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Robust Anisotropic Power-Functions-based Filtrations for Clustering.

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¹ — Abstract

- ² We consider robust power-distance functions that approximate the distance function to a compact
- 3 set, from a noisy sample. We pay particular interest to robust power-distance functions that are
- 4 anisotropic, in the sense that their sublevel sets are unions of ellipsoids, and not necessarily unions
- 5 of balls. Using persistence homology on such power-distance functions provides robust clustering
- ⁶ schemes. We investigate such clustering schemes and compare the different procedures on synthetic
- 7 and real datasets. In particular, we enhance the good performance of the anisotropic method for
- ⁸ some cases for which classical methods fail.

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Lines 479

1 Introduction

¹⁰ Often data can be represented as a point cloud X in a Euclidean space \mathbb{R}^d . Grouping data ¹¹ into clusters as homogeneous and well-separated as possible is the purpose of clustering. ¹² When no label is know in advance, we talk about unsupervised clustering. Topological data ¹³ analysis (TDA) tools are designed to understand the shape of the data. Thereby, such tools ¹⁴ may help to understand the shape of clusters in which to group the data. In this paper, we ¹⁵ develop and study a TDA-based unsupervised clustering scheme. In addition, our method ¹⁶ detects and removes points that do not really belong to any cluster; the outliers.

Clustering datasets is of extreme importance in multiple domains including medicine and 17 social networks among others. The classical k-means method clusters data into isotropic 18 clusters. In particular, the trimmed version of k-means of [14] that removes outliers, supplies 19 balls-shaped clusters. These two algorithms have been extended by [2, 5] for Bregman-balls-20 shaped clusters, see also tclust [17] for ellipsoidal clusters. Such methods are well-suited for 21 data generated according to mixtures of distributions which sublevel-set are Bregman balls 22 themselves. For more general datasets, for instance, a sample of point from a disconnected 23 manifold, these methods are no longer appropriate. Spectral clustering methods [27] perform 24 such tasks, but are not robust to outliers. DBSCAN [19] is an algorithm based on a fixed 25 upper-level set of an approximation of the density, and consequently, does not provide a 26 multiscale information. Via a dendrogram, the classical single-linkage hierarchical clustering 27 algorithm provides such a multiscale information. The dendrogram encodes information about 28 the connectivity of unions of balls centered at points in X, or equivalently, of the sublevel 29 sets of the distance function to X. For a fixed radius r, the Čech complex is a simplicial 30 complex defined as the collection of simplices (vertex, edge, triangle, tetrahedron) for which 31 the r-balls centered at the vertices have a non-empty common intersection. We call 1-skeleton 32

its subcomplex (a graph) that contains only vertices and edges. The non-decreasing family 33 of such graphs indexed by $r \in \mathbb{R}$ is called a filtration. Single-linkage is a persistence-based 34 method since is based on the persistence, prominence or equivalently lifetime of the connected 35 components into this graph filtration, however, it is not robust to outliers. The algorithm 36 ToMATo in [12] is robust and persistence-based. Indeed, it is based on a graph filtration 37 built from a neighborhood graph and a (robust) distance-like function whose values guide 38 the appearance of vertices and edges in the graph filtration. An example of robust distance 39 function that Chazal et al. consider in [12] is given by the distance-to-measure (DTM) [10]. 40 Note that the graph is a priori not intrinsic to the distance function, which may cause bad 41 clustering. For instance, an edge that links two vertices with small distance-function value 42 but intersects an area with large distance function value, may link two clusters that should 43 not be. This problem was the cause of failure of the single-linkage method for data corrupted 44 by outliers. Alternative filtrations that do not suffer from this problem are the DTM-filtration 45 [1], or the power filtrations [7], based on the 1-skeleton of the Čech filtration associated to 46 the sublevel sets of a power distance function: a function of type $x \mapsto \min_{i \in I} ||x - m_i||^2 + \omega_i$ 47 for some $(m_i)_{i \in I}$ in \mathbb{R}^d and $(\omega_i)_{i \in I}$ in \mathbb{R} . Some approximations of the DTM that are power 48 functions have been introduced and studied in the literature: the k-witnessed distance [18], 49 the power distance [7], the c-PDTM [6] whose sublevel sets are unions of c balls, and the 50 c-PLM [4] whose sublevel sets are unions of c ellipsoids, with c possibly much smaller than 51 the sample size. The last two functions are robust to outliers since their construction is 52 based on the principle of trimmed least squares [26]. 53

54 Contributions

⁵⁵ By replacing balls with ellipsoids, we enlarge the notion of weighted Čech filtration into the ⁵⁶ anisotropic weighted Čech filtration. We derive an expression for the radius of intersection of ⁵⁷ two ellipsoids. We introduce a clustering algorithm based on persistence. Such a clustering ⁵⁸ algorithm can be run from any graph filtration, in particular, from the 1-skeleton of the ⁵⁹ anisotropic weighted Čech filtration, which corresponds to the filtration of sublevel sets of an ⁶⁰ anisotropic power function. We experiment this algorithm on the filtration of the *c*-PLM [4].

61 Practical interests

A clustering algorithm based on the persistence filtration of the sublevel sets of a power 62 function is pertinent since unlike ToMATo, the graph is intrinsic to the distance function. 63 So, no additional parameters are required for the algorithm. The main advantage of using 64 an anisotropic power function is that its sublevel sets are ellipsoids. Much less ellipsoids are 65 required than balls to Hausdorff-approximate a compact manifold with intrinsic dimension 66 smaller than the ambient dimension. The clustering scheme can also be applied to decompose 67 a set of points generated on a polygonal line into segments. Once the ellipsoids computed, 68 the persistence algorithm runs fast. Its complexity in terms of number of comparisons is at 69 worst $O(c^4)$, with c, the number of ellipsoids, which is much smaller than the sample size. 70 Most importantly, the robustness of the persistence algorithm relies on the robustness of 71 the distance function. The c-PLM [4] is robust to outliers. The guaranty for the clustering 72 method follows from the $\|\cdot\|_{\infty}$ -distance closeness between the power distance function and the 73 distance function to the underlying manifold \mathcal{X} , relatively to the minimal distance between 74 the connected components of \mathcal{X} . Note that such a proximity condition is sufficient but not 75 necessary, as illustrated by the different numerical examples, with the c-PLM. 76

77 Organisation of the paper

In Section 2, we recall the notions of power function and weighted Čech filtration, the 78 filtration of the nerves of its sublevel sets, that we extend to anisotropic power functions. 79 We prove some stability and approximation properties for such filtrations. Examples of 80 robust power filtrations are also displayed. The main clustering algorithm, Algorithm 1 is 81 given in Section 3. This algorithm applies to any filtration of graphs, including the graph 82 filtrations obtained as the 1-skeleton of a weighted Čech filtration. We enumerate other types 83 of filtrations that fit into this framework. Finally, we implement Algorithm 1 with the robust 84 anisotropic aforementioned power function in Section 4. We compare this method to other 85 clustering methods on synthetic and real datasets. 86

