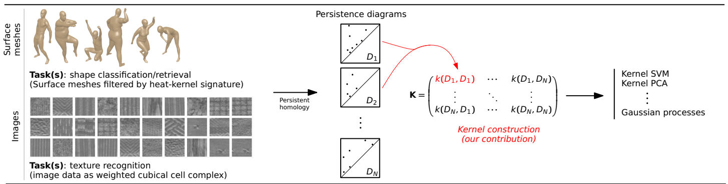


Figure 1: Overview of **our contribution**.

**Persistence diagrams.** *Persistence diagrams* are a concise description of the topological changes occurring in a growing sequence of shapes, called *filtration*. In particular, during the growth of a shape, holes of different dimension (*i.e.*, gaps between components, tunnels, voids, etc.) may appear and disappear. Intuitively, a $k$-dimensional hole, born at time $b$ and filled at time $d$, gives rise to a point $(b,d)$ in the $k^{\text{th}}$ persistence diagram. A persistence diagram is thus a multiset of points in $\mathbb{R}^2$.

**Filtrations from functions.** A standard way of obtaining a filtration is to consider the *sublevel sets* $f^{-1}(-\infty, t]$ of a function $f\colon \Omega \to \mathbb{R}$ defined on some domain $\Omega$, for $t \in \mathbb{R}$. It is easy to see that the sublevel sets indeed form a filtration parametrized by $t$. We denote the resulting persistence diagram by $D_f$. *Example(s):* Consider a grayscale image, where $\Omega$ is the rectangular domain of the image and $f$ is the grayscale value at any point of the domain (*i.e.*, at a particular pixel). A sublevel set would thus consist of all pixels of $\Omega$ with value up to a certain threshold $t$. Another example would be a piecewise linear function on a triangular mesh $\Omega$, such as the popular heat kernel signature [6]. Yet another commonly used filtration arises from point clouds $P$ embedded in $\mathbb{R}^n$, by considering the distance function $d_P(x) = \min_{p \in P} \|x - p\|$ on $\Omega = \mathbb{R}^n$. The sublevel sets of this function are unions of balls around $P$.

**The persistence scale-space (PSS) kernel.** We propose a stable *multi-scale* kernel $k_\sigma$ for the set of persistence diagrams $\mathcal{D}$. This kernel will be defined via a *feature map* $\Phi_\sigma\colon \mathcal{D} \to L_2(\Omega)$, with $\Omega \subset \mathbb{R}^2$ denoting the closed half plane above the diagonal, *i.e.*, $\Omega = \{x = (x_1, x_2) \in \mathbb{R}^2 \colon x_2 \geq x_1\}$.

Since, a persistence diagram $D$ can be uniquely represented as a sum of Dirac delta distributions, we use the sum as an initial condition for a heat diffusion problem with a Dirichlet boundary condition on the diagonal. The solution of this partial differential equation (see paper) is an $L_2(\Omega)$ function for any chosen scale parameter $\sigma > 0$. We define the feature map (see Fig. 2 for an illustration) $\Phi_\sigma\colon \mathcal{D} \to L_2(\Omega)$ at scale $\sigma > 0$ of a persistence diagram $D$ as $\Phi_\sigma(D) = u|_{t=\sigma}$ with $u\colon \Omega \times \mathbb{R}_{\geq 0} \to \mathbb{R}$

$$u(x,t) = \frac{1}{4\pi t} \sum_{p \in D} \exp\left(-\frac{\|x-p\|^2}{4t}\right) - \exp\left(-\frac{\|x-\overline{p}\|^2}{4t}\right) \tag{1}$$

being the closed-form solution to the aforementioned partial differential equation. This map yields the persistence scale space kernel $k_\sigma$ on $\mathcal{D}$ as

$$k_\sigma(F,G) = \langle \Phi_\sigma(F), \Phi_\sigma(G) \rangle_{L_2(\Omega)} \tag{2}$$

This is an extended abstract. The full paper is available at the Computer Vision Foundation webpage or on arXiv at http://arxiv.org/abs/1412.6821.

and we can derive a simple expression for evaluating the kernel:

$$\boxed{k_\sigma(F,G) = \frac{1}{8\pi\sigma} \sum_{\substack{p \in F \\ q \in G}} \exp\left(-\frac{\|p-q\|^2}{8\sigma}\right) - \exp\left(-\frac{\|p-\overline{q}\|^2}{8\sigma}\right)} \tag{3}$$

where $\overline{q} = (b,a)$ is $q = (a,b)$ mirrored at the diagonal.

