# INTRINSIC PERSISTENT HOMOLOGY VIA DENSITY-BASED METRIC LEARNING

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ABSTRACT. We address the problem of estimating intrinsic distances in a manifold from a finite sample. We prove that the metric space defined by the sample endowed with a computable metric known as sample Fermat distance converges a.s. in the sense of Gromov–Hausdorff. The limiting object is the manifold itself endowed with the population Fermat distance, an intrinsic metric that accounts for both the geometry of the manifold and the density that produces the sample. This result is applied to obtain intrinsic persistence diagrams, which are less sensitive to the particular embedding of the manifold in the Euclidean space. We show that this approach is robust to outliers and deduce a method for pattern recognition in signals, with applications in real data.

#### 1. INTRODUCTION

1.1. Motivation and problem statement. Let  $X_n$  be a set of n sample points with common density f supported on a smooth compact Riemannian manifold  $\mathcal{M}$  embedded in  $\mathbb{R}^{D}$ . We are interested in recovering topological features of  $\mathcal{M}$  from the sample  $\mathbb{X}_{n} \subseteq \mathbb{R}^{D}$ in a setting in which both  $\mathcal{M}$  and f are assumed to be unknown. A standard approach to accomplish this task consists in applying a computational technique known as *persistent* homology to  $X_n$ . Here, the sample  $X_n$  is considered as a metric space endowed with some computable distance, such as the Euclidean distance or an estimator of the inherited geodesic distance. Although the topological information carried by  $\mathcal{M}$  remains the same when endowed with any Riemannian metric, the output of the application of persistent homology to  $\mathbb{X}_n$  strongly depends on the particular distance function employed. In this article, we consider a computable estimator defined over  $\mathbb{X}_n$  of a certain Riemannian metric on  $\mathcal{M}$  that takes into account the density f, which was called *Fermat distance* in [35]. We show that the use of this density based intrinsic metric in the computation of persistent homology can lead to result that overcome simultaneously certain weaknesses of standard approaches, such as the sensitivity to outliers and the dependence on the embedding of the sample in the ambient space.

Persistent homology [9, 25, 27, 51, 61] is a central technique in Topological Data Analysis (TDA) that allows to infer the homology groups of a space by studying a sample  $X_n$  at all scales of resolution at the same time. As a result, this method yields an object called *persistence diagram* associated to the sample. Under mild conditions, the homology groups of the underlying topological space can be read off the persistence diagram [27]. In [12, 14], the authors provide a general framework that allows to define persistence diagrams for infinite metric spaces instead of just finite approximations (samples). Thus, one can view the persistence diagram associated to a sample of a space as an estimate of a limiting object, namely, the persistence diagram of the entire space. When the distinction is needed, we

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will call these diagrams sample persistence diagram and population persistence diagram respectively.

Our main result states that, under reasonable conditions, there is convergence as metric spaces of the sample  $X_n$  endowed with a computable estimator of the Fermat distance towards the manifold  $\mathcal{M}$  (equipped with the Fermat distance) in the sense of Gromov– Hausdorff as the size n grows. This extends and streamlines methods and results from [35, 46]. When combined with the well-known *stability theorem* [12, 15, 21], this approximation result as metric spaces allows to deduce the convergence of the corresponding persistence diagrams. For this purpose, the space of diagrams is naturally equipped with the *bottleneck distance*. Approximation results that include convergence rates and confidence regions have been established when the metric of the target space is known (see [29] where the Euclidean distance is considered for both the samples and the space and also [16], where a general metric is used but assumed to be known in advance).

Persistence diagrams are known to be sensitive to the presence of outliers [5, 6, 11, 13]. In [5, 13], the authors propose filtrations of point clouds regarded as empirical measures in the ambient Euclidean space — called DTM-filtrations — to achieve a robust computation of ambient persistent homology. This theory was later extended to general metric spaces in [11]. On the other hand, intrinsic versions of the classical Čech and Vietoris–Rips filtrations were developed with the aim of capturing topological properties of manifolds sitting in an Euclidean space which are independent of the embedding. The approach exhibited in this article handles both difficulties at the same time. Indeed, we show that sample persistence diagrams computed using the estimator of the (intrinsic) Fermat distance are both robust to outliers for positive degree and display the correct homology of the manifold for a longer parameter interval as compared with the use of ambient Euclidean distance.

We refer the reader to [33] for a video containing an introductory exposition of the contents of this article.

1.2. Contributions. Let  $(\mathcal{M}, \rho)$  be a smooth *d*-dimensional Riemannian manifold embedded in  $\mathbb{R}^D$  with density  $f : \mathcal{M} \to \mathbb{R}_{>0}$  and a Riemannian density-based distance  $\rho$  (mainly, it will be the Fermat distance  $d_{f,p}$  defined below).

For p > 1, the population Fermat distance is defined as

$$d_{f,p}(x,y) = \inf_{\gamma} \int_{I} \frac{1}{f(\gamma_t)^{(p-1)/d}} |\dot{\gamma_t}| dt.$$

Here  $x, y \in \mathcal{M}$ ,  $|\cdot|$  denotes the Euclidean distance and the infimum is taken over all piecewise smooth curves  $\gamma: I = [0, 1] \to \mathcal{M}$  with  $\gamma(0) = x$ , and  $\gamma(1) = y$ . In the special case when f is uniform, the population Fermat distance reduces to (a multiple of) the inherited Riemannian distance  $d_{\mathcal{M}}$  from the ambient Euclidean space. When this is not the case, this distance takes into account the density, which can be advantageous in certain situations [35, 55]. This metric was also considered in [39, 46].

Given a finite set of points  $X_n$ , the sample Fermat distance between x, y is defined as

$$d_{\mathbb{X}_n,p}(x,y) = \inf_{\gamma} \sum_{i=0}^{\prime} |x_{i+1} - x_i|^p$$

where the infimum is taken over all paths  $\gamma = (x_0, x_1, \dots, x_{r+1})$  with  $x_0 = x$ ,  $x_{r+1} = y$ and  $\{x_1, x_2, \dots, x_r\} \subseteq \mathbb{X}_n$ .

Our main result states the Gromov-Hausdorff convergence (a.s.) of the sample endowed with the sample Fermat distance, appropriately re-scaled, to  $(\mathcal{M}, d_{f,p})$ .

**Theorem.** Let  $\mathcal{M}$  be a smooth, closed d-dimensional Riemannian manifold embedded in  $\mathbb{R}^D$ . Let  $f : \mathcal{M} \to \mathbb{R}_{>0}$  be a smooth density function. Let  $\mathbb{X}_n = \{x_1, x_2, \ldots, x_n\} \subseteq \mathcal{M}$  be a set of n independent sample points in  $\mathcal{M}$  with common density f. Given p > 1, there exists a constant  $\mu = \mu(p, d)$  such that for every  $\lambda \in ((p-1)/pd, 1/d)$  and  $\varepsilon > 0$  there exist  $\theta > 0$  satisfying

$$\mathbb{P}\left(d_{GH}\left(\left(\mathcal{M}, d_{f, p}\right), \left(\mathbb{X}_{n}, \frac{n^{(p-1)/d}}{\mu} d_{\mathbb{X}_{n}, p}\right)\right) > \varepsilon\right) \le \exp\left(-\theta n^{(1-\lambda d)/(d+2p)}\right)$$

for n large enough, where  $d_{GH}$  stands for the Gromov-Hausdorff distance between metric spaces.

As a consequence of this result and the stability theorem for persistence diagrams we deduce the following convergence result.

**Corollary.** Let  $\varepsilon > 0$  and  $\lambda \in ((p-1)/pd, 1/d)$ . There exists a constant  $\theta > 0$  such that

$$\mathbb{P}\Big(d_b\big(\operatorname{dgm}(\operatorname{Filt}(\mathcal{M}, d_{f,p})), \operatorname{dgm}(\operatorname{Filt}(\mathbb{X}_n, \frac{n^{(p-1)/d}}{\mu}d_{\mathbb{X}_n,p}))\big) > \varepsilon\Big) \le \exp\left(-\theta n^{(1-\lambda d)/(d+2p)}\right)$$

for n large enough.

Here Filt(·) denotes either the Vietoris–Rips or Cech filtration, dgm(·) the associated persistence diagram and  $d_b$  is the bottleneck distance (see Section 3 for precise definitions). Since  $(\mathcal{M}, d_{f,p})$  is a Riemannian manifold, its population persistence diagram dgm(Filt $(\mathcal{M}, d_{f,p})$ ) displays the correct homology up to the convexity radius conv $(\mathcal{M}, d_{f,p})$ . In contrast, for  $(\mathcal{M}, |\cdot|)$  this is guaranteed only up to the reach  $\tau_{\mathcal{M}}$ . It is easy to find examples of manifolds in which conv $(\mathcal{M}, d_{f,p})$  is much larger than  $\tau_{\mathcal{M}}$ .

On the other hand, we prove that for a reasonable upper bound r on the filtration parameter,  $\operatorname{dgm}(\operatorname{Rips}_{< r}(\mathbb{X}_n, d_{\mathbb{X}_n, p}))$  is robust to outliers for homology degree greater than 0.

**Proposition.** Let  $\mathbb{X}_n$  be a sample of  $\mathcal{M}$  and let  $Y \subseteq \mathbb{R}^D \setminus \mathcal{M}$  be a finite set of outliers. Let  $\delta = \min \{ \min_{y \in Y} d_E(y, Y \setminus \{y\}, d_E(\mathbb{X}_n, Y) \}, where d_E denotes the Euclidean distance between sets. For all <math>k > 0$  and p > 1,

 $\operatorname{dgm}_{k}(\operatorname{Rips}_{<\delta^{p}}(\mathbb{X}_{n}\cup Y, d_{\mathbb{X}_{n}\cup Y, p})) = \operatorname{dgm}_{k}(\operatorname{Rips}_{<\delta^{p}}(\mathbb{X}_{n}, d_{\mathbb{X}_{n}, p})),$ 

where  $\operatorname{Rips}_{<\delta^p}$  stands for the Rips filtration up to parameter  $\delta^p$  and  $\operatorname{dgm}_k$  for the persistent homology of degree k.

The threshold  $\delta^p$  is restrictive if it is below diam $(\mathbb{X}_n, d_{\mathbb{X}_n, p})$ . However, we will show that under a natural model for the outliers,  $\delta^p > \operatorname{diam}(\mathbb{X}_n, d_{\mathbb{X}_n, p})$  for large enough p.

1.3. Applications to signal analysis. The study of time series — specially, derived from dynamical systems — through the inference of homology groups of a certain associated space called *delay embedding* was pioneered in [52, 53]. The construction of the delay embedding of a time series heavily depends on the dimension or number of independent variables of the underlying system. It often leads to analyse subspaces of a sufficiently high dimensional Euclidean space, which makes the inference of topological information unstable.

In first place, by means of a concrete example involving the Lorenz attractor, we show that the use of Fermat distance in this method can lead to a more robust inference of the topological features of delay embeddings. The reason behind this is that the Fermat distance is less prone, compared to the Euclidean distance, to the effect known as *curse*  of dimensionality. We also describe a method to detect change-points in the time series through the study of the evolution in time of the persistence diagrams of the corresponding time-delay embeddings. This is applied to discover anomalies in electrocardiogram signals and different patterns in the song of canaries corresponding to different syllables.

The code to replicate the computational examples and applications can be found at [32].

1.4. **Related work.** The sample Fermat distance was introduced independently in [35, 55]. The study of approximations of density based metric from samples was suggested in [60] and developed in [54]. In [19, 20], the authors analyze a general family of metrics that includes the population Fermat distance and deeply study the case p = 2 of sample Fermat distance, which was also called power weighted shortest distance in [46]. In [35], it is proved that it is possible to recover the population Fermat distance  $d_{f,p}$  for d-dimensional manifolds which are isometrically embedded (closures of) open sets of  $\mathbb{R}^d$  in  $\mathbb{R}^D$  as the limit of the sample Fermat distance. In the related work [39] it was shown that in the same context, a statistic that is similar to the sample Fermat distance but uses the inherited Riemannian distance  $d_{\mathcal{M}}$  between consecutive points in a path instead of the Euclidean one to measure its cost, also converges almost surely to the Fermat distance. We remark that this statistic can not be computed from the sample since the inherited distance is not assumed to be known in advance. In both works, the authors prove uniform convergence with concrete exponential bounds for all  $x, y \in \mathcal{M}$  which are at least at a fixed distance b > 0 apart.