⁸⁷ 2 Power-functions-based filtrations for robust clustering

In the sequel, we will recall the notion of filtration for subsets of \mathbb{R}^d (equipped with the 88 Euclidean norm $\|\cdot\|$) and for simplicial complexes. We will consider a class of functions for 89 which filtrations associated to sublevel sets are easily represented by filtrations of simplicial 90 complexes, making the evolution of their connected components tractable: the power functions. 91 In addition, we will give an example of robust power-functions [6] that can be built from 92 a probability distribution or a pointset X. Their sublevel sets are unions of c balls, with c93 possibly much smaller than the size of X. Most importantly, we will also give an example of 94 a robust anisotropic power-function, whose sublevel sets are unions of c ellipsoids [4]. Both 95 of these power functions will be considered in the next sections for clustering purposes. 96

97 2.1 Generalities on filtrations

A filtration indexed by a time set $T \subset \mathbb{R}$ is a family $(V^t)_{t \in T}$ of subsets of \mathbb{R}^d , non-decreasing for the inclusion (i.e. $\forall t \leq t', V^t \subset V^{t'}$). A typical example is the filtration of the sub-level sets of a function $f : \mathbb{R}^d \to \mathbb{R}$, $(f^{-1}((-\infty, t]))_{t \in T}$. For any simplex S with finite vertex set \mathbb{X} , a filtration of simplicial complexes of S is a non-decreasing family $(S^t)_{t \in T}$ of subcomplexes of S, meaning that for every $t \leq t'$, any simplex of S^t is also a simplex of $S^{t'}$.

The interleaving pseudo-distance between two filtrations $(V^t)_{t\in T}$ and $(W^t)_{t\in T}$ is defined as the smallest $\epsilon > 0$ such that $(V^t)_{t\in T}$ and $(W^t)_{t\in T}$ are ϵ -interleaved, i.e. such that: $\forall t \in T, V^t \subset W^{t+\epsilon}$ and $W^t \subset V^{t+\epsilon}$. This definition extends to simplicial complexes. Note that the sub-level-sets filtrations of two functions f and g satisfying $||f - g||_{\infty} \leq \epsilon$ are ϵ -interleaved. We will see in Section 3 that the notion of interleaving is primordial, since it measures the difference of topology between two filtrations. In particular, the stability of our sub-level-sets-based clustering scheme will be guarantied from the closeness of the functions.

110 2.2 Power-functions-based filtrations

In this paper, we consider classes of functions whose sub-level sets filtration has a sparse
representation, the power functions. The sublevel sets of these functions can be represented
by simplicial complexes in so-called weighted Čech filtrations. We will consider two types of
power functions, the isotropic and the anisotropic ones.

115 2.2.1 The isotropic case

An isotropic power function is a function $f_{\mathbf{m},\boldsymbol{\omega}} : \mathbb{R}^d \to \mathbb{R}$ defined from an index set $I = \llbracket 1, c \rrbracket$, a family of centers $\mathbf{m} = (m_i)_{i \in I}$ in \mathbb{R}^d and a family of weights $\boldsymbol{\omega} = (\omega_i)_{i \in I}$ in \mathbb{R} by

 $f_{\mathbf{m},\boldsymbol{\omega}}: x \mapsto \min_{i \in I} \|x - m_i\|^2 + \omega_i$. A simple example of power function is the squared 118 Euclidean distance function to a set of points \mathbb{X} , $d_{\mathbb{X}}^2 : x \in \mathbb{R}^d \mapsto \min_{m \in \mathbb{X}} ||x - m||^2$. The 119 sublevel sets of $f_{\mathbf{m},\boldsymbol{\omega}}, V_{\mathbf{m},\boldsymbol{\omega}}^t = f_{\mathbf{m},\boldsymbol{\omega}}^{-1}((-\infty,t])$, are unions of at most c balls $\mathcal{B}_i^t = \overline{\mathrm{B}}(m_i,\sqrt{t-\omega_i})$ 120 with $\overline{B}(m,r) = \{x \in \mathbb{R}^d \mid ||x-m|| \le r\}$. Note that \mathcal{B}_i^t is empty for $t < \omega_i$ and two balls 121 $\mathcal{B}_i^t \text{ and } \mathcal{B}_j^t \text{ intersect if and only if } t \ge t_{i,j} \text{ with } t_{i,j} = \frac{(\omega_j - \omega_i)^2 + 2(\omega_j + \omega_i)||m_j - m_i||^2 + ||m_j - m_i||^4}{4||m_j - m_i||^2}.$ 122 The connectivity of $V_{\mathbf{m},\boldsymbol{\omega}}^t$ can be encoded in a graph $\mathcal{G}_{\mathbf{m},\boldsymbol{\omega}}^t$, whose vertices are indices $i \in I$ 123 such that $\omega_i \leq t$ and whose edges are pairs of vertices [i, j] such that $t_{i,j} \leq t$. Indeed, $\mathcal{G}_{\mathbf{m},\omega}^t$ 124 and $V_{\mathbf{m},\boldsymbol{\omega}}^t$ have the same number of connected components, and m_i and m_j are in the same 125 connected component in $V_{\mathbf{m},\omega}^t$ if and only if *i* and *j* are also in the same component in $\mathcal{G}_{\mathbf{m},\omega}^t$. 126 More generally, the topological information of $V_{\mathbf{m},\boldsymbol{\omega}}^{t}$ (number of connected components, 127

loops, voids etc.) can be encoded in the weighted Čech complex $\operatorname{Cech}_{\mathbf{m},\boldsymbol{\omega}}(t)$, defined as 128 the nerve of the union of balls $(\mathcal{B}_i^t)_{i \in I}$: Cech_{**m**, $\boldsymbol{\omega}$} $(t) = \{ \sigma \subset I \mid \bigcap_{i \in \sigma} \mathcal{B}_i^t \neq \emptyset \}, [1, 7, 3].$ 129 According to the Nerve Lemma [20, Corollary 4G.3], any sublevel set $V_{\mathbf{m},\boldsymbol{\omega}}^t$ is homotopic 130 to $\operatorname{Cech}_{\mathbf{m},\boldsymbol{\omega}}(t)$ and thus contains the same topological information. For computational 131 reasons, the weighted Vietoris-Rips filtration is frequently considered as a provably good 132 surrogate for the weighted Čech filtration $(\operatorname{Cech}_{\mathbf{m},\boldsymbol{\omega}}(t))_{t\in T}$. The weighted Vietoris-Rips 133 complex $\operatorname{VR}_{\mathbf{m},\boldsymbol{\omega}}(t)$ is the flag complex of $\mathcal{G}_{\mathbf{m},\boldsymbol{\omega}}^t$ ($\mathcal{G}_{\mathbf{m},\boldsymbol{\omega}}^t$ is the 1-skeleton of the weighted Čech 134 complex): $\operatorname{VR}_{\mathbf{m},\boldsymbol{\omega}}(t) = \{ \sigma \subset I \mid \forall i, j \in \sigma, \mathcal{B}_i^t \cap \mathcal{B}_j^t \neq \emptyset \}$. Indeed, as a direct consequence of 135 [3, Theorem 3.2] which is a generalization of the non-weighted case in [15, Theorem 2.5.], if 136 the weights in $\boldsymbol{\omega}$ are non-negative, then these two filtrations are interleaved: 137