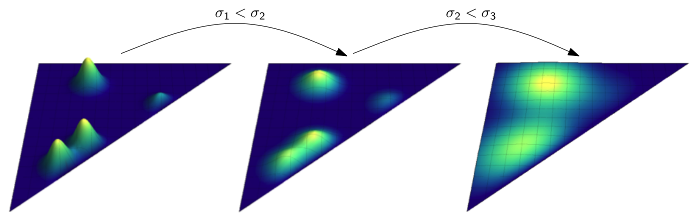


Figure 2: The feature map $\Phi_\sigma(D)$ as a function in $L_2(\Omega)$ at growing $\sigma$.

With the *p-Wasserstein distance* (for positive real $p$) defined as

$$d_{W,p}(F,G) = \left( \inf_\gamma \sum_{x \in F} \|x - \gamma(x)\|_\infty^p \right)^{\frac{1}{p}}, \tag{4}$$

we prove the following result:

**Theorem 1** *The kernel $k_\sigma$ is* 1*-Wasserstein stable.*

We further prove that Theorem 1 is *sharp* in the sense that *no* non-trivial (*i.e.*, $\forall F, G \in \mathcal{D}\colon k(F,G) \neq 0$) additive kernel (see paper for definition) can be stable w.r.t. the $p$-Wasserstein distance when $p > 1$.

**Evaluation.** In the paper, we report results on two vision tasks where persistent homology has already been shown to provide valuable discriminative information [3]: *shape classification/retrieval* (on SHREC 2014 [5]) and *texture image classification* (on the `Outex_TC_00000` benchmark [4]); see Fig. 3 for an illustration of the datasets. We primarily compare against a kernel that can be constructed based on Bubenik's concept of *persistence landscapes* [2], a representation of persistence diagrams as functions in the Banach space $L_p(\mathbb{R}^2)$. For $p = 2$, we can use the Hilbert space structure of $L_2(\mathbb{R}^2)$ to construct a kernel analogously to (2). Our experimental results are listed in the paper.

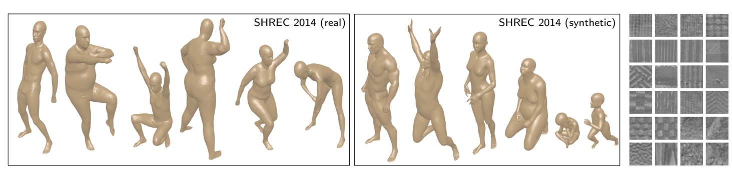


Figure 3: Datasets used in our experiments (see paper).

**Implementation.** DIPHA [1] is freely available at http://goo.gl/EXSpm1, the kernel implementation (compatible with DIPHA) will be made available right after the conference.

[1] U. Bauer, M. Kerber, and J. Reininghaus. Distributed computation of persistent homology. In *ALENEX*, 2014.

[2] P. Bubenik. Statistical topological data analysis using persistence landscapes. arXiv, available at http://arxiv.org/abs/1207.6437, 2012.

[3] C. Li, M. Ovsjanikov, and F. Chazal. Persistence-based structural recognition. In *CVPR*, 2014.

[4] T. Ojala, T. Mäenpää, M. Pietikäinen, J. Viertola, J. Kyllonen, and S. Huovinen. OuTeX – new framework for empirical evaluation of texture analysis algorithms. In *ICPR*, 2002.

[5] Pickup, D. *et al.*. SHREC '14 track: Shape retrieval of non-rigid 3d human models. In *Proceedings of the 7th Eurographics workshop on 3D Object Retrieval*, EG 3DOR'14. Eurographics Association, 2014.

[6] J. Sun, M. Ovsjanikov, and L. Guibas. A concise and probably informative multi-scale signature based on heat diffusion. In *SGP*, 2009.