The problem of learning geodesic distances from samples for submanifolds of the Euclidean space, specially with the aim of reducing dimensionality and visualizing data, has a long history (see for instance [47, 58]). On the other hand, the problem of estimating the persistence diagram of a submanifold of an Euclidean space from a sample has been studied in [16, 29], where the underlying metric is assumed to be known. In this setting, both the authors from [16] and [29] were able to prove the following satisfying result: the persistence diagrams computed using the sample converge almost surely (in the sense of bottleneck distance) to the persistence diagram of the desired metric space. Moreover, they gave exponentially small bounds in the size of the sample for the probability of the bottleneck distance between the corresponding persistence diagrams being larger than some positive number (see [16, Corollary 3] and [29, Lemma 4], where in addition confidence sets for persistence diagrams of submanifolds of an Euclidean space using alternative metrics (more specifically, metrics based on diffusion geometry and random walks) were explored experimentally in [6].

1.5. Structure of the paper. In Section 2 we prove our main result Theorem 2.5 regarding the Gromov-Hausdorff convergence of metric spaces using, respectively, the sample and the population Fermat distance. Section 3 includes an introduction to the persistent homology and is devoted to the study of persistence diagrams of manifolds endowed with Fermat distance. We deduce in first place the convergence of sample persistence diagrams to population persistence diagrams. Then, we show that by using these intrinsic metrics the topological features last longer in the persistence diagrams. Finally, we show that Fermat-based persistence diagrams are robust to the presence of outliers for positive homology degree. In Section 4 we present a method for pattern recognition in time series, which is applied to real data from electrocardiograms and songs of canaries. The closing Section 5 contains the proofs of some technical results (Proposition 2.4 and Lemma 2.6), required as intermediate steps to prove Theorem 2.5.

#### 2. Density-based Distance Learning

In this section we prove the main theorem of the article, which states that the sample  $X_n$ , considered as a metric space with the sample Fermat distance (appropriately re-scaled), converges almost surely to  $(\mathcal{M}, d_{f,p})$  in the sense of Gromov–Hausdorff.

We begin by introducing the population Fermat distance for a smooth closed Riemannian manifold without boundary  $\mathcal{M}$  of dimension d > 1 with Riemannian metric tensor gtogether with a positive  $C^{\infty}$  density function  $f : \mathcal{M} \to \mathbb{R}_{>0}$ . For p > 1, consider the deformed metric tensor  $g_p = f^{2(1-p)/d}g$  given by a conformal transformation of the original metric g. Since f is smooth,  $g_p$  is a Riemannian metric tensor. Thus,  $\mathcal{M}$  has a metric space structure given by the geodesic distance with respect to  $g_p$ , denoted by  $d_{f,p}$ .

**Definition 2.1.** [35, 39] For p > 1, the population Fermat distance between  $x, y \in \mathcal{M}$  is defined as

$$d_{f,p}(x,y) = \inf_{\gamma} \int_{I} \frac{1}{f(\gamma_t)^{(p-1)/d}} \sqrt{g(\dot{\gamma}_t, \dot{\gamma}_t)} dt$$

where the infimum is taken over all piecewise smooth curves  $\gamma \colon I \to \mathcal{M}$  with  $\gamma_0 = x$ , and  $\gamma_1 = y$ .

Notice that geodesics in  $\mathcal{M}$  respect to the distance  $d_{f,p}$  are more likely to lie in regions with high values of f. The name Fermat distance comes from the analogy with optics, in which  $d_{f,p}$  is the optical distance as defined by Fermat principle when the refraction index is given by  $f^{-(p-1)/d}$ .

Consider now a set  $\mathbb{X}_n = \{x_1, x_2, \ldots, x_n\} \subseteq \mathcal{M}$  of n sample points in  $\mathcal{M}$  with common density f. Suppose that  $\mathcal{M}$  is embedded in  $\mathbb{R}^D$  and it is endowed with the standard inherited Riemannian metric. Our aim is to approximate  $d_{f,p}(x, y)$ , assuming no knowledge about  $\mathcal{M}$  and the Riemannian distance defined on it. To achieve this, we will define an estimator for this distance over the sample. We denote by |x - y| the Euclidean distance between points  $x, y \in \mathcal{M}$ .

**Definition 2.2.** [35, 46] For p > 1, the sample Fermat distance between  $x, y \in \mathcal{M}$  is defined as

$$d_{\mathbb{X}_n,p}(x,y) = \inf_{\gamma} \sum_{i=0}^r |x_{i+1} - x_i|^p$$

where the infimum is taken over all paths  $\gamma = (x_0, x_1, \dots, x_{r+1})$  of finite length with  $x_0 = x$ ,  $x_{r+1} = y$  and  $\{x_1, x_2, \dots, x_r\} \subseteq \mathbb{X}_n$ .

Since p > 1, geodesics respect to this distance are also likely to lie in regions with high density of points in  $X_n$ . This is due to the fact that paths with short edges are favored even if they have large total (euclidean) length.

We remark here that, for technical reasons, we adopt a slightly different definition for the sample Fermat distance than the original one from [35]. Namely, in the original setting, only paths completely contained in  $X_n$  are considered, including the endpoints. Points that are are not in the sample  $X_n$  are projected to the nearest point in  $X_n$ . In consequence, our sample Fermat distance here does not generally induce a pseudometric over  $\mathcal{M}$ , but only a metric when restricted to  $X_n$ .

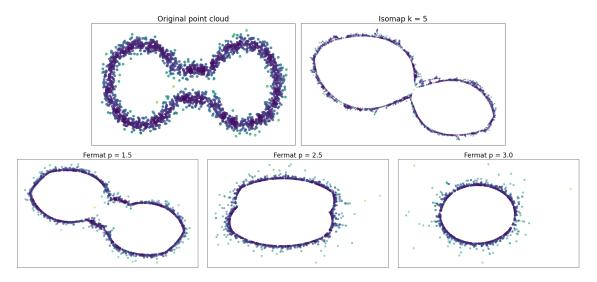


Figure 1. Top: A sample with noise of 2000 points of the eyeglasses dataset and Isomap projection with k = 5 (similar results are obtained for other values of k). Points are coloured according to local density. Bottom: MDS embedding in  $\mathbb{R}^2$  using Fermat distance for p = 1.5, 2.5, 3.0.

**Example 2.3** (Eyeglasses). The effect of taking different values of p for the sample Fermat distance  $d_{\mathbb{X}_n,p}$  in the geometry of a manifold is illustrated below. Concretely, the *eyeglasses* curve in  $\mathbb{R}^2$  uniformly sampled and perturbed with Gaussian noise is considered (see Figure 1). We compute the sample Fermat distance between each pair of points for a series of values of p > 1 and embed the sampled points in  $\mathbb{R}^2$  in such a way that the Euclidean distance in the embedding reflects the Fermat distance, using the Multidimensional Scaling algorithm (MDS). As p becomes larger, the geometry of the data overcomes the bottleneck region and it deforms into a circle. We also compute the Isomap embedding [7] in  $\mathbb{R}^2$  (that is, the MDS projection with an estimator of the inherited Riemannian distance based in the k-NN graph<sup>1</sup> as input distances). Due to the noise near the bottleneck region, some points that are far in the sense of the inherited Riemannian distance become close in the distance estimated from the k-NN graph. Note that Isomap embedding is sensitive to noise, while with Fermat distance the points lying in low density regions are mapped to points that are far from the rest of the sample. The larger the power p, the stronger this effect. This feature allows Fermat distance to reconstruct the underlying topology of the manifold in the present case, even with noise.

Our first result, Proposition 2.4, shows that the sample Fermat distance converges to the population Fermat distance for closed (i.e. compact and without boundary) submanifolds of  $\mathbb{R}^D$ . A related result was previously proved for isometrically embedded (closures of) open sets of  $\mathbb{R}^d$  [35]. Here we extend the class of manifolds to any compact manifold without boundary embedded in  $\mathbb{R}^D$ . Moreover, Proposition 2.4 states a *uniform* convergence for

<sup>&</sup>lt;sup>1</sup>Given  $\mathbb{X}_n \subset \mathbb{R}^D$  and  $k \in \mathbb{N}$ , the k nearest neighbors (k-NN) graph  $G_k$  is the (undirected) graph whose vertices are the points of  $\mathbb{X}_n$ , and with an edge between x and y if x is among the k nearest neighbors of y or vice-versa, in the sense of the Euclidean distance. The k-NN estimator of the inherited geodesic distance is computed as  $d_{\mathbb{X}_n,k}(x,y) = \inf_{\gamma} \sum_{i=0}^r |x_{i+1} - x_i|$ , where the infimum is taken over all paths  $\gamma = (x_0, x_1, \ldots, x_{r+1})$  in  $G_k$  such that  $x_0 = x, x_{r+1} = y$ .

any two points in the manifold (not only pointwise, as stated in [35]). This feature is essential to study both the manifold and the sample endowed with the (population and sample respectively) Fermat distance as *single* objects — metric spaces — and to prove convergence in the sense of Gromov–Hausdorff.

Let us fix some notations and general hypotheses. Hereafter,  $\mathcal{M}$  will denote a smooth ddimensional closed Riemannian submanifold of  $\mathbb{R}^D$  endowed with the inherited Riemannian distance  $d_{\mathcal{M}}$ . We will consider a set  $\mathbb{X}_n \subseteq \mathcal{M}$  of n independent random points with common smooth density  $f: \mathcal{M} \to \mathbb{R}_{>0}$ . We will denote by  $M_f$  and  $m_f$  the maximum and minimum values attained by f on  $\mathcal{M}$ , respectively. Observe that  $0 < m_f < M_f < \infty$ . Finally, given p > 1 we set  $\alpha = 1/(d+2p)$ .

**Proposition 2.4.** For every p > 1 and  $\lambda \in ((p-1)/pd, 1/d)$ , given  $\varepsilon > 0$  there exist  $\mu, \theta > 0$  such that

$$\mathbb{P}\left(\sup_{x,y}\left|n^{(p-1)/d}d_{\mathbb{X}_n,p}(x,y)-\mu d_{f,p}(x,y)\right| > \varepsilon\right) \le \exp\left(-\theta n^{(1-\lambda d)\alpha}\right)$$

for n large enough. The supremum is taken over  $x, y \in \mathcal{M}$ .

The constant  $\mu$  depends only on p and d and is defined in [38]. We defer the proof of Proposition 2.4 to Section 5.

This result will allow us to estimate the Gromov-Hausdorff distance between the metric space  $\mathbb{X}_n$  with an appropriate re-scaling of the sample Fermat distance  $d_{\mathbb{X}_n,p}$  and  $\mathcal{M}$ endowed with the population Fermat distance  $d_{f,p}$ . Recall that the *Gromov-Hausdorff* distance  $d_{GH}$  is a metric on the (isometry classes of) compact metric spaces that, roughly speaking, quantifies how difficult it is to match every point of a metric space  $(\mathbb{X}, \rho_{\mathbb{X}})$  with some point of another space  $(\mathbb{Y}, \rho_{\mathbb{Y}})$ . More formally, it is defined as

$$d_{GH}((\mathbb{X}, \rho_{\mathbb{X}}), (\mathbb{Y}, \rho_{\mathbb{Y}})) := \inf\{d_H(h_1(\mathbb{X}), h_2(\mathbb{Y}))\}$$

where the infimum is over all the isometric embeddings  $h_1: \mathbb{X} \to \mathbb{W}, h_2: \mathbb{Y} \to \mathbb{W}$  in a common metric space  $\mathbb{W}$  and  $d_H$  stands for the Hausdorff distance. We will employ the following equivalent characterization of the Gromov-Hausdorff distance, which is often more convenient:

(1) 
$$d_{GH}((\mathbb{X},\rho_{\mathbb{X}}),(\mathbb{Y},\rho_{\mathbb{Y}})) = \frac{1}{2} \inf_{R} \sup_{(x,y),(x',y')\in R} |\rho_{\mathbb{X}}(x,x') - \rho_{\mathbb{Y}}(y,y')|,$$

where the infimum is taken over subsets  $R \subseteq \mathbb{X} \times \mathbb{Y}$  such that the projections  $\pi_{\mathbb{X}}(R) = \mathbb{X}$ ,  $\pi_{\mathbb{Y}}(R) = \mathbb{Y}$ .

We are now ready to state our main theorem. For notational convenience, we set  $d_{n,p} = \frac{n^{(p-1)/d}}{\mu} d_{\mathbb{X}_n,p}$ , the re-scaled sample Fermat distance on  $\mathbb{X}_n$ .