¹³⁸
$$\forall 0 < t' \leq \frac{d+1}{2d} t, \operatorname{VR}_{\mathbf{m},\boldsymbol{\omega}}(t') \subset \operatorname{Cech}_{\mathbf{m},\boldsymbol{\omega}}(t) \subset \operatorname{VR}_{\mathbf{m},\boldsymbol{\omega}}(t).$$
 (1)

¹³⁹ These notions can all be extended to anisotropic power functions.

¹⁴⁰ 2.2.2 The anisotropic case

Consider $I = [\![1, c]\!]$, centers $\mathbf{m} = (m_i)_{i \in I}$ in \mathbb{R}^d , weights $\boldsymbol{\omega} = (\omega_i)_{i \in I}$ in \mathbb{R} and matrices $\Sigma = (\Sigma_i)_{i \in I}$ in \mathcal{M}_d , the set of definite positive symmetric matrices. An anisotropic power function is a function $f_{\mathbf{m}, \boldsymbol{\omega}, \boldsymbol{\Sigma}} : \mathbb{R}^d \to \mathbb{R}$ defined from I, $\mathbf{m}, \boldsymbol{\omega}$ and Σ by $f_{\mathbf{m}, \boldsymbol{\omega}, \boldsymbol{\Sigma}} : x \mapsto$ $\min_{i \in I} \|x - m_i\|_{\Sigma_i^{-1}}^2 + \omega_i$. For any matrix $\Sigma \in \mathcal{M}_d$ and $x \in \mathbb{R}^d$, $\|x\|_{\Sigma^{-1}} = \sqrt{x^T \Sigma^{-1} x}$ denotes the Σ -Mahalanobis norm of x. The sublevel sets of $f_{\mathbf{m}, \boldsymbol{\omega}, \boldsymbol{\Sigma}}$, $V_{\mathbf{m}, \boldsymbol{\omega}, \boldsymbol{\Sigma}}^t = f_{\mathbf{m}, \boldsymbol{\omega}, \boldsymbol{\Sigma}}^{-1}((-\infty, t])$, are unions of at most c ellipsoids $\mathcal{E}_i^t = \overline{B}_{\Sigma_i}(m_i, \sqrt{t - \omega_i}) = \{x \in \mathbb{R}^d \mid \|x - m_i\|_{\Sigma_i^{-1}}^2 \leq t - \omega_i\}$. Again, \mathcal{E}_i^t is empty for $t < \omega_i$ and the intersection time $t_{i,j}$ of \mathcal{E}_i^t and \mathcal{E}_j^t is given below. The relative question of the emptiness of the intersection of two ellipsoids is tackled in [28, 25].

▶ Proposition 1. Consider two ellipsoids $\mathcal{E}_{i}^{t} = \overline{\mathbb{B}}_{\Sigma_{i}}(m_{i}, \sqrt{t-\omega_{i}})$ and $\mathcal{E}_{j}^{t} = \overline{\mathbb{B}}_{\Sigma_{j}}(m_{j}, \sqrt{t-\omega_{j}})$ with $\omega_{i} \leq \omega_{j}$ in \mathbb{R} , m_{i} and m_{j} in \mathbb{R}^{d} , $\Sigma_{i} = P_{i}D_{i}P_{i}^{T}$ and $\Sigma_{j} = P_{j}D_{j}P_{j}^{T}$ in \mathcal{M}_{d} , with two positive diagonal matrices D_{i} and D_{j} and two orthogonal matrices P_{i} and P_{j} from the spectral theorem. Set $\tilde{\Sigma} = \sqrt{D_{i}}P_{i}^{T}\Sigma_{j}^{-1}P_{i}\sqrt{D_{i}} = \tilde{P}\tilde{D}\tilde{P}^{T}$, for orthogonal and diagonal matrices \tilde{P} and $\tilde{D} = diag(\lambda_{1}, \lambda_{2}, ..., \lambda_{d})$, and $\tilde{m} = \tilde{P}^{T}\sqrt{D_{i}^{-1}}P_{i}^{T}(m_{j} - m_{i})$. Ellipsoids \mathcal{E}_{i}^{t} and \mathcal{E}_{j}^{t} intersect if and only if $t \geq t_{i,j}$ for $t_{i,j} = \omega_{j}$ when $\|\tilde{m}\| \leq \sqrt{\omega_{j} - \omega_{i}}$, and $t_{i,j} = \omega_{j} + \sum_{k=1}^{d} \left(\frac{\lambda \tilde{m}_{k}}{\lambda + \lambda_{k}}\right)^{2} \lambda_{k}$ when $\|\tilde{m}\| > \sqrt{\omega_{j} - \omega_{i}}$. The positive number λ is the unique solution of the following equation: 154

$$\sum_{k=1}^{a} \frac{\lambda_k - \lambda^2}{(\lambda + \lambda_k)^2} \lambda_k \tilde{m}_k^2 = \omega_j - \omega_i.$$
(2)

The proof of Proposition 1 is to be found in Section A. It is based on the fact that the 158 ellipsoids \mathcal{E}_i^t and \mathcal{E}_i^t are tangent at their first intersection point, and the corresponding 159 gradients are collinear. In the context of isotropy (i.e. for $\Sigma_i = \Sigma_j = I_d$, the identity 160 matrix of \mathbb{R}^d) $\tilde{m} = m_j - m_i$, and when $||m_j - m_i|| > \sqrt{\omega_j - \omega_i}$, (2) has a unique positive 161 solution given by $\lambda = \frac{\omega_i - \omega_j + ||m_j - m_i||^2}{\omega_j - \omega_i + ||m_j - m_i||^2}$. We recover the merging time $t_{i,j}$ given in Section 162 2.2.1. Now, define $\mathcal{G}_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}^t$, $\operatorname{Cech}_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}(t)$ and $\operatorname{VR}_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}(t)$, the anisotropic counterparts of 163 $\mathcal{G}_{\mathbf{m},\boldsymbol{\omega}}^t$, Cech_{m,\boldsymbol{\omega}}(t) and VR_{m,\boldsymbol{\omega}}(t). The nerve lemma still applies, since unions of ellipsoids 164 are contractible. Although this paper is mostly based on the study of connected components 165 for clustering, anisotropic weighted Čech and Vietoris-Rips filtrations are primordial to have 166 a tractable estimation of the topology of compact sets from suitable approximations as 167 finite unions of ellipsoids. In fact, as their isotropic counterparts (1), these filtrations are 168 interleaved, provided that the eigenvalues of the matrices in Σ are positive. 169

▶ Proposition 2. If ω is a set on non-negative weights in \mathbb{R} and Σ a family of matrices with eigenvalues in $[\lambda_{\min}, \lambda_{\max}]$ for some $\lambda_{\min} > 0$, then for every t > 0 and $0 < t' \leq \frac{\lambda_{\min}}{\lambda_{\max}} \frac{d+1}{2d}t$,

¹⁷²
$$\operatorname{VR}_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}(t') \subset \operatorname{Cech}_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}(t) \subset \operatorname{VR}_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}(t).$$
 (3)

The condition of non-negative weights is not too restrictive since for general weights, it suffices to replace $\boldsymbol{\omega}$, t and t' by $\boldsymbol{\omega} - \min_{i \in I} \omega_i$, $t - \min_{i \in I} \omega_i$ and $t' - \min_{i \in I} \omega_i$ in the proposition. Then, the condition on t' becomes $\min_{i \in I} \omega_i < t' \leq \frac{\lambda_{\min}}{\lambda_{\max}} \frac{d+1}{2d} t + \left(1 - \frac{\lambda_{\min}}{\lambda_{\max}} \frac{d+1}{2d}\right) \min_{i \in I} \omega_i$. As noted in [15], when λ_{\min} equals λ_{\max} and the weights in $\boldsymbol{\omega}$ are null, the term $\frac{\lambda_{\min}}{\lambda_{\max}} \frac{d+1}{2d}$ is optimal. When \mathbf{m} is the set of vertices of a regular d-simplex, the left inclusion is an equality. The proof of Proposition 2 is available in Section B.

Often, less ellipsoids than balls are required to describe a compact set \mathcal{X} , for a fixed level of precision (e.g. for the Hausdorff distance). For instance, a segment in \mathbb{R}^2 , and more generally, any d'-dimensional submanifold in \mathbb{R}^d , with d' < d. For this reason, anisotropic Čech and Vietoris-Rips filtrations are pertinent tools to compute and store the topological information about \mathcal{X} efficiently. The requisite condition is that we dispose of an anisotropic power function that is a good approximation of $d^2_{\mathcal{X}}$. Such examples of functions follow.

¹⁸⁵ 2.3 Examples of filtrations based on robust power functions

186 2.3.1 Isotropic robust power functions

Set X, a set of n points generated on the neighborhood of a compact subset \mathcal{X} of \mathbb{R}^d . In order 187 to face the non robustness of the distance function to \mathbb{X} , $d_{\mathbb{X}}$, Chazal et al. have introduced 188 the notion of distance-to-measure (DTM), in [10]. The DTM is a counterpart of d_X robust 189 to noise and outliers. Its robustness follows from some parameter $k \in [1, n]$, the number 190 of nearest-neighbors X^1, X^2, \ldots, X^k of x in \mathbb{X} , used to estimate $d_{\mathbb{X}}(x)$. The DTM $d_{\mathbb{X},k}$ is defined by $d_{\mathbb{X},k}^2 : x \mapsto \frac{1}{k} \sum_{i=1}^k ||x - X^i||^2 = ||x - m_{x,k}||^2 + v_{x,k}$ with $m_{x,k} = \sum_{i=1}^k X^i$, the 191 192 mean of the k nearest neighbours of x in X and $v_{x,k} = \frac{1}{k} \sum_{i=1}^{k} ||X^i - m_{x,k}||^2$ their variance. 193 Note that $d_{X,1}$ coincides with d_X and is not robust, whereas $d_{X,n}(x)$ is the distance of x to 194 the barycenter of the point cloud X, up to some factor, which is robust, but very poor in 195 terms of topological information. The DTM is actually a weighted power function [18]: 196

¹⁹⁷
$$d^2_{\mathbb{X},k}(x) = \inf_{y \in \mathbb{R}^d} ||x - m_{y,k}||^2 + v_{y,k}.$$
 (4)

This follows from the fact that the mean distance between x and its k nearest neighbors is not larger than the mean distance between x and the k nearest neighbors of any other point

 $y \in \mathbb{R}^d$. This infimum is actually a minimum over a set of c points $\mathbf{y} = (y_i)_{i \in [1,c]}$ in \mathbb{R}^d , with $\binom{n}{k}$. A power approximation of the DTM, the k-witnessed distance, was defined c of order 201 in [18] by replacing \mathbb{R}^d by X in (4). Its sublevel sets are unions of n balls. An approximation 202 of the DTM with c (possibly much smaller than n) balls, the c-PDTM, was defined in [6], by 203 replacing \mathbb{R}^d by a set $\mathbf{y}_{c,k}$ of c points in \mathbb{R}^d . This set $\mathbf{y}_{c,k}$ is a minimum of a "k-means"-type 204 criterion [24], $\mathbf{y} \mapsto \sum_{i=1}^{n} \min_{y \in \mathbf{y}} ||X_i - m_{y,k}||^2 + v_{y,k}$, for \mathbf{y} with cardinality c. Morally, $\mathbf{y}_{c,k}$ is chosen such that on average on \mathbb{X} , $x \mapsto \min_{y \in \mathbf{y}} ||x - m_{y,k}||^2 + v_{y,k}$ is small. Note that the 205 206 graph of the c-PDTM is necessarily above the graph of the DTM. According to [6], for a 207 sample on a regular d'-dimensional manifold, c can be chosen of order $n^{\frac{d'}{d'+4}}$, which is much 208 smaller than n. Moreover, the c-PDTM is a good approximation of $d^2_{\mathcal{X}}$, despite noise. 209