**Theorem 2.5.** Let  $\varepsilon > 0$  and  $\lambda \in ((p-1)/pd, 1/d)$ . There exists a constant  $\theta > 0$  such that

$$\mathbb{P}(d_{GH}((\mathcal{M}, d_{f,p}), (\mathbb{X}_n, d_{n,p})) > \varepsilon) \le \exp\left(-\theta n^{(1-\lambda d)\alpha}\right)$$

for n large enough and  $\alpha = 1/(d+2p)$ .

Before presenting the proof of Theorem 2.5, we will need a preliminary lemma which asserts that, with high probability, no point of  $\mathcal{M}$  is too far from the nearest point of the sample. The argument of this proof is standard, but we include it in Section 5 for the reader's convenience.

**Lemma 2.6.** For any  $\kappa > 0$ , the event

$$\left\{\sup_{x\in\mathcal{M}}d_{\mathcal{M}}(x,\mathbb{X}_n)\geq n^{(\kappa-1)/d}\right\}$$

holds with probability at most  $\exp(-\theta n^{\kappa})$  for some constant  $\theta > 0$  if n is large enough.

We are now in position to prove Theorem 2.5.

Proof of Theorem 2.5. In order to compute the Gromov–Hausdorff distance between  $(\mathcal{M}, d_{f,p})$ and  $(\mathbb{X}_n, d_{n,p})$ , we consider in (1) the relation

$$R = \{ (x_i, x_i) \colon x_i \in \mathbb{X}_n \} \cup \{ (x_y, y) \colon y \in \mathcal{M}, d_{f,p}(x_y, y) = d_{f,p}(\mathbb{X}_n, y) \}.$$

By a simple application of the triangle inequality we get that

(2) 
$$d_{GH}((\mathcal{M}, d_{f,p}), (\mathbb{X}_n, d_{n,p})) \leq \frac{1}{2} \left( \sup_{x,y \in \mathbb{X}_n} |d_{f,p}(x,y) - d_{n,p}(x,y)| + 2 \sup_{y \in \mathcal{M}} d_{f,p}(\mathbb{X}_n, y) \right)$$

Observe that the two terms on the right hand side of the previous inequality can be bounded above by Proposition 2.4 and Lemma 2.6 respectively.

Given  $\varepsilon > 0$ , by (2) we have that

$$\mathbb{P}\left(d_{GH}\left((\mathcal{M}, d_{f,p}), (\mathbb{X}_n, d_{n,p})\right) > \varepsilon/2\right)$$
  
$$\leq \mathbb{P}\left(\sup_{x,y \in \mathbb{X}_n} |d_{f,p}(x,y) - d_{n,p}(x,y)| > \varepsilon/2\right) + \mathbb{P}\left(\sup_{y \in \mathcal{M}} d_{f,p}(\mathbb{X}_n, y) > \varepsilon/4\right)$$

To bound the first term, we apply Proposition 2.4 to get

$$\mathbb{P}\left(\sup_{x,y\in\mathbb{X}_n} |d_{f,p}(x,y) - d_{n,p}(x,y)| > \varepsilon/2\right) \le \exp\left(-\theta n^{(1-\lambda d)\alpha}\right)$$

for some positive constant  $\theta$  and n sufficiently large. As for the second term, notice that since

$$d_{f,p}(x,y) \le m_f^{-(p-1)/d} d_{\mathcal{M}}(x,y),$$

Lemma 2.6 implies

$$\mathbb{P}\left(\sup_{y\in\mathcal{M}}d_{f,p}(\mathbb{X}_n,y)>n^{(\alpha-1)/d}m_f^{(p-1)/d}\right)\leq\exp(-\theta n^{\alpha})$$

for n large. The proof follows by noticing that the sequence  $n^{(\alpha-1)/d}m_f^{-(p-1)/d}$  converges to 0 as n goes to infinity.

## 3. Fermat-based Persistent Homology

In this section we explore the use of Fermat distance as input in the computation of the persistence diagram associated to a sample of a manifold. We deduce the almost sure convergence of persistence diagrams of the sample  $X_n$  with the (re-scaled) sample Fermat distance towards the persistence diagram of  $(\mathcal{M}, d_{f,p})$ . We also show that we expect to read the correct homology of  $\mathcal{M}$  for a longer parameter interval in the diagram associated to the sample  $X_n$  computed with Fermat distance as compared with the use of Euclidean distance. Finally, we prove that Fermat-based persistence diagrams are robust to the presence of outliers for homology degree greater than 0.

3.1. Convergence of persistence diagrams. We start by briefly recalling the main concepts and results in persistent homology theory and refer the reader to [14, 15] for a more thorough exposition.

For the computation of the persistent homology of a point cloud, one imagines each point as a *ball* (that is, representing a small surrounding region) and builds a combinatorial model for the space connecting the points according to whether the corresponding regions intersect. More precisely, for every fixed value of a parameter or *scale* that controls the size of the region that each point represents, one gets a *simplicial complex* (i.e., a higher dimensional analogue of a graph). This family of simplicial complexes, also known as a *filtration*, is the input of the procedure to compute persistent homology. Indeed, the topological features of this family of complexes change as the scale parameter grows: different connected components join in one, some loops are filled, new cavities appear, etc. By analyzing these transitions, we are able to assign a *birth* and a *death* value to each of these features represent *topological signatures*, whereas the shortest intervals may be considered as *noise*. The output of this procedure is summarized in an object called *persistence diagram*. We next give the formal definitions.

Given a (possibly infinite) metric space  $(\mathbb{X}, \rho)$ , a filtration over the real numbers  $\operatorname{Filt}(\mathbb{X}, \rho) =$  $(\operatorname{Filt}_{\epsilon}(\mathbb{X},\rho))_{\epsilon\in\mathbb{R}}$  is a family of simplicial complexes with vertex set  $\mathbb{X}$  such that  $\operatorname{Filt}_{\epsilon}(\mathbb{X})\subseteq$  $\operatorname{Filt}_{\epsilon'}(\mathbb{X})$  whenever  $\epsilon \leq \epsilon'$ . For the purposes of this article, we are going to consider only some natural filtrations that are strongly linked to the metric  $\rho$ . The Cech filtration consists of a family of simplicial complexes  $(\operatorname{\check{C}ech}_{\epsilon}(\mathbb{X}))_{\epsilon \in \mathbb{R}}$  where a set of points  $[x_0,\ldots,x_k]$  forms a k-simplex of  $\check{\mathrm{Cech}}_{\epsilon}(\mathbb{X})$  if the intersection of the k+1 closed balls  $\bar{B}_{\rho}(x_i,\epsilon)$  is non empty. Equivalently,  $\check{C}ech_{\epsilon}(\mathbb{X})$  is the *nerve* of the cover  $\{\bar{B}_{\rho}(x,\epsilon): x \in \mathbb{X}\}$ . The Cech complex is the most natural way to build a simplicial complex associated to a space, since in favourable cases, it allows to recover its homotopy type as a consequence of the Nerve Theorem [36, §4.G]. However, the construction of the Cech complex is expensive from a computational point of view, since it requires to check for a large number of intersections. To circumvent this issue, one can instead consider the Vietoris-Rips filtration  $(\operatorname{Rips}_{\epsilon}(\mathbb{X}))_{\epsilon \in \mathbb{R}}$ . The k-simplices of  $\operatorname{Rips}_{\epsilon}(\mathbb{X})$  are sets  $[x_0, \ldots, x_k]$  such that  $\rho(x_i, x_j) \leq \epsilon$  for all  $0 \leq i, j \leq k$ . If X is a subset of the Euclidean space  $\mathbb{R}^D$ , then one have  $\check{\operatorname{Cech}}_{\epsilon}(\mathbb{X}) \subseteq \operatorname{Rips}_{2\epsilon}(\mathbb{X}) \subseteq \check{\operatorname{Cech}}_{\sqrt{2D/(D+1)\epsilon}}(\mathbb{X})$  (e.g. see Theorem 2.5. in [24]). In this sense, the Rips complex is a computationally efficient approximation of the Čech complex. Other filtrations involving lower dimensional simplices, such as the Alpha filtration (see [26]), can also be considered in our context.

For any filtration as above, it is clear that the topology of the complexes  $\operatorname{Filt}_{\epsilon}(\mathbb{X})$  will typically change as  $\epsilon$  increases. This evolution is appropriately captured by considering the homology groups (over a field **k**) of the nested family of simplicial complexes. One gets in this way a sequence of vector spaces  $(H_{\bullet}(\operatorname{Filt}_{\epsilon}(\mathbb{X})))_{\epsilon \in \mathbb{R}}$ , where the inclusions  $\operatorname{Filt}_{\epsilon}(\mathbb{X}) \subseteq$  $\operatorname{Filt}_{\epsilon'}(\mathbb{X})$  induce canonical linear maps  $H_{\bullet}(\operatorname{Filt}_{\epsilon}(\mathbb{X})) \to H_{\bullet}(\operatorname{Filt}_{\epsilon'}(\mathbb{X}))$  in homology. Under some conditions, such as finiteness of  $\mathbb{X}$  [27, 61], this sequence can be decomposed as a direct sum of *intervals*  $I[\epsilon_b, \epsilon_d]$  defined as

$$0 \xrightarrow{0} \cdots \xrightarrow{0} 0 \xrightarrow{0} \underbrace{\mathbf{k}} \xrightarrow{\mathbb{1}} \cdots \xrightarrow{\mathbb{1}} \mathbf{k}}_{[\epsilon_b, \epsilon_d]} \xrightarrow{0} 0 \xrightarrow{0} \cdots \xrightarrow{0} 0$$

Every interval is determined by the *birth* and *death* parameters  $\epsilon_b$  and  $\epsilon_d$  respectively, and it can be interpreted as a *topological feature* of X with an associated *lifetime*  $\epsilon_d - \epsilon_b$ (note that  $\epsilon_d$  may be infinite, in that case the feature has infinite lifetime). The (multi)set of points ( $\epsilon_b, \epsilon_d$ ) is called the *persistence diagram* of (X,  $\rho$ ) and is denoted dgm(Filt(X,  $\rho$ )) (or simply dgm(Filt(X)) if  $\rho$  is clear from the context). Persistence diagrams are contained in the half (extended) plane above the diagonal  $\Delta = \{(x, y) : x = y\}$ . For technical reasons, the diagonal  $\Delta$  is considered as part of every persistence diagram with infinite multiplicity. In [12, 14, 15], the authors prove that, within a more abstract persistent framework, it is possible to extend the definition of persistence diagrams to some cases where the sequence might not be interval-decomposable. In particular, it is shown in [15] that if X is a compact metric space, for every value of  $\epsilon$  at most a finite number of new topological features appear (even though the vector spaces  $(H_{\bullet}(\text{Filt}_{\epsilon}(X)))_{\epsilon \in \mathbb{R}}$  may be infinite-dimensional) and hence dgm(Filt(X)) is well-defined. Notice also that all the definitions can be extended to filtrations indexed over connected subsets of the real line.

**Example 3.1** (Eyeglasses). We compute the persistence diagram associated to the sample points from Example 2.3, Figure 1. We compare the results obtained with different distance choices: the Euclidean distance, the k-NN estimator of the inherited Riemannian distance and the sample Fermat distance for p = 2.5, p = 3 and p = 3.5. The homology of the eyeglasses curve has one generator of  $H_0$  and one generator of  $H_1$ . However, it can be noticed that for either Euclidean and k-NN distance for  $k \ge 5$ , the persistence diagram displays two salient generators for the first homology group  $H_1$ , which can be attributed to the small reach of the manifold. As it can be seen in Figure 2, smaller values of k fail to capture the geometry of the eyeglasses manifold. With the Fermat distance for different choices of p the diagram shows accurately only one persistent generator for  $H_1$ . On the other hand, the number of noticeable connected components increases with p. This effect is caused by the presence of noisy points in regions of extremely low density, becoming isolated points (or outliers) as p evolves (cf. Remark 3.9).