210 2.3.2 An anisotropic robust power function

An anisotropic version of the c-PDTM has been introduced in [4], the c-power likelihood to 211 measure (c-PLM). It consists in replacing Euclidean norms with Mahalanobis norms. For 212 every $x \in \mathbb{R}^d$ and $\Sigma \in \mathcal{M}_d$, set $X^1, X^2, \dots X^k$ the k-nearest neighbors of x in X, for the 213 Σ^{-1} -Mahalanobis norm: $\|X^i - x\|_{\Sigma^{-1}} \leq \|X^j - x\|_{\Sigma^{-1}}$ for every $i \leq j$. Denote by $m_{x,\Sigma,k}$ their mean, and by $v_{x,\Sigma,k} = \frac{1}{k} \sum_{i=1}^k \|X^i - m_{x,\Sigma,k}\|_{\Sigma^{-1}}^2$ their variance, relative to the Σ -Mahalanobis 214 215 norm. Set $\boldsymbol{\theta}_{c,k}$, a family of c pairs $(y, \Sigma) \in \mathbb{R}^{\overline{d}} \times \mathcal{M}_d$ that minimizes (or which criterion is as 216 close as possible to the optimal criterion, in case of non existence of a minimum) the following 217 "k-means"-type criterion $R_{c,k}$ among all $\boldsymbol{\theta}$ s of cardinality c: $R_{c,k}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \min_{(y,\Sigma) \in \boldsymbol{\theta}} \|X_i - X_i\|_{1}$ 218 $m_{y,\Sigma,k}\|_{\Sigma^{-1}}^2 + v_{y,\Sigma,k} + \log(\det(\Sigma))$. The term $\log(\det(\Sigma))$ prevents optimal covariance matrices 219 to be degenerated, with Σ^{-1} going to 0. In some sense, minimizing such a criterion boils 220 down to fit Gaussian distributions to the data set X, at best. The c-PLM is the power 221 function defined from $\boldsymbol{\theta}_{c,k}$ by: $x \mapsto \min_{(y,\Sigma) \in \boldsymbol{\theta}_{c,k}} \|x - m_{y,\Sigma,k}\|_{\Sigma^{-1}}^2 + v_{y,\Sigma,k} + \log(\det(\Sigma))$. A 222 modification of the criterion $R_{c,k}$ has been introduced in [4], to remove some datapoints 223 (|X| - sig for some parameter sig), when X is corrupted with outliers. The criterion is given by 224 $R_{c,k,sig}(\theta) = \min_{(i_1,i_2,\dots,i_{sig}) \in [\![1,|\mathbb{X}|]\!]} \sum_{j=1}^{sig} \min_{(y,\Sigma) \in \theta} \|X_{i_j} - m_{y,\Sigma,k}\|_{\Sigma^{-1}}^2 + v_{y,\Sigma,k} + \log(\det(\Sigma)).$ 225 Iterative Lloyd-type algorithms [22] provide local minima $\tilde{\theta}_{c,k}$ and $\tilde{\theta}_{c,k,sig}$ for the criteria 226 $R_{c,k}$ and $R_{c,k,sig}$ [4]. These algorithms run in $O(ncd^2 + nkd^2 + n\log(n)c)it$ operations, with 227

it the number of iterations of the algorithm. They consist, given $\boldsymbol{\theta} = (\mathbf{y}, \boldsymbol{\Sigma})$, in splitting the space \mathbb{R}^d into weighted $\boldsymbol{\Sigma}$ -curved Voronoi cells, replacing centers \mathbf{y} by the centroid of the cells, and updating the matrices in $\boldsymbol{\Sigma}$ by a close formula from the points in the cells and ellipsoids. To compute $\tilde{\boldsymbol{\theta}}_{c,k,sig}$, a trimming step is added at each iteration. For clustering, disposing of a local minimum is enough, as enhanced in the numerical illustration section, since we can remove bad centers in $\tilde{\boldsymbol{\theta}}_{c,k,sig}$ with the parameter *Threshold* in Algorithm 1.

²³⁴ **3** Persistence-based clustering from power-functions-based filtrations

3.1 Persistence for power-functions-based filtrations

Set $f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}: x \in \mathbb{R}^d \mapsto \min_{i \in I} ||x - m_i||_{\Sigma_i^{-1}}^2 + \omega_i$, an anisotropic power-function indexed by a set $I = [\![1,c]\!]$ and with the ω_i s sorted in non-decreasing order. As above-mentioned, the sublevel sets $V^t = f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}^{-1}((-\infty,t])$ are unions of at most c ellipsoids $\mathcal{E}_i^t = B_{\Sigma_i}(m_i,\sqrt{t-\omega_i})$, non empty as soon as $t \ge \omega_i$. In particular, each sublevel set of $f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}$ contains at most cconnected components. Each connected component of V^t, V_i^t is indexed by the smallest index $i \in I$ such that m_i belongs to the component. With a language abuse, we call connected component V_i , the family of connected components $(V_i^t)_{t\in T}$ that gets born at time $t = b_i = \omega_i$

and dies at a time $t = d_i$ when V_i^t merges with another connected component V_j^t for some $j \leq i$. Note that $d_1 = \infty$. The lifetime of the component V_i^t , $d_i - b_i$, is called persistence or prominence of the component *i*. This merging information is encoded in a barcode or a dendrogram. In these two representations, each line is associated to a component V_i , has length $d_i - b_i$, and begins at the height b_i . The dendrogram is obtained from the barcode by linking the bars associated to merging components, at a height given by the merging time.

When **m** is a point set \mathbb{X} , $\Sigma_i = I_d$ and $\omega_i = 0$ for every *i*, clustering points accordingly 249 to the connected components of V^t boils down to the classical single-linkage clustering 250 procedure, with t > 0, calibrated in accordance with the dendrogram. This procedure is not 251 robust to outliers. In this paper, we consider an adjacent procedure, similar to the ToMATo 252 algorithm [12], based on the prominence of components. To be precise, in the clustering 253 scheme, a component V_i cannot merge with another component V_j at a time t larger than 254 $\omega_i + Stop$, for some parameter Stop. In other words, components with large prominence will 255 never die in this clustering procedure. This is the purpose of Algorithm 1 in the next section. 256 257

In order to better visualize the prominence of the components, we represent their lifetimes 258 in a persistence diagram. A persistence diagram is a multiset of points $(b_i, d_i) \in \mathbb{R}^2$ that lie 259 above the diagonal b = d. Each point (b_i, d_i) is associated to a connected component V_i . The 260 notion of persistence diagram was introduced by Edelsbrunner et al. in [16], in the broader 261 framework of homology, and allows to compute lifetimes of additionnal features such as loops, 262 voids etc. It is defined for filtrations that are regular enough, on triangulable spaces such 263 as \mathbb{R}^d . The proper notion of regularity is the notion of q-tameness [11]. In [7, Proposition 264 [3.5], Buchet et al. proved that the DTM is q-tame. The proof of [7] can be straightforwardly 265 adjusted for distance functions to compact sets and most importantly, for anisotropic power 266 functions, provided that the eigenvalues of the matrices Σ_i are all positive. A sketch of proof 267 is given in the Appendix, in Section C. 268

Since distance to compact sets, distance-to-measure and anisotropic power functions are q-tame, the persistence diagrams associated to their filtrations are well defined. They can be compared through the bottleneck distance, a distance between two diagrams D and D'defined as the minimal value of $\max_{x \in D, y \in D'} |y - \phi(x)|_{\infty}$ among functions ϕ that pair points in D with points in D', with some points potentially paired to diagonal points. Diagrams associated to interleaved filtrations are close, according to the following theorem.

▶ **Theorem 3** (Stability of persistence diagrams [11, 9, 13]). If two filtrations V and W are q-tame and ϵ -interleaved, then the persistence diagrams of these filtrations are ϵ -close in bottleneck distance.

According to Theorem 3, the persistence diagram of any anisotropic power function 278 $f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}$ that is $\epsilon - \|\cdot\|_{\infty}$ close to $d_{\mathcal{X}}$ is ϵ -bottleneck close to the persistence diagram of the 279 sublevel sets of $d_{\mathcal{X}}$. Consequently, prominence of the connected components of \mathcal{X} can be 280 deduced from the diagram associated to $f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}$, for ϵ small enough. This bottleneck closeness 281 occurs with large probability for a regular manifold \mathcal{X} for the c-PDTM built from a noisy 282 sample from \mathcal{X} , according to [6]. No such result has been proved yet for the c-PLM. Anyway, 283 intuitively, its sublevel sets are good approximations of the manifold \mathcal{X} , with the advantage 284 that they are made of less ellipsoids, and that these ellipsoids are oriented accordingly to 285 the manifold, i.e. with large eigenvalues on the tangent space and small eigenvalues on its 286 orthogonal. This will be confirmed in the numerical illustrations section. 287

²⁸⁸ By construction, the persistence diagram (for connected components) associated to the ²⁸⁹ filtration of the sublevel sets of $f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}$ coincides with the persistence diagram associated to ²⁹⁰ the anisotropic weighted Čech complex Cech $(f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}})$. Consequently, we can forget about the

ellipsoids and focus on the simplicial complex filtration, which can be computed and stored efficiently, in a $c \times c$ matrix Mat = $(t_{i,j})_{i,j\in I}$. Such a matrix contains the times of appearance of vertices and of merging of connected components in $\operatorname{Cech}(f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}})$. The clustering scheme of this paper exposed just below is based on such a merging matrix Mat.

²⁹⁵ 3.2 An algorithm for persistence-based clustering

Consider $(\mathcal{G}^t)_{t\in\mathbb{R}}$ a filtration of sub-graphs of \mathcal{G} , a graph with c nodes. Based on this filtration, 296 we define an algorithm, strongly inspired from the ToMATo algorithm [12]. The clustering 297 scheme is guided by the persistence of the connected components in $(\mathcal{G}^t)_{t\in\mathbb{R}}$, and preserves 298 components with large prominence. We assume that the nodes of $\mathcal G$ are labeled such that the 299 node labeled i gets born before the node labeled j, when $i \leq j$. The procedure is as follows. 300 A connected component gets born when a node gets born, with the same label. A component 301 changes of label at each time t for which it merges with a component with smaller label in \mathcal{G}^t , 302 unless its prominence is larger than some parameter Stop. The prominence of a node or a 303 component is defined as the lifetime of the component in the filtration (i.e. the elapsed time 304 between the birth of the node and the time t such that a node with smaller index is present 305 in its connected component in \mathcal{G}^t). The resulting clustering is given by the label of the nodes 306 at time $t = +\infty$. It contains exactly labels of edges with a prominence larger than Stop. In 307 this clustering scheme, we decide that nodes born after some time parameter Threshold are 308 not relevant; they are removed. This procedure is implemented in Algorithm 1. 309

```
310 Data: Mat, Threshold, Stop
311 Result: Color, Birth, Death
312 Initialization;
\operatorname{Mat}[i,i] \leq \operatorname{Threshold}; Mat \leftarrow \operatorname{Mat}[1:c,1:c];
<sup>314</sup> Birth \leftarrow [Mat[i,i] for i in 1:c]; Death \leftarrow [\infty for i in 1:c];
   indice \leftarrow 1; I \leftarrow 1; time \leftarrow \text{Mat}[I,I]; Color \leftarrow [];
315
    while time < \infty do
316
        if time = Mat/I, I then
317
             Component I appears ;
318
             indice \leftarrow indice +1; Mat[I,I] \leftarrow \infty; Color[I] \leftarrow I;
319
        else
320
             (col_max, col_min) \leftarrow (max(Color[I], Color[J]), min(Color[I], Color[J]));
321
             if time - Birth/col_max \le Stop then
322
                 Components col_max and col_min merge;
323
                 Replace all entries col_max by col_min in Color;
324
                 Death[col max] \leftarrow time;
325
             else
326
                 Component col_max will never die ;
327
            end
328
             Mat[i,j] \leftarrow \infty for every i, j \leq min(indice,c) such that
329
             (Color[i], Color[j]) \in \{(col\_min, col\_max), (col\_max, col\_min)\};
330
        end
331
        I,J \leftarrow \arg\min_{i,j \leq \min(indice,c)} \operatorname{Mat}[i,j] \ ; \ time \leftarrow \operatorname{Mat}[I,J]
332
333 end
```

This algorithm requires a merging matrix $\text{Mat} = (t_{i,j})_{i,j \in I}$, with $I = \llbracket 1, c \rrbracket$. We define its coefficients by $t_{i,i}$, the birth time of the node *i* in the filtration $(\mathcal{G}^t)_{t \in T}$; for i > j, $t_{i,j}$ the

birth time of the edge [i, j] and for i < j, $t_{i,j} = \infty$. The vector *Color* contains the resulting clustering, the vector *Birth*, the birth time of the components and *Death* their death time. Note that *Death*[1] is always $+\infty$. When $(\mathcal{G}_t)_{t\in T}$ is the filtration of the sublevel sets of some power function $f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}$, the matrix Mat has coefficients given by $t_{i,i} = \omega_i$ and for $i > j \ge 1$, $t_{i,j}$ the intersecting time of the ellipsoids \mathcal{E}_i^t and \mathcal{E}_j^t , given by Proposition 1.

In practice, to label points in \mathbb{X} (generated around \mathcal{X}), we consider an approximation 318 of $d_{\mathcal{X}}^2$ based on a family **m** of c centers. Set **m'**, the centers not removed and labeled by 319 Algorithm 1, and ω' and Σ' the corresponding parameters. Clustering points in X is made 320 accordingly to these labels and to the Voronoi decomposition of \mathbb{R}^d , based on $\mathbf{m}', \boldsymbol{\omega}'$ and $\boldsymbol{\Sigma}'$: 321 $x \in \mathbb{X}$ has the same label as m'_i if $\|x - m'_i\|_{\Sigma'_i^{-1}}^2 + \omega'_i \leq \|x - m'_j\|_{\Sigma'_j^{-1}}^2 + \omega'_j$ for every j. 322 Since $f_{\mathbf{m}^*,\boldsymbol{\omega}^*,\boldsymbol{\Sigma}^*}$ approximates $d_{\mathcal{X}}^2$, in order to deal with outliers, we remove (i.e. assign the 323 label 0) the points $x \in \mathbb{X}$ for which $f_{\mathbf{m}', \boldsymbol{\omega}', \boldsymbol{\Sigma}'}(x)$ is the largest. Note that a power function is 324 homogeneous to the square of a distance function. Therefore, for positive weights $\boldsymbol{\omega}$, it could 325 be more appropriate to consider the filtration of sublevel sets of $\sqrt{f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}}$ instead of $f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}$. 326 The best complexity of Algorithm 1 ($O(c^3)$ comparisons) is obtained when $Stop = \infty$, 327 with 2c iterations of the algorithm. The worst complexity $(O(c^4))$ is obtained when Stop = 0, 328 with $O(c^2)$ iterations. This is fast when c is much smaller than the sample size (e.g. for 329 c-PLM and c-PDTM), and does not depend on the dimension. In the experiments of Section 330 4, Algorithm 1 runs much faster than the computation of the c-PLM and the c-PDTM. 331 332