Since in our setup we usually only get an approximation of the metric space under consideration, we will be interested in comparing persistence diagrams built on top of different metric spaces. In this sense, the *bottleneck distance* is a frequently used quantity to measure the difference between two persistence diagrams. Given persistence diagrams dgm<sub>1</sub> and dgm<sub>2</sub>, consider all perfect matchings  $M \subseteq \text{dgm}_1 \times \text{dgm}_2$  such that every point of dgm<sub>1</sub>  $\setminus \Delta$  and dgm<sub>1</sub>  $\setminus \Delta$  is paired exactly once in M. The bottleneck distance  $d_b(\text{dgm}_1, \text{dgm}_2)$  is then defined as the infimum, over all such matchings M as before, of the largest  $\ell_{\infty}$ -distance between matched pairs. That is,

$$d_b(\operatorname{dgm}_1, \operatorname{dgm}_2) = \inf_M \max_{(x,y) \in M} |x - y|_{\infty}.$$

The stability theorem [15, 21] ensures continuity (more precisely, Lipschitz continuity) in the process of computing persistence diagrams for a metric space. This means that small perturbations in the original metric space (in the sense of Gromov–Hausdorff) will translate into an at most proportional perturbation in the corresponding persistence diagram (in the

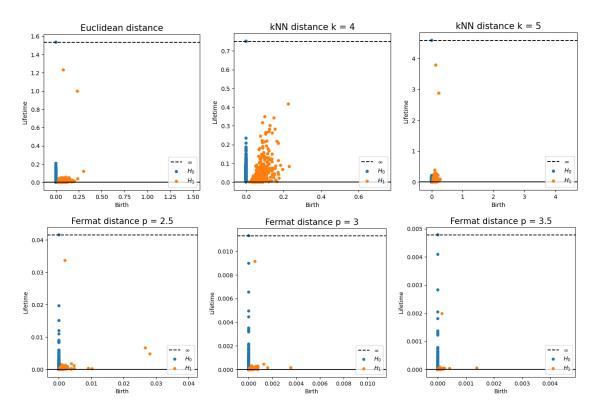


Figure 2. Persistence diagrams (lifetime) associated to the eyeglasses point cloud with noise for different distances. Top: Euclidean distance and k-NN distance with k = 4 and k = 5. Bottom: Fermat distance with p = 2.5 p = 3 and p = 3.5.

sense of the bottleneck distance). Formally, it states that for any two precompact metric spaces  $\mathbb X$  and  $\mathbb Y$ 

(3) 
$$d_b \Big( \operatorname{dgm} \big( \operatorname{Filt}(\mathbb{X}, \rho_{\mathbb{X}}) \big), \operatorname{dgm} \big( \operatorname{Filt}(\mathbb{Y}, \rho_{\mathbb{Y}}) \big) \Big) \leq 2d_{GH} \big( (\mathbb{X}, \rho_{\mathbb{X}}), (\mathbb{Y}, \rho_{\mathbb{Y}}) \big).$$

This fact is exploited in [16, 29] to establish the almost sure convergence (in the sense of bottleneck distance) of the persistence diagrams associated to samples of a compact metric space drawn according to a measure satisfying certain hypotheses to the persistence diagram of the space. In these works the distance function of the underlying metric space is assumed to be known, and it is inherited by the sample.

We are able to obtain convergence of persistence diagrams in our context, in which only an estimator of the underlying metric is available. Concretely, given the metric spaces  $(\mathcal{M}, d_{f,p})$  and  $(\mathbb{X}_n, d_{n,p})$ , from the estimation of its Gromov-Hausdorff distance of Theorem 2.5 and the stability theorem (3) we deduce the following result.

**Corollary 3.2.** Let  $\varepsilon > 0$  and  $\lambda \in ((p-1)/pd, 1/d)$ . There exists a constant  $\theta > 0$  such that

$$\mathbb{P}\Big(d_b\big(\mathrm{dgm}(\mathrm{Filt}(\mathcal{M}, d_{f,p})), \mathrm{dgm}(\mathrm{Filt}(\mathbb{X}_n, d_{n,p}))\big) > \varepsilon\Big) \le \exp\left(-\theta n^{(1-\lambda d)\alpha}\right)$$

for n large enough and  $\alpha = 1/(d+2p)$ .

3.2. Homology inference. The content of Corollary 3.2 is that dgm(Filt( $X_n, d_{n,p}$ )) is (asymptotically) a good estimator of dgm(Filt( $\mathcal{M}, d_{f,p}$ )). On the other hand, if we were to employ the Euclidean distance  $|\cdot|$ , it follows from [16] that the sample persistence diagrams dgm(Filt( $X_n, |\cdot|$ )) converge to dgm(Filt( $\mathcal{M}, |\cdot|$ )) under reasonable hypotheses. We are therefore interested in comparing for how long we may expect to read the correct homology of  $\mathcal{M}$  in each of the diagrams dgm(Filt( $\mathcal{M}, d_{n,p}$ )) and dgm(Filt( $\mathcal{M}, |\cdot|$ )) in terms of two natural geometric measures associated to the manifold, namely, the reach and the convexity radius (see also [17, 37, 41, 51]). In this section we show that the homology of ( $\mathcal{M}, d_{f,p}$ ) can be recovered correctly from its persistence diagram up to the convexity radius conv( $\mathcal{M}, d_{f,p}$ ), whereas for ( $\mathcal{M}, |\cdot|$ ) this is guaranteed only up to its reach  $\tau_{\mathcal{M}}$ . Notice that the reach of a submanifold of an Euclidean space depends strongly on the particular embedding, whereas the convexity radius is an intrinsic quantity linked to the geometry of the manifold. There are simple examples of manifolds in which this distinction is relevant to correctly recover its homology from a sample (see Examples 2.3 and 3.4).

Recall that given  $\mathbb{X} \subseteq \mathbb{R}^D$  a closed subset, the *medial axis* Med( $\mathbb{X}$ ) of  $\mathbb{X}$  is defined as

$$\operatorname{Med}(\mathbb{X}) := \{ y \in \mathbb{R}^D : d_E(y, \mathbb{X}) = |p - y| \text{ for at least two different points } p \in \mathbb{R}^D \}$$

where  $d_E(y, \mathbb{X}) = \inf_{x \in \mathbb{X}} |y - x|$ . The reach  $\tau_{\mathbb{X}}$  of  $\mathbb{X}$ , first introduced in [30], is the minimum distance from  $\mathbb{X}$  to Med( $\mathbb{X}$ ), that is,

$$\tau_{\mathbb{X}} := \inf_{x \in \mathbb{X}} d_E(x, \operatorname{Med}(\mathbb{X})).$$

Given a Riemannian manifold  $(\mathcal{N}, g)$ , we will say that a subset  $S \subseteq \mathcal{N}$  is geodesically convex if for every two points in S, there is a unique geodesic segment that connects them and it is completely contained in S. The convexity radius  $\operatorname{conv}(\mathcal{N}, x)$  at a point  $x \in \mathcal{N}$ is the supremum over those r > 0 for which the ball B(x, r) is geodesically convex. The convexity radius  $\operatorname{conv}(\mathcal{N})$  of the manifold  $\mathcal{N}$  is defined as

$$\operatorname{conv}(\mathcal{N}) := \inf_{x \in \mathcal{N}} \operatorname{conv}(\mathcal{N}, x).$$

**Proposition 3.3.** Let  $\mathcal{M}$  be a compact submanifold of  $\mathbb{R}^D$ . Then,

- $\check{\operatorname{Cech}}_{\epsilon}(\mathcal{M}, |\cdot|) \simeq \mathcal{M}$  for  $\epsilon < \tau_{\mathcal{M}}$  and  $\operatorname{Rips}_{\epsilon}(\mathcal{M}, |\cdot|) \simeq \mathcal{M}$  for  $\epsilon < 2\sqrt{\frac{D+1}{2D}}\tau_{\mathcal{M}}$ , and both bounds are optimal, in the sense that there exist examples for which the homotopy equivalence does not hold for larger values of  $\epsilon$ .
- $\operatorname{\check{Cech}}_{\epsilon}(\mathcal{M}, d_{f,p}) \simeq \mathcal{M} \text{ and } \operatorname{Rips}_{\epsilon}(\mathcal{M}, d_{f,p}) \simeq \mathcal{M} \text{ for } \epsilon < \operatorname{conv}(\mathcal{M}, d_{f,p}).$

Moreover, if  $d_{f,p}$  coincides up to a constant with  $d_{\mathcal{M}}$  (i.e. f is uniform), we have the estimate

$$\operatorname{conv}(\mathcal{M}, d_{f,p}) = \operatorname{Vol}(\mathcal{M}, d_{\mathcal{M}})^{(p-1)/d} \operatorname{conv}(\mathcal{M}, d_{\mathcal{M}}) \ge \operatorname{Vol}(\mathcal{M}, d_{\mathcal{M}})^{(p-1)/d} \frac{\pi}{2} \tau_{\mathcal{M}}.$$

Proof. The fact that  $\operatorname{Cech}_{\epsilon}(\mathcal{M}, |\cdot|)$  is homotopy equivalent to  $\mathcal{M}$  for  $\epsilon < \tau_{\mathcal{M}}$  is an immediate consequence of the Nerve Theorem. The same result implies that  $\operatorname{Cech}_{\epsilon}(\mathcal{M}, d_{f,p}) \simeq \mathcal{M}$  for  $\epsilon < \operatorname{conv}(\mathcal{M}, d_{f,p})$ , since geodesically convex sets are always contractible and the intersection of geodesically convex sets is again geodesically convex. Regarding the Vietoris–Rips filtration, the fact that the simplicial complex  $\operatorname{Rips}_{\epsilon}(\mathcal{M}, |\cdot|)$  is homotopy equivalent to  $\mathcal{M}$ for  $\epsilon < 2\sqrt{\frac{D+1}{2D}}\tau_{\mathcal{M}}$  can be deduced from [40, Theorem 20]. Finally, since  $d_{f,p}$  is a Riemannian distance on  $\mathcal{M}$ , by [37] there is an explicit homotopy equivalence  $\operatorname{Rips}_{\epsilon}(\mathcal{M}, d_{\mathcal{M}}) \simeq \mathcal{M}$ for  $\epsilon < \operatorname{conv}(\mathcal{M}, d_{f,p})$  (see also [41]). The optimality of the bound  $\epsilon < \tau_{\mathcal{M}}$  for  $\operatorname{\check{Cech}}_{\epsilon}(\mathcal{M}, |\cdot|)$  is clear (think of a unit sphere in  $\mathbb{R}^{D}$ ), and indeed, typically the topology of  $\operatorname{\check{Cech}}_{\epsilon}(\mathcal{M}, |\cdot|)$  changes when  $\epsilon$  attains  $\tau_{\mathcal{M}}$ . A critical example for the Vietoris–Rips complex is the standard 1-dimensional circle  $\mathbb{S}^{1}$ , and it can be derived from the main result in [2], similarly as in [40, Example 24].

The last assertion in the statement follows directly from the inequalities

$$\operatorname{conv}(\mathcal{M}, d_{\mathcal{M}}) \ge \min\left\{\frac{\pi}{2\sqrt{\sup K}}, \frac{1}{2}\operatorname{inj}(\mathcal{M}, d_{\mathcal{M}})\right\}$$

 $(\text{see} [18, \S5.14])$  and

$$\operatorname{inj}(\mathcal{M}, d_{\mathcal{M}}) \ge \pi \tau_{\mathcal{M}}, \, K \le \frac{1}{\tau_{\mathcal{M}}^2}$$

(see [1, Proposition A.1]). Here  $\operatorname{inj}(\mathcal{M}, d_{\mathcal{M}})$  is the injectivity radius of  $\mathcal{M}$  and K is the sectional curvature.

**Example 3.4.** Consider a planar ellipse  $E_{R,\varepsilon}$  with minor axis of length  $\varepsilon$  and major axis of length  $R \geq \varepsilon$ . By letting  $R \to +\infty$  and/or  $\varepsilon \to 0$ , we see that the convexity radius of a closed submanifold of  $\mathbb{R}^2$  can be arbitrarily large while its reach can be arbitrarily small. A similar example can be constructed in  $\mathbb{R}^D$ , being  $\mathcal{M}$  a *d*-dimensional ellipsoid for any d < D. The same phenomenon can be achieved by constructing different *eyeglasses* curves with arbitrarily large length and constant reach, Figure 3. Its population persistence diagrams differ as predicted by Theorem 3.3. The persistence diagram computed with the Euclidean distance captures the right homology only for  $\varepsilon$  less that the reach. In contrast, for the Fermat distance the correct homology is captured for radii as large as (a multiple of) the convexity radius, which can be made large enough by enlarging the bridge between the glasses.

3.3. Robustness to outliers. Persistence diagrams are highly sensitive to outliers [5, 6, 11, 13]. We will see that the computation of persistence homology using Fermat distance is robust to the presence of outliers for positive degree. Concretely, given a sample  $\mathbb{X}_n \subseteq \mathcal{M}$  and  $Y \subseteq \mathbb{R}^D \setminus \mathcal{M}$  a finite set of points in the complement of  $\mathcal{M}$  in the ambient Euclidean space — the *outliers* — we prove that  $\operatorname{dgm}_k(\operatorname{Rips}(\mathbb{X}_n \cup Y, d_{\mathbb{X}_n \cup Y,p}))$  coincides with  $\operatorname{dgm}_k(\operatorname{Rips}(\mathbb{X}_n, d_{\mathbb{X}_n,p}))$  for k > 0 up to some reasonable filtration parameter. First we need a definition.