In practice, just as Chazal et al. [12], we recommend to run Algorithm 1 several times. A 333 first time with $Threshold = Stop = \infty$ to calibrate the parameter Threshold, in order to 334 remove bad nodes (i.e. nodes with late birth and short lifetime). A second time with this 335 parameter Threshold and $Stop = \infty$, to measure the prominence of the components and 336 select the number of clusters (via the parameter Stop), as the number of components with 337 prominence much larger than others. More details on the calibration of these two parameters, 338 from the persistence diagrams $(Birth[i], Death[i])_{i \in I}$, are given in Section 4.1. The final 339 clustering is obtained from *Color*, after running Algorithm 1 with these two parameters. 340

Giving a sense to an optimal minimal prominence *Stop* is possible for distance functions. 341 For instance, for the sublevel-sets filtration of $d_{\mathcal{X}}$, Stop can be chosen as half of the minimal 342 distance between two distinct components of \mathcal{X} . Consequently, for any $\epsilon - \| \cdot \|_{\infty}$ -close 343 approximation of $d_{\mathcal{X}}$, taking $Stop - \epsilon$ leads to a perfect clustering, provided that $2\epsilon < Stop$. 344 The parameter *Threshold* is primordial, especially for the *c*-PLM function. Indeed, the 345 algorithm for the c-PLM is based on $\hat{\theta}_{c,k}$, a local minimizer of the criterion $R_{c,k}$. Consequently, 346 some ellipsoids \mathcal{E}_i are far from the support, or in a wrong direction. Thus, their weight 347 ω_i (and thus Birth[i]) is large with respect to other well-placed ellipsoids, due to a large 348 variance term $y_{y_i, \Sigma_i, k}$. Such bad ellipsoids are removed for a suitable parameter *Threshold*. 349

350 3.3 Connection to other persistence-based clustering methods

In the sequel, we display different graph filtrations, to be used for persistence-based clustering, with Algorithm 1. For each of these filtrations, we give a summarize of the corresponding matrices Mat, in Table 1, with the convention that $t_{i,i} \leq t_{j,j}$ when $i \leq j$.

ToMATo Algorithm [12] rests on a graph filtration based on a graph \mathcal{G} and a function *f* defined on the nodes of \mathcal{G} . Morally, \mathcal{G}^t is the sub-graph of \mathcal{G} that contains the nodes *i* such that $f(i) \leq t$, and the edges [i, j] if and only if *i* and *j* are in \mathcal{G}^t . Chazal et al. mostly studied this method for \mathcal{G} , a Rips graph of a set $\mathbb{X} \subset \mathbb{R}^d$, and for f(i), the DTM to \mathbb{X} at X_i . The DTM-filtration [1] corresponds to the 1-skeleton of the nerve of the union of balls

 $(\bigcup_{x \in \mathbb{X}} \overline{B}(x, r_t(x)))_{t>0} \text{ with } r_t(x) = -\infty \text{ for } t < d_{\mathbb{X},k}(x) \text{ and } r_t(x) = (t^p - d_{\mathbb{X},k}^p(x))^{\frac{1}{p}} \text{ for } t \ge d_{\mathbb{X},k}(x), \text{ for some } p \ge 1 \text{ and with the convention that } \overline{B}(x, -\infty) \text{ is empty. In Table 1, we } give the coefficients for <math>p = 1$. The DTM-filtration with p = 2 was actually introduced in [7], leading to what we call Power filtration, which coincides with the sublevel-sets filtration of the square of a power distance. We also consider additional power-functions-based filtrations, from the k-witnessed distance [18], the c-PDTM [6] and the c-PLM [4].

Table 1 Coefficients of Mat for the different methods, with the notation $f = d_{\mathbb{X},k}$ for the DTM to \mathbb{X} with number of nearest neighbors parameter k.

| 367 | Method | $t_{i,i}$ $t_{i,j}$ for $i < j$ | | | | | | | |
|-----|--|--|---|--|--|--|--|--|--|
| 368 | ToMATo | f(i) | $f(i) \qquad \max(f(i), f(j))(\mathbb{1}_{[i,j]\in\mathcal{G}})^{-1}$ | | | | | | |
| 369 | DTM-filtration | f(i) | $i) \left(\frac{\ X_i - X_j\ + f(i) + f(j)}{2}\right) \mathbb{1}_{\ X_i - X_j\ > f(i) - f(j) } + f(i) \mathbb{1}_{f(i) - f(j) \ge \ X_i - X_j\ }$ | | | | | | |
| 370 | $f_{{f m},{m \omega}}$ | ω_i | $\frac{(\omega_j - \omega_i)^2 + 2(\omega_j + \omega_i) \ m_j - m_i\ ^2 + \ m_j - m_i\ ^4}{4\ m_j - m_i\ ^2}$ | | | | | | |
| 371 | $\sqrt{f_{\mathbf{m}, \boldsymbol{\omega}}}$ | $\sqrt{\omega_i}$ | $\sqrt{\frac{(\omega_j - \omega_i)^2 + 2(\omega_j + \omega_i) \ m_j - m_i\ ^2 + \ m_j - m_i\ ^4}{4\ m_j - m_i\ ^2}}$ | | | | | | |
| 372 | $f_{\mathbf{m}, \boldsymbol{\omega}, \boldsymbol{\Sigma}}$ | ω_i | Given by Proposition 1 | | | | | | |
| 373 | Power filtration | $\sqrt{f_{\mathbf{m},\boldsymbol{\omega}}}$ with $\mathbf{m} = \mathbb{X}$ and $\boldsymbol{\omega} = (f^2(x))_{x \in \mathbb{X}}$ | | | | | | | |
| 374 | Witnessed | $\sqrt{f_{\mathbf{m},\boldsymbol{\omega}}}$ with $(\mathbf{m},\boldsymbol{\omega}) = (m_{x,k}, v_{x,k})_{x \in \mathbb{X}}$ | | | | | | | |
| 375 | $c	ext{-PDTM}$ | $f_{\mathbf{m},\boldsymbol{\omega}}$ with $(\mathbf{m},\boldsymbol{\omega}) = (m_{y,k}, v_{y,k})_{y \in \mathbf{y}_{c,k}}$ | | | | | | | |
| 376 | c-PLM | $f_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}$ with $(\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}) = (m_{y,\Sigma,k}, v_{y,\Sigma,k} + \log(\det(\Sigma)), \Sigma)_{(y,\Sigma)\in\theta_{c,k}}$ | | | | | | | |