**Definition 3.5.** Given a finite set of points  $S \subseteq \mathbb{R}^D$ , define the minimal spacing of S as

$$\kappa(S) = \min_{x \in S} d_E(x, S \setminus \{x\}),$$

where  $d_E$  denotes the Euclidean distance between sets.

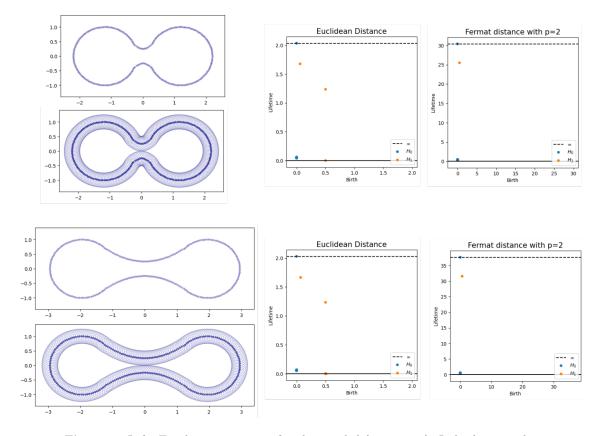
**Proposition 3.6.** Let  $\delta = \min\{\kappa(Y), d_E(\mathbb{X}_n, Y)\}$  and p > 1. Then, for every  $\epsilon < \delta^p$ 

$$\operatorname{Rips}_{\epsilon}(\mathbb{X}_n \cup Y, d_{\mathbb{X}_n \cup Y, p}) = \operatorname{Rips}_{\epsilon}(\mathbb{X}_n, d_{\mathbb{X}_n, p}) \cup Y$$

In particular, for all k > 0

$$\operatorname{dgm}_{k}(\operatorname{Rips}_{<\delta^{p}}(\mathbb{X}_{n}\cup Y, d_{\mathbb{X}_{n}\cup Y, p})) = \operatorname{dgm}_{k}(\operatorname{Rips}_{<\delta^{p}}(\mathbb{X}_{n}, d_{\mathbb{X}_{n}, p})),$$

where  $\operatorname{Rips}_{<\delta^p}(\mathbb{X}, \rho_{\mathbb{X}})$  stands for  $\left(\operatorname{Rips}_{\epsilon}(\mathbb{X}, \rho_{\mathbb{X}})\right)_{\epsilon < \delta^p}$ , *i.e.*, the Rips filtration up to parameter  $\delta^p$  of a metric space  $(\mathbb{X}, \rho_{\mathbb{X}})$ .



**Figure 3.** Left: Eyeglasses curves, uniformly sampled (250 points). In both cases, the reach is 0.5. Below each curve, we plot a thickening of the samples with Euclidean balls of radius slightly greater than the reach. Right: Persistence diagrams (lifetime) associated to the Vietoris–Rips filtration for both the Euclidean distance and the re-scaled Fermat distance  $d_{n,p}$  with p = 2. While  $H_0$  is correctly estimated in both cases by reading the persistence diagrams, the ones computed with the Euclidean distance displays two salient generators for the first homology group  $H_1$ , inaccurately suggesting two cycles. The second cycle's birth is at the level of twice the reach. For the (re-scaled) Fermat distance, the diagrams shows correctly only one persistent generator for  $H_1$ .

*Proof.* Let us estimate the distance between two given points in  $\mathbb{X}_n \cup Y$  with respect to  $d_{\mathbb{X}_n \cup Y,p}$  in terms of  $\delta$  and  $d_{\mathbb{X}_n,p}$ .

If  $x \in \mathbb{X}_n$  and  $y \in Y$ ,

$$d_{\mathbb{X}_n \cup Y, p}(x, y) \ge d_{\mathbb{X}_n \cup Y, p}(\mathbb{X}_n, Y) = d_E(\mathbb{X}_n, Y)^p \ge \delta^p.$$

If  $y, y' \in Y$ ,

$$d_{\mathbb{X}_n \cup Y, p}(y, y') \ge d_{\mathbb{X}_n \cup Y, p}(y, Y \setminus \{y\}) \ge \delta^p.$$

For the second inequality, notice that if  $\tilde{y} \in Y$  is such that  $d_{\mathbb{X}_n \cup Y, p}(y, Y \setminus \{y\}) = d_{\mathbb{X}_n \cup Y, p}(y, \tilde{y}) = \operatorname{len}(\gamma)$ , the geodesic  $\gamma$  between y and  $\tilde{y}$  either involves only points from Y or there exist some point  $x \in \mathbb{X}_n$  in  $\gamma$ . In the first case  $d_{\mathbb{X}_n \cup Y, p}(y, \tilde{y}) \geq \kappa(Y)^p$  whereas in the second case  $d_{\mathbb{X}_n \cup Y, p}(y, \tilde{y}) \geq 2d_E(\mathbb{X}_n, Y)^p$ .

Given  $x, x' \in \mathbb{X}_n$ , let  $\gamma$  be a minimal path between x, x', so that  $d_{\mathbb{X}_n \cup Y, p}(x, x') = \operatorname{len}(\gamma)$ . If  $d_{\mathbb{X}_n \cup Y, p}(x, x') < \epsilon$ , then  $\gamma$  only involves points in  $\mathbb{X}_n$  since otherwise  $\epsilon \geq \operatorname{len}(\gamma) \geq 2d_E(\mathbb{X}_n, Y) \geq 2\delta^p$ , which is a contradiction. Hence,  $d_{\mathbb{X}_n \cup Y, p}(x, x') = d_{\mathbb{X}_n, p}(x, x')$ .  $\Box$  We define now a geometric notion of outliers. Recall that given  $\mathbb{X}_n \subseteq \mathbb{R}^D$ , the  $\varepsilon$ -graph  $G_{\varepsilon}(\mathbb{X}_n)$  is the undirected graph with the points of  $\mathbb{X}_n$  as vertices and an edge connecting  $x_i$  and  $x_j \in \mathbb{X}_n$  whenever  $|x_i - x_j| < \varepsilon$ .

**Definition 3.7.** Let  $\mathbb{X}_n \subseteq \mathcal{M}$  be a sample of  $\mathcal{M} \subseteq \mathbb{R}^D$  and  $Y \subseteq \mathbb{R}^D \setminus \mathcal{M}$  be a finite set of points. Let  $\varepsilon_* := \min\{\varepsilon > 0 : G_{\varepsilon}(\mathbb{X}_n) \text{ is connected}\}$  and  $\delta = \min\{\kappa(Y), d_E(\mathbb{X}_n, Y)\}$ . We say that Y are *(geometric) outliers* if  $\delta > \varepsilon_*$ .

We show next that for this notion of outliers, the upper bound on the parameter for the Rips filtration of Proposition 3.6 is not restrictive for sufficiently large p. Indeed, let diam<sub>p</sub>( $\mathbb{X}_n$ ) be the diameter of ( $\mathbb{X}_n, d_{\mathbb{X}_n,p}$ ). Note that for every  $\epsilon \geq \text{diam}_p(\mathbb{X}_n)$  the simplicial complex Rips<sub> $\epsilon$ </sub>( $\mathbb{X}_n, d_{\mathbb{X}_n,p}$ ) equals the standard (n-1)-simplex  $\Delta^{n-1}$ , with trivial topology (and hence persistence diagrams are not interesting for scales larger than this threshold). The next result states that provided that p is large enough, the persistence diagrams of ( $\mathbb{X}_n, d_{\mathbb{X}_n,p}$ ) and ( $\mathbb{X}_n \cup Y, d_{\mathbb{X}_n \cup Y,p}$ ) coincide up to the filtration parameter diam<sub>p</sub>( $\mathbb{X}_n$ ).

**Corollary 3.8.** Given  $\mathbb{X}_n$  a sample of  $\mathcal{M}$  and  $Y \subseteq \mathbb{R}^D$  a finite set of outliers, then for all k > 0

$$\operatorname{dgm}_k(\operatorname{Rips}_{<\operatorname{diam}_p(\mathbb{X}_n)}(\mathbb{X}_n\cup Y, d_{\mathbb{X}_n\cup Y, p})) = \operatorname{dgm}_k(\operatorname{Rips}_{<\operatorname{diam}_p(\mathbb{X}_n)}(\mathbb{X}_n, d_{\mathbb{X}_n, p})).$$

for p sufficiently large.

*Proof.* There is an upper bound  $\operatorname{diam}_p(\mathbb{X}_n) \leq n\varepsilon_*^p$ . Since Y are outliers,  $\varepsilon_* < \delta$ . Hence  $\left(\frac{\delta}{\varepsilon_*}\right)^p > n$  for p sufficiently large and consequently,  $\operatorname{diam}_p(\mathbb{X}_n) < \delta^p$ . The result now follows from Proposition 3.6.

Remark 3.9. In general, the persistence diagram of  $(\mathbb{X}_n \cup Y, d_{\mathbb{X}_n \cup Y,p})$  for degree k = 0 does not coincide with the diagram of the metric space without outliers  $(\mathbb{X}_n, d_{\mathbb{X}_n,p})$ . However, if Y is a set of geometric outliers, it is related to the corresponding persistence diagrams of  $\mathbb{X}_n$  and Y through the following formula:

 $\mathrm{dgm}_{0}(\mathrm{Rips}(\mathbb{X}_{n}\cup Y, d_{\mathbb{X}_{n}\cup Y, p})) = \mathrm{dgm}_{0}^{<\infty}(\mathrm{Rips}(\mathbb{X}_{n}, d_{\mathbb{X}_{n}, p})) \cup \mathrm{dgm}_{0}(\mathrm{Rips}(Q, d_{Q}))$ 

Here, dgm<sup> $<\infty$ </sup> denotes the bounded persistence intervals and  $Q = (Y \cup \mathbb{X}_n)/\mathbb{X}_n$  is the quotient metric space endowed with the induced metric  $d_Q$ , defined as

$$d_Q(q,q') = \inf_{\gamma} \left\{ \sum_{i=0}^r \tilde{d}_{\mathbb{X}_n \cup Y, p}(q_i, q_{i+1}) \right\}$$

where the infimum is taken over all paths  $\gamma = (q_0, q_2, \dots, q_{r+1})$  in  $\mathbb{X}_n \cup Y$  such that  $q_0 = q, q_{r+1} = q'$  and

$$\tilde{d}_{\mathbb{X}_n \cup Y, p}(q_i, q_{i+1}) = \begin{cases} 0 & \text{if } q_i, q_{i+1} \in \mathbb{X}_n, \\ d_{\mathbb{X}_n \cup Y, p}(q_i, q_{i+1}) & \text{otherwise.} \end{cases}$$

**Example 3.10** (Trefoil). Consider the embedding of a topological circle  $\mathbb{S}^1$  in  $\mathbb{R}^3$  given by the *trefoil knot*. In particular, it is homeomorphic to  $\mathbb{S}^1$  and its homology has just one generator in  $H_0$  (one connected component) and one generator in  $H_1$  (one 1-dimensional cycle). Given a (noisy) sample of 1500 points from the trefoil knot with 10 outliers, Figure 4, we compute its persistence diagram for different choices of distances and compare them with the case without the outliers, Figure 5. For Euclidean distance, the small reach of the embedding produces a persistence diagram with four persistent generators for  $H_1$  in both cases, with and without outliers (cf. Example 3.4). For k-NN distances, the presence of outliers affects the performance of the topological features captured in the persistence diagram, which presents four salient generators for  $H_1$  instead of the single generator recovered from the sample without outliers. Finally, the persistence diagram computed with Fermat distance for degree 1 remains unaffected in presence of outliers (Corollary 3.8), and it shows correctly a single salient generator of  $H_1$ . For degree 0, the diagram is related to the diagram of the sample without the outliers and the diagram of the outliers themselves (cf. Remark 3.9).

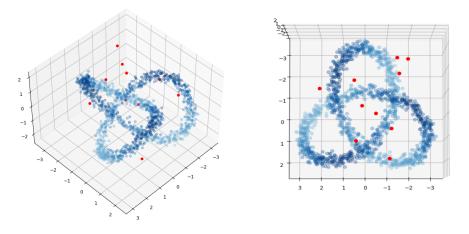


Figure 4. A sample of 1500 points from the trefoil knot with outliers (red).

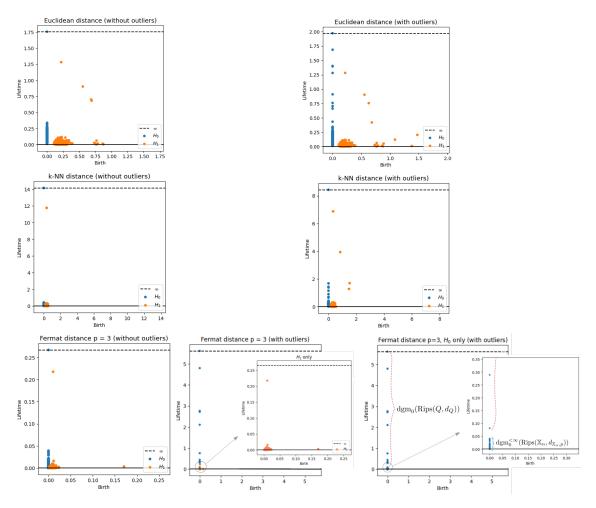
## 4. Applications to signal analysis

In this section we present a method for change-point detection and pattern recognition in time series through the analysis of topological features. This method is illustrated by a series of experiments in both synthetic and real data. In the experiments, the use of Fermat distance (as opposed to Euclidean distance) is observed to lead to more robust inference of the topology of the underlying space. We remark that in these examples the data does not necessarily verify the i.i.d. assumption. (see also [45, 52, 53])

We clarify some computational details before presenting the examples. To start with, we compute the matrix of pairwise sample Fermat distances between points in  $\mathbb{X}_n$  as the input of the persistence homology algorithm. This procedure has complexity  $\mathcal{O}(n^3)$  (but can be reduced to  $\mathcal{O}(n^2 \log^2 n)$  with high probability) [35]. In any case, the precomputation of the sample Fermat distance in  $\mathbb{X}_n$  does not increase the complexity of the total persistent homology computation, which runs in  $\mathcal{O}(n^{3(k+2)})$  for degree k (see [50]).

The Fermat and the k-NN distance are computed using the library Fermat [31], while Ripser [59] is employed for the computation of persistence diagrams associated to Vietoris– Rips filtrations. All the computations are over the field  $\mathbf{k} = \mathbb{Z}_2$ . The code for all the examples and experiments can be found in [32].

4.1. Topological analysis of time series. Time-delay embeddings of scalar time-series data is a well-known technique to recover the underlying dynamics of a system. Takens' theorem [57] gives conditions under which a smooth attractor can be reconstructed from



**Figure 5.** Persistence diagrams associated to the sample of the trefoil knot for Euclidean distance, k-NN distance with k = 10, and Fermat distance with p = 3 of the sample without outliers  $\mathbb{X}_n$  (left) and the sample with outliers  $\mathbb{X}_n \cup Y$  (right) respectively. When Fermat distance is used, the persistence diagram of  $\mathbb{X}_n \cup Y$  for degree 1 equals the diagram of  $\mathbb{X}_n$  (without outliers). For degree 0, it decomposes as the union of the subdiagram of finite intervals of  $\mathbb{X}_n$ ,  $\dim_0^{\infty}(\operatorname{Rips}(\mathbb{X}_n, d_{\mathbb{X}_n, p}))$ , and the diagram  $\dim_0(\operatorname{Rips}(Q, d_Q))$  of the quotient space  $Q = (Y \cup \mathbb{X}_n)/\mathbb{X}_n$ .

a generic observable function, with dimensional bounds related to those of the Whitney Embedding Theorem. It implies in particular that if X(t) is a real valued signal (which is assumed to be one of the coordinates of a flow given by a system of differential equations), then the *delay coordinate map* 

$$t \mapsto \left( X(t), X(t+\tau), X(t+2\tau) \dots, X(t+(D-1)\tau) \right)$$

is an embedding of an orbit. Here D is the embedding dimension and  $\tau$  is the time delay. From a theoretical point of view, D is the number of variables of the original system. However, in practice the underlying equations describing the dynamical system are not available — and, indeed, this is one of the main goals of the research in the area —. Thus, dynamics are often analyzed by studying the topology of their *attractors* (i.e., invariant subsets of the phase space towards which the system tends to evolve) [8, 34, 56]. If the attractor is a smooth manifold  $\mathcal{M}$  of dimension d, under certain conditions Taken's theorem [57] implies that the delay embedding of the signal with  $D \geq 2d + 1$  is diffeomorphic to  $\mathcal{M}$ .

We describe now an approach — based on intrinsic persistent diagrams — to study geometry of attractors and pattern recognition in time series by means of the analysis of the time evolving topological organization of the embedded flow. Let  $(x_1, x_2, \ldots, x_n)$  be a time series, i.e. a finite sample of a signal  $X : [0,T] \to \mathbb{R}$  such that for evenly spaced points  $0 = t_1 < t_2 < \cdots < t_n = T$ ,  $x_i = X(t_i)$  for all  $1 \le i \le n$ . Given D and  $\tau$ , compute the delay embedding of the time series

$$\mathbb{X}_{n} = \{ (x_{i}, x_{i+\tau}, x_{i+2\tau}, \dots, x_{i+(D-1)\tau}) : 1 \le i \le n - (D-1)\tau \} \subseteq \mathbb{R}^{D}.$$

Then, for p > 1, endow  $\mathbb{X}_n$  with a metric space structure induced by the sample Fermat distance  $d_{\mathbb{X}_n,p}$ . The persistence diagram of the delay embedding  $(\mathbb{X}_n, d_{\mathbb{X}_n,p})$  quantifies information about the homology of the attractor associated to the underlying dynamical system.

**Example 4.1** (Reconstruction of Lorenz attractor). The parameters associated to the delay coordinate reconstruction for a time series can be determined following some heuristics (e.g. *false nearest neighbors* to determine the embedding dimension). However, in case of noisy data, the embedding dimension is often over-estimated and it may have a great impact on the phase space reconstruction. Indeed, in high dimensional spaces, any two points of a typical large set are at similar Euclidean distance [3]. This phenomenon is part of what is known as the *curse of dimensionality*. For this reason, the choice of an intrinsic distance is crucial to recover the right topological features of a space embedded in high dimension.

Consider the strange attractor associated to the Lorenz system [44]

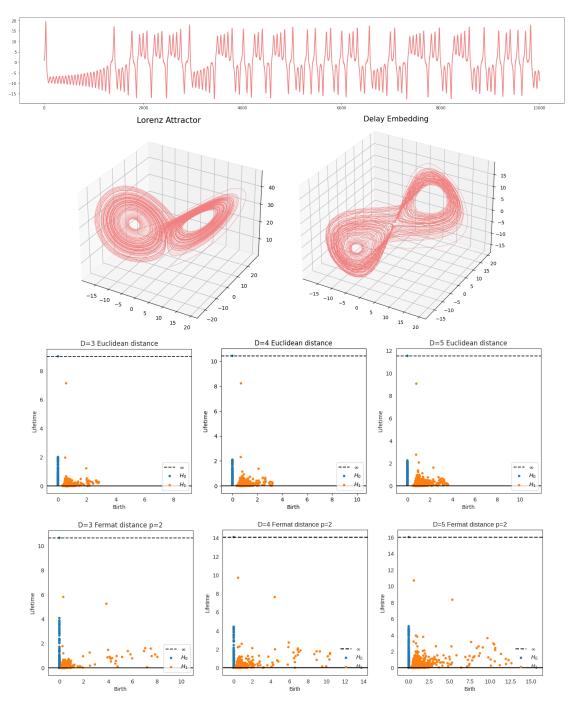
(4) 
$$\begin{cases} \dot{x} = \sigma(y - x), \\ \dot{y} = x(\rho - z) - y \\ \dot{z} = xy - \beta z \end{cases}$$

when  $(\sigma, \rho, \beta) = (10, 28, 8/3)$ .

In Figure 6 we take a numerical integration  $\varphi(t, v_0)$  of (4) with dt = 0.01, satisfying the initial condition  $\varphi(0, v_0) = v_0$  with  $v_0 = (1, 1, 1)$ . We inspect the time series corresponding to the *x*-coordinate with added Gaussian noise with variance 0.1, and recover topological information of the attractor from the delay embedding (see also [45]). Notice that in this case, although the number of variables in the underlying system is 3, the dimension of the attractor is d = 2 so the embedding dimension estimated by Taken's theorem is greater than or equal to 5.

The persistence diagram of the delay embedding reconstruction is computed with time delay  $\tau = 10$  and embedding dimensions D = 3, 4 and 5, Figure 6. The Lorenz attractor is homotopy equivalent to the *eight-space* with two holes corresponding to the equilibrium points that the trajectory never reaches. As Figure 6 reveals, the use of Fermat distance leads to robustly capturing the intrinsic two 1-cycles for the different embedding dimensions, while this is not the case for the Euclidean distance.

In order to identify changes in patterns of time series, we investigate the topological evolution in time of the delay embedding. For every sample time  $t_j \in [0, T]$   $(1 \le j \le 1)$ 



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**Figure 6.** From top to bottom: The *x*-coordinate time series with Gaussian noise (variance = 0.1) of the Lorenz attractor. The original trajectory and the delay embedding of the noisy *x*-coordinate time series with D = 3 and  $\tau = 10$ . Persistence diagrams associated to the delay embedding computed with Euclidean and Fermat distances for embedding dimension D = 3, D = 4 and D = 5 and time delay  $\tau = 10$ .

 $n - (D-1)\tau$ ), consider the delay embedding  $\mathbb{X}_j$  of the restriction of the time series up to time  $t_j$ , with the metric structure inherited from  $(\mathbb{X}_n, d_{\mathbb{X}_n, p})$ . That is,

$$\mathbb{X}_j := \{ (x_i, x_{i+\tau}, x_{i+2\tau}, \dots, x_{i+(D-1)\tau}) : 1 \le i \le j \} \subseteq \mathbb{X}_n.$$

If  $\mathcal{M}[0, t]$  is the delay embedding of the restricted signal  $X|_{[0,t]}$ , the time evolving series of diagrams  $\{\operatorname{dgm}(\operatorname{Rips}(\mathbb{X}_i)): 1 \leq j \leq n - (D-1)\tau\}$  is a sample of an approximation of the curve

(5) 
$$t \mapsto \operatorname{dgm}(\operatorname{Rips}(\mathcal{M}[0, t]))$$

where  $\mathcal{M}[0, t]$  is considered a metric subspace of  $\mathcal{M} = \mathcal{M}[0, T]$  endowed with the population Fermat distance. Finally, compute

$$\frac{d_b(\operatorname{dgm}(\operatorname{Rips}(\mathbb{X}_i)) - d_b(\operatorname{dgm}(\operatorname{Rips}(\mathbb{X}_{i-1})))}{t_i - t_{i-1}}$$

as an approximate the 'first order derivative' of (5). Shifts in patterns in the signal can be detected from the sample as peaks in the bottleneck distance between consecutive persistence diagrams.

Some applications of this technique follow below.

**Example 4.2** (Anomaly detection in ECG). The purpose of this example is to present a computational method of automated detection of abnormal heartbeats (arrhythmia) through the topological analysis of a delay embedding of ECG signals. We consider the record *sel102* of the *QT Database* from the freely-available repository of medical research data PhysioNet [49], Figure 7.

Regular heartbeats are characterized by a periodic pattern ([43, Ch.4]). The delay embedding in  $\mathbb{R}^3$  of a normal ECG has hence a cyclic topology induced by the periodic behavior of the time series (see also [28, 52]). However, every time that an irregular heartbeat occurs, a new cycle arises in the embedding. We compute the associated persistence diagram for a normal period and for a period that includes an anomalous heartbeat. By using Fermat distance with p = 2, a second cycle in the irregular period that accounts for the anomaly is distinctly detected (here, the choice of p is related to the weight we give to the density when computing Fermat distances, that is, we set p so that the exponent  $\frac{p-1}{d}$ equals 1 where d = 1 is the dimension of the curve). Moreover, the moment immediately following the occurrence of the anomaly can be detected using persistent homology of time evolving delay embeddings. Indeed, the bottleneck distance between consecutive diagrams features a prominent peak when the topology of the embedding changes.

**Example 4.3** (Pattern recognition in birdsongs). During song production, canaries use a set of air sac pressure gestures with characteristic shapes to generate different patterns of sound (or syllables). Pressure patterns of different syllables constitute a diverse set: they can be either almost harmonic oscillations, high frequency fluctuations or oscillations presenting wiggles. The recognition of song syllables from the air sac pressure series is a well-studied problem in non-linear dynamical systems [4, 48].

We provide a topological method to detect the number of different syllables in a canary song from the (noisy) record of the fluctuations of its air sac pressure X(t), Figure 8 (data provided by the Laboratory of Dynamical Systems from the Department of Physics of the University of Buenos Aires). Given the time delay embedding of the time series X(t) with  $\tau = 500$  and D = 3, its associated persistence diagram computed using Fermat distance with p = 1.5 shows four prominent generators for the first homology group, which are in

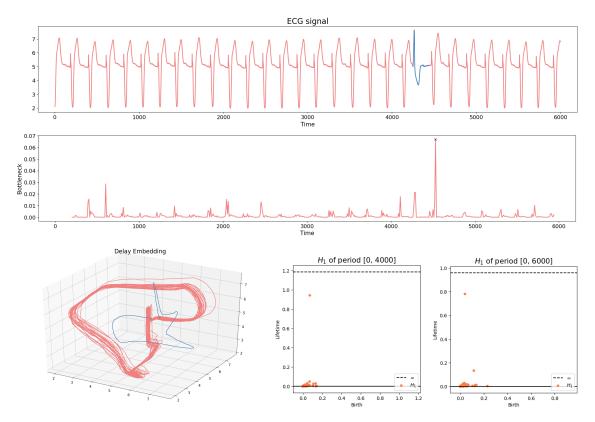


Figure 7. Top: ECG signal (anomaly in blue). Middle: Bottleneck distance between consecutive persistence diagrams associated to time evolving embeddings of the ECG signal. Bottom: Delay embedding in  $\mathbb{R}^3$  with  $\tau = 15$ . The associated persistence diagrams at degree 1 using Fermat distance with p = 2 for the embedding of the signal in the periods of time [0, 4000] and [0, 6000].

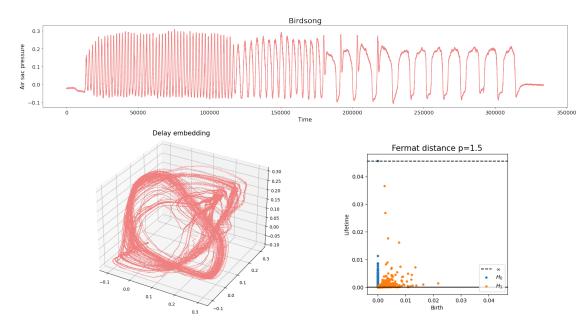
correspondence with the four different patterns observed in the time series (see Figure 9). Indeed, the embedding of each syllable is topologically a cycle (see [52, 53]). However, this decomposition is not available beforehand so the study of the global topology of the embedding of the entire time series is necessary in order to analyze the complete song. Here, prior to the computation of the persistence diagram, we down-sampled the original time series at evenly spaced times with stride t = 100, obtaining a subsample of size ~ 3000 from the original  $T \sim 300000$  points.

We can also detect the moments at which changes of syllables take place during the song. The bottleneck distance between consecutive persistence diagrams associated to the time evolving delay embeddings presents peaks each time a new pattern arises, Figure 9.

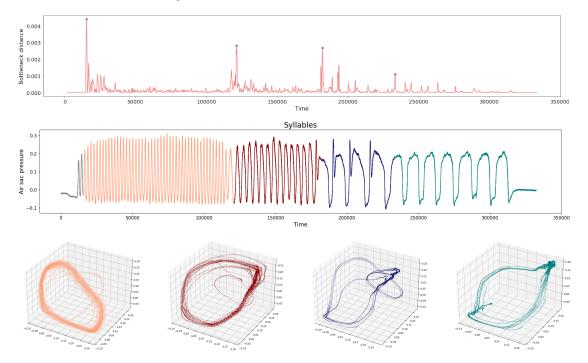
## 5. PROOF OF AUXILIARY RESULTS

The purpose of this section is to present formal proofs of Proposition 2.4 and Lemma 2.6. Recall that  $\mathcal{M} \subseteq \mathbb{R}^D$  is a closed submanifold of dimension  $d \leq D$  and  $\mathbb{X}_n \subseteq \mathcal{M}$  is an i.i.d. sample of size n with common density f > 0. Given p > 1, we set  $\alpha = 1/(d+2p)$ .

In [39] the authors establish the convergence of an estimator known as the *power-weighted* shortest path to the population Fermat distance. For p > 1 and points  $x, y \in \mathcal{M}$ , the



**Figure 8.** Top: Record of the air sac pressure of canary during a song. Bottom: Delay embedding in  $\mathbb{R}^3$  with the delay  $\tau = 500$  and its associated persistence diagram using Fermat distance with p = 1.5.



**Figure 9.** Top: Bottleneck distance between consecutive persistence diagrams associated to time evolving embeddings (moving average curve with window of time 500). Peaks are related to changes in the pattern of the air sac pressure record of the canary song. Bottom: Delay embedding of each detected syllable.

power-weighted shortest path between x, y is defined as

$$L_{\mathbb{X}_n,p}(x,y) = \inf_{\gamma} \sum_{i=0}^k d_{\mathcal{M}}(x_{i+1},x_i)^p$$

where the infimum is taken over all paths  $\gamma = (x_0, \ldots, x_{k+1})$  in  $\mathbb{X}_n$  of finite length with  $x_0 = x, x_{k+1} = y$ .

**Theorem 5.1.** [39, Theorem 1] Let p > 1 and  $\varepsilon > 0$ . Suppose that  $(b_n)_{n \ge 1}$  is a sequence of positive real numbers such that  $\frac{\log(n)}{nb_n^d} \to 0$  as n goes to infinity. Then, there exists a constant  $\theta > 0$  (which depends on  $\varepsilon$ ) such that

$$\mathbb{P}\left(\sup_{\substack{x,y\in\mathcal{M}\\d_{\mathcal{M}}(x,y)\geq b_{n}}}\left|\frac{n^{(p-1)/d}L_{\mathbb{X}_{n},p}(x,y)}{d_{f,p}(x,y)}-\mu\right|>\varepsilon\right)\leq\exp(-\theta(nb_{n}^{d})^{\alpha})$$

for all sufficiently large n, where the supremum is taken over  $x, y \in \mathcal{M}$  with  $d_{\mathcal{M}}(x, y) \geq b_n$ .

The constant  $\mu = \mu(d, p)$  from the statement is fixed and depends only on p and d. It was originally defined in [38, Lemma 3]. As explained in the paragraph following Theorem 1 in [39, p. 2793], the requirement that  $\frac{\log(n)}{nb_n^d} \to 0$  is necessary in order to obtain a nontrivial upper bound for the probability.

Note that in Theorem 5.1, the convergence holds for the set of points  $x, y \in \mathcal{M}$  with  $d_{\mathcal{M}}(x, y)$  greater than some sequence  $(b_n)$ . However, in order to study Gromov-Hausdorff convergence of the associated metric spaces, it is necessary to have uniform control of the convergence of the estimated distance for *all* points in the manifold. The uniform convergence with similar rate is one of the main improvements upon Theorem 5.1 we show in Proposition 2.4. Also, notice that the proposed estimator  $L_{\mathbb{X}_n,p}$  of  $d_{f,p}$  is based on the previous knowledge of the inherited Riemannian distance  $d_{\mathcal{M}}$ . In the general data analysis setting, only a sample of points in a Euclidean space is given. Under the assumption that points lie on an (unknown) manifold  $\mathcal{M}$ , the goal is to find an estimator of the intrinsic distance  $d_{f,p}$  that can be completely computed from the sample. In Proposition 2.4, we prove that sample Fermat distance  $d_{\mathbb{X}_n,p}$  is indeed a good estimator of  $d_{f,p}$ .

The proof of Proposition 2.4 will take most of this section. The idea of the next results is to show that any segment that is part of any shortest path with respect to  $d_{\mathbb{X}_{n,p}}$  will be arbitrarily small with high probability if n is large enough. This will allow us to prove that the power-weighted distance is well approximated by the sample Fermat distance.

**Proposition 5.2.** Given b > 0 and  $\varepsilon > 0$ , there exists  $\theta > 0$  such that

$$\mathbb{P}\left(\sup_{x,y}\left(\frac{n^{(p-1)/d}d_{\mathbb{X}_n,p}(x,y)}{d_{f,p}(x,y)}-\mu\right)>\varepsilon\right)\leq\exp(-\theta n^{\alpha})$$

for n large enough, where the supremum is taken over all  $x, y \in \mathcal{M}$  with  $d_{\mathcal{M}}(x, y) \geq b$ .

*Proof.* Given  $\varepsilon > 0$  and b > 0, by Theorem 5.1 there exists  $\theta > 0$  such that for every  $x, y \in \mathcal{M}$  with  $d_{\mathcal{M}}(x, y) \ge b$ 

(6) 
$$\frac{n^{(p-1)/d}L_{\mathbb{X}_n,p}(x,y)}{d_{f,p}(x,y)} - \mu > \varepsilon$$

with probability at most  $\exp(-\theta n^{\alpha})$  (notice that here we set the sequence  $b_n$  to be constantly b).

Let  $x, y \in \mathcal{M}$  and let  $\gamma = (x_0, \ldots, x_{k+1})$  be the shortest path between x, y with respect to  $L_{\mathbb{X}_n,p}$ . That is,

$$L_{\mathbb{X}_n,p}(x,y) = \sum_{i=0}^{\kappa} d_{\mathcal{M}}(x_{i+1},x_i)^p$$

Since  $|x_{i+1} - x_i| \le d_{\mathcal{M}}(x_{i+1}, x_i)$ ,

$$L_{\mathbb{X}_{n,p}}(x,y) \ge \sum_{i=0}^{k} |x_{i+1} - x_i|^p \ge d_{\mathbb{X}_{n,p}}(x,y).$$

Thus, by (6), the inequality

$$\frac{n^{(p-1)/d}d_{\mathbb{X}_n,p}(x,y)}{d_{f,p}(x,y)} - \mu > \varepsilon$$

holds with probability bounded by  $\exp(-\theta n^{\alpha})$ .

**Corollary 5.3.** Let  $b_0 > 0$ . Let  $x, y \in \mathcal{M}$  be such that they belong to some minimal path between points in  $\mathcal{M}$  respect to  $d_{\mathbb{X}_n,p}$ . Then,

$$\mathbb{P}(|x-y| > b_0) \le \exp(-\theta n^{\alpha})$$

for some constant  $\theta > 0$ , provided n is large enough.

*Proof.* Fix  $\varepsilon_0 > 0$ . By Proposition 5.2, there exists a constant  $\theta > 0$  such that

$$\mathbb{P}\left(\sup_{u,v}\frac{n^{(p-1)/d}d_{\mathbb{X}_n,p}(u,v)}{d_{f,p}(u,v)} > \mu + \varepsilon_0\right) \le \exp(-\theta n^{\alpha})$$

for all n sufficiently large, where the supremum is taken over  $u, v \in \mathcal{M}$  such that  $d_{\mathcal{M}}(u, v) \geq b_0$ .

On the other hand, note that since  $\mathcal{M}$  is compact the diameter  $\operatorname{diam}_p(\mathcal{M})$  of  $\mathcal{M}$  with respect to the distance  $d_{f,p}$  is finite. Hence,

$$\frac{d_{f,p}(u,v)}{n^{(p-1)/d}}(\mu+\varepsilon_0) \le \frac{\operatorname{diam}_p(\mathcal{M})}{n^{(p-1)/d}}(\mu+\varepsilon_0) \le b_0^p$$

for all  $u, v \in \mathcal{M}$  with  $d_{\mathcal{M}}(u, v) \geq b_0$  and all *n* sufficiently large.

Suppose now that  $x, y \in \mathcal{M}$  belong to some shortest path between points of  $\mathcal{M}$  with respect to  $d_{\mathbb{X}_n,p}$ , say u and v, but that  $|x-y| > b_0$ . Then, clearly  $d_{\mathbb{X}_n,p}(u,v) \ge |x-y|^p$  and  $d_{\mathcal{M}}(u,v) > b_0$  (since otherwise  $d_{\mathbb{X}_n,p}(u,v) \le |u-v|^p < b_0^p$ ). We remark here that x and y do not necessarily belong to the sample  $\mathbb{X}_n$ . From the previous computations, it follows that whenever n is large enough, with probability at least  $1 - \exp(-\theta n^{\alpha})$ ,

$$|x-y|^p \le d_{\mathbb{X}_n,p}(u,v) \le \frac{d_{f,p}(u,v)}{n^{(p-1)/d}}(\mu+\varepsilon_0) \le b_0^p,$$

as we wanted to show.

Remark 5.4. (see [7, Corollary 4] or [10, Lemma 3]) Let  $(\mathcal{M}, g)$  be a smooth compact Riemannian manifold embedded in  $\mathbb{R}^D$ . Given  $\delta > 0$ , there exists  $\varepsilon > 0$  such that for every  $x, y \in \mathcal{M}$  with  $|x - y| < \varepsilon$ ,

$$d_{\mathcal{M}}(x,y) \le (1+\delta)|x-y|.$$

We are now able to prove a new version of Theorem 5.1 in which the proposed estimator of  $d_{f,p}$  is the sample Fermat distance (rather than the power-weighted shortest path).

**Proposition 5.5.** Fix  $\varepsilon > 0$  and a sequence of positive real numbers  $(b_n)_{n\geq 1}$  satisfying that  $\frac{\log(n)}{nb_n^d} \to 0$  when  $n \to \infty$ . Then, for every p > 1, there exists  $\theta > 0$  such that

$$\mathbb{P}\left(\sup_{x,y} \left| \frac{n^{(p-1)/d} d_{\mathbb{X}_n,p}(x,y)}{d_{f,p}(x,y)} - \mu \right| > \varepsilon \right) \le \exp\left(-\theta (nb_n^d)^{\alpha}\right)$$

for n large enough, where the supremum is taken over  $x, y \in \mathcal{M}$  with  $d_{\mathcal{M}}(x, y) \geq b_n$ .

*Proof.* Let  $\delta > 0$  be a small number to be fixed later. The strategy of the proof consists of showing that, with probability exponentially high in  $(nb_n^d)^{\alpha}$ ,  $L_{\mathbb{X}_n,p}(x,y)$  and  $d_{\mathbb{X}_n,p}(x,y)$ coincide up to a factor of  $(1 + \delta)^p$  for all  $x, y \in \mathcal{M}$  with  $d_{\mathcal{M}}(x,y) \geq b_n$ . Once that is established, the proof follows readily by applying Theorem 5.1.

Notice in first place that by Remark 5.4, there exists  $\eta > 0$  such that  $d_{\mathcal{M}}(x, y) \leq (1+\delta)|x-y|$  whenever  $x, y \in \mathcal{M}, |x-y| < \eta$ . By Corollary 5.3, we may assume that  $|u-v| < \eta$  for every  $u, v \in \mathcal{M}$  belonging to a minimal path with probability exponentially high in  $n^{\alpha}$ . Let  $x, y \in \mathcal{M}$  be two points with  $d_{\mathcal{M}}(x, y) \geq b_n$ . Since by our assumptions every segment in a shortest path from x to y with respect to  $d_{\mathbb{X}_n,p}$  has Euclidean length at most  $\eta$ , it is not difficult to see that

(7) 
$$d_{\mathbb{X}_n,p}(x,y) \le L_{\mathbb{X}_n,p}(x,y) \le (1+\delta)^p d_{\mathbb{X}_n,p}(x,y).$$

Now, by Theorem 5.1, the probability that

(8) 
$$\left|\frac{n^{(p-1)/d}L_{\mathbb{X}_n,p}(x,y)}{d_{f,p}(x,y)} - \mu\right| < \frac{\varepsilon}{2}$$

is exponentially high in  $(nb_n^d)^{\alpha}$ , provided n is large enough. We will check that for  $\delta > 0$  sufficiently small, the desired inequality for  $d_{\mathbb{X}_n,p}$  follows if we assume that the event from (8) occurs. It is clear by (7) and (8) that

$$\frac{n^{(p-1)/d}d_{\mathbb{X}_n,p}(x,y)}{d_{f,p}(x,y)}-\mu<\frac{\varepsilon}{2}.$$

As for the other inequality, notice that

$$-\frac{\varepsilon}{2} < (1+\delta)^p \left(\frac{n^{(p-1)/d} d_{\mathbb{X}_n, p}(x, y)}{d_{f, p}(x, y)} - \mu\right) + ((1+\delta)^p - 1)\mu.$$

Hence, for  $\delta > 0$  small enough we have

$$-\varepsilon < \frac{n^{(p-1)/d} d_{\mathbb{X}_n,p}(x,y)}{d_{f,p}(x,y)} - \mu$$

as desired.

Finally, we promote the convergence of the sample Fermat distance from Proposition 5.5 to a *uniform* convergence in probability (that is, for any pair of points  $x, y \in \mathcal{M}$  regardless of the distance between them). Such uniform convergence may be accomplished by choosing a sequence  $(b_n)_{n\geq 1}$  which converges to 0 at an adequate rate. This step is

instrumental in order to prove the Gromov-Hausdorff convergence of the sample metric spaces  $(\mathbb{X}_n, d_{n,p})$  to  $(\mathcal{M}, d_{f,p})$  (see Theorem 3.2 and its proof).

*Proof of Proposition 2.4.* Roughly, the strategy of the proof consists in bounding the quantity

$$|n^{(p-1)/d}d_{\mathbb{X}_n,p}(x,y) - \mu d_{f,p}(x,y)|$$

splitting in two cases according to whether the distance  $d_{\mathcal{M}}(x, y)$  is greater than or smaller than some appropriately chosen sequence  $b_n > 0$ . More precisely, we will set  $b_n = n^{-\lambda}$  for some  $\lambda \in ((p-1)/pd, 1/d)$ . Let  $\varepsilon > 0$ . Since  $\lambda < 1/d$ , clearly the sequence  $\left(\frac{\log(n)}{nb_n^d}\right)_{n\geq 1}$ converges to 0 as n goes to infinity and hence, by Proposition 5.5 the bound

$$\left|\frac{n^{(p-1)/d}d_{\mathbb{X}_n,p}(x,y)}{d_{f,p}(x,y)} - \mu\right| > \varepsilon'$$

holds with probability at most  $\exp(-\theta(nb_n^d)^{\alpha}) = \exp(-\theta n^{(1-\lambda d)\alpha})$  for some  $\theta > 0$  and all  $x, y \in \mathcal{M}$  with  $d_{\mathcal{M}}(x, y) \ge n^{-\lambda}$  provided n is large enough (here  $\varepsilon' > 0$  is a small number to be determined). Denote by diam( $\mathcal{M}$ ) the diameter of  $\mathcal{M}$  respect to the distance  $d_{\mathcal{M}}$ . Since  $d_{f,p}(x, y) \le m_f^{-(p-1)/d} d_{\mathcal{M}}(x, y) \le m_f^{-(p-1)/d} \operatorname{diam}(\mathcal{M})$ , we see that the event

$$|n^{(p-1)/d} d_{\mathbb{X}_n,p}(x,y) - \mu d_{f,p}(x,y)| > m_f^{-(p-1)/d} \operatorname{diam}(\mathcal{M})\varepsilon'$$

also holds with probability bounded from above by  $\exp(-\theta n^{(1-\lambda d)\alpha})$  for the same  $\theta > 0$  as before, whenever  $d_{\mathcal{M}}(x, y) \ge n^{-\lambda}$ . By setting  $\varepsilon' = \varepsilon (m_f^{-(p-1)/d} \operatorname{diam}(\mathcal{M}))^{-1}$  we obtain the desired bound for  $x, y \in \mathcal{M}$  with  $d_{\mathcal{M}}(x, y) \ge n^{-\lambda}$ . For the remaining case, take  $x, y \in \mathcal{M}$ satisfying  $d_{\mathcal{M}}(x, y) \le n^{-\lambda}$  and notice in first place that

$$d_{f,p}(x,y) \le m_f^{-(p-1)/d} d_{\mathcal{M}}(x,y) \le m_f^{-(p-1)/d} n^{-\lambda}.$$

Hence, for n sufficiently large,  $\mu d_{f,p}(x,y) \leq \varepsilon/2$ . On the other hand, since by definition of  $d_{\mathbb{X}_n,p}$  it is

$$d_{\mathbb{X}_n,p}(x,y) \le |x-y|^p \le d_{\mathcal{M}}(x,y)^p \le n^{-\lambda p},$$

we see that  $n^{(p-1)/d} d_{\mathbb{X}_n,p}(x,y) \leq n^{(p-1)/d-\lambda p}$ . The hypothesis on  $\lambda$  implies that the exponent of n in the last inequality is negative and thus  $n^{(p-1)/d} d_{\mathbb{X}_n,p}(x,y) \leq \varepsilon/2$  provided n is large. Summing up, we conclude that there exists  $n_0$  such that for all  $x, y \in \mathcal{M}$  with  $d_{\mathcal{M}}(x,y) \leq n^{-\lambda}$  and  $n \geq n_0$ ,

$$|n^{(p-1)/d}d_{\mathbb{X}_n,p}(x,y) - \mu d_{f,p}(x,y)| \le \varepsilon$$

which completes the proof of the proposition.

We turn now to the proof of Lemma 2.6, which follows ideas from [23] and [47, Section 5].

Proof of Lemma 2.6. Since  $\mathcal{M}$  is compact, its injectivity radius  $\operatorname{inj}(\mathcal{M})^2$  is strictly positive. Then, by an inequality of Croke (see [22, Proposition 14]), there exists a constant c = c(d) > 0 such that every metric ball B in  $\mathcal{M}$  of radius  $r < \frac{\operatorname{inj}(\mathcal{M})}{2}$  has volume at least  $c(d)r^d$ . Since we can assume that  $\kappa < 1$  without loss of generality, for all n sufficiently large we have

<sup>&</sup>lt;sup>2</sup>Given  $(\mathcal{N}, g)$  a Riemannian manifold, the *injectivity radius*  $\operatorname{inj}(\mathcal{N})$  is defined as  $\operatorname{inj}(\mathcal{N}) := \inf_{x \in \mathbb{N}} \operatorname{inj}(\mathcal{N}, x)$ , where  $\operatorname{inj}(\mathcal{N}, x)$  is the largest radius for which the exponential map is a diffeomorphism (see [42, Chapter 5]).

 $n^{(\kappa-1)/d} < \frac{\operatorname{inj}(\mathcal{M})}{2}$ . From this point, we follow the strategy from the proof of [23, Theorem 3]. Let  $P_n$  be the maximum number of disjoint balls of radius  $\frac{n^{(\kappa-1)/d}}{4}$  contained in  $\mathcal{M}$  (this is known as *packing number*, see for example [51, Section 5]) and take  $\{B_1, \ldots, B_{P_n}\}$  a set of disjoint balls of radius  $\frac{n^{(\kappa-1)/d}}{4}$  in  $\mathcal{M}$ . It is clear then that

$$P_n \le \frac{\operatorname{Vol}(\mathcal{M})}{\min_{1 \le j \le P_n} \operatorname{Vol}(B_j)} \le \frac{\operatorname{Vol}(\mathcal{M})4^d}{c(d)} n^{1-\kappa},$$

for n so large that  $n^{(\kappa-1)/d} < \frac{\operatorname{inj}(\mathcal{M})}{2}$ . Now, suppose that  $x \in \mathcal{M}$  verifies  $d_{\mathcal{M}}(x, \mathbb{X}_n) > n^{(\kappa-1)/d}$ . Since the balls  $2B_1, \ldots, 2B_{P_n}$  cover  $\mathcal{M}$  (where  $2B_j$  stands for the ball with the same center as  $B_j$  but with twice the radius) the distance from x to some center of these balls is at most  $\frac{n^{(\kappa-1)/d}}{2}$  and thus there should be no point from the sample in some ball  $2B_j$ . A simple computation reveals that the probability that some random variable  $\mathbf{x}_i \in \mathbb{X}_n$  does not belong to  $2B_j$  is at most  $1 - m_f \cdot \operatorname{Vol}(2B_j)$ . By the independence of the random variables  $\mathbf{x}_1, \ldots, \mathbf{x}_n$ , if n is large enough

$$\mathbb{P}\left(\bigcap_{i=1}^{n} \{\mathbf{x}_i \notin 2B_j\}\right) \le \left(1 - m_f \cdot \operatorname{Vol}(2B_j)\right)^n \le \left(1 - m_f c(d) n^{\kappa - 1}\right)^n.$$

We conclude that

$$\mathbb{P}\left(\left\{\sup_{x\in\mathcal{M}}d_{\mathcal{M}}(x,\mathbb{X}_n)\geq n^{(\kappa-1)/d}\right\}\right)\leq \sum_{j=1}^{P_n}\mathbb{P}\left(\bigcap_{i=1}^n\{\mathbf{x}_i\notin 2B_j\}\right)\leq (1-m_fc(d)n^{\kappa-1})^nP_n.$$

Since  $P_n$  grows at most like a polynomial in n,  $(1 - m_f c(d) n^{\kappa-1})^n P_n \leq \exp(-\theta n^{\kappa})$  for an appropriate  $\theta > 0$  and n big enough, as we wanted to show.

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