377 **4** Numerical illustrations

4.1 A complete illustration of the method

Consider the target \mathcal{X} , a set of three curves in \mathbb{R}^2 . We generate $\mathbb{X} = (X_i)_{i \in [1, N_s + N_o]}$, 379 a set of $N_s = 500$ signal points $(X_i = Y_i + Z_i)_{i \in [\![1,N_s]\!]}$, with Y_i uniform on \mathcal{X} and Z_i 380 Gaussian with standard deviation $\sigma = 0.02$; corrupted by $N_o = 200$ outliers, uniform on 381 $[-1.5, 2.5]^2$. We compare the clustering scheme based on Algorithm 1 with the sublevel 382 sets of the c-PLM, to the target labels in Figure 2 (left). Parameters are set to c = 50383 centers, k = 10 nearest neighbors, sig = 520 points to consider as signal, and it = 100384 iterations and $n_{ini} = 10$ initializations to compute a suitable local optimum $\hat{\theta}_{c,k,siq}$ of the 385 c-PLM-criterion $R_{c,k,sig}$. Since the DTM $d_{\mathbb{X},k}$ is large for outliers, we select sig from the 386 curve $([d_{X,k}(X_i), i \in [1, N_s + N_o]])$ in non-decreasing order), as the point of slope break; see 387 Figure 1 (left). The DTM can be replaced by any not-trimmed approximation of the c-PLM. 388 We run Algorithm 1 a first time with the parameters $Threshold = \infty$ and $Stop = \infty$, and 390 display the persistence diagram $(Birth[i], Death[i])_{i \in [1,c]}$, in Figure 1 (middle). In order to 391 have 3 clusters, we select Stop = 5.62, the height of a line parallel to the diagonal, separating 392 3 points from the others. We run Algorithm 1 a second time with this new parameter, which 393 results in the clustering C_1 of Figure 2 (middle). A sublevel set of the function $f_{\tilde{\theta}_{ch}}$ is 394 represented by the union of ellipses. Note that some ellipses have a bad position. This results 395 in a bad clustering. We use the parameter *Threshold* to remove them. In Figure 1 (middle), 396 6 points are on the right side, separated from the other points with a vertical line (of abscissa 397 -10.27). Then, we run Algorithm 1 with Threshold = -10.27 and $Stop = \infty$. According to 398 the persistence diagram in Figure 1 (right), since 3 points are well-separated from the other 399 ones with a large band parallel to the diagonal (containing a line parallel to the diagonal, 400 with height 12), we recover the number of clusters, 3, and set Stop = 12. The clustering C_2 401



³⁸⁹ **Figure 1** Parameters selection heuristics

obtained with Threshold = -10.27 and Stop = 12 is represented in Figure 2 (right). The bad ellipses have been removed. Denote by $\tilde{\boldsymbol{\theta}}'_{c,k,sig}$, the subfamily of $\tilde{\boldsymbol{\theta}}_{c,k,sig}$ made of centers not removed by the procedure. The color of any point x in Figure 2 (right) is given by the label in *Color* (label returned by the Algorithm 1) of its associated center (y, Σ) in $\tilde{\boldsymbol{\theta}}'_{c,k,sig}$. This is the center (y, Σ) such that $f_{\tilde{\boldsymbol{\theta}}'_{c,k,sig}}(x) = ||x - m_{y,\Sigma,k}||_{\Sigma^{-1}}^2 + v_{y,\Sigma,k} + \log(\det(\Sigma)))$. The labels of the $|\mathbb{X}| - sig$ points with largest $f_{\tilde{\boldsymbol{\theta}}'_{c,k,sig}}$ -value are set to 0.

Note that for large datasets, computing $\theta'_{c,k,sig}$ may take some time. We can compute it from a sub-sample of X, run Algorithm 1, and label points in X accordingly.



410 **Figure 2** Two resulting clusterings, with ellipses

We compare the performance of the two clusterings C_1 and C_2 . In terms of outliers 411 detection, this can be assessed via the proportion of signal points labeled as outliers (0.034)412 for \mathcal{C}_1 , 0.016 for \mathcal{C}_2) and as the proportion of outliers labeled as signal points (0.185 for \mathcal{C}_1 , 413 0.14 for C_2). As expected from Figure 2, removing bad ellipses reduces these proportions 414 and thus improves the outliers detection performance. In terms of clusters recovering, the 415 normalized mutual information (NMI) is classically used. It equals 1 for a perfect clustering 416 and 0 for a terrible clustering. When considering outliers as a cluster with label 0, we got 417 NMI = 0.586 for C_1 and NMI = 0.841 for C_2 . The NMI computed on the signal points 418 labeled as signal points is NMI = 0.634 for C_1 and NMI = 1 for C_2 , a perfect clustering. 419

420 4.2 Comparison of the different methods on synthetic datasets

We compare different clustering methods on two synthetic datasets : the previous dataset with 3 curves, and datapoints from a polygonal curve of 14 segments, as in [8]. We set parameters to $N_s = 500$, $N_o = 200$, $\sigma = 0.02$, c = 50, k = 10, it = 100, $n_ini = 10$ and *Threshold* chosen such that 10 means are removed from the *c*-PLM-centers $\hat{\theta}_{c,k,sig}$. For the Tomato algorithm we set r = 0.12, the radius of the Rips graph. We used the function dbscan from the R packages dbscan [19], with parameters eps = 0.15 and minPts = 10; tclust and specc from the tclust [17] and kernlab [21] R packages.



428 **Figure 3** Violin plots representing the NMI computed on signal points, detected as signal points.

For the three curves, the parameter r for ToMATo is chosen such that the graph is not 429 connected, the clusterings are acceptable but have more than 3 clusters. The c-PLM often 430 performs perfectly, and sometimes performs poorly, since the number of bad ellipses removed 431 is fixed to 10 and not calibrated according to the heuristics, and their is some instability. We 432 observe the same clustering problem as in Figure 2 (middle) for the other methods since the 433 lines are close, compared to the distance between sample points from the same line. For the 434 polygonal line of 14 segments, all methods except the c-PLM and tclust put centers of clusters 435 on massive parts of X (the center and the intersections of 3 segments). For the c-PLM and 436 tclust, most clusters coincide with segments. Nonetheless, their is some instability (much 437 less pronounced for the *c*-PLM), since the algorithms are based on local minimizers. 438

439 4.3 Applications to real datasets

440 4.3.1 Recovering fleas species, based on 6 measurements

We picked the dataset flea from the R-package tourr [29], initially from [23]. This dataset 441 contains records of 6 measurements for 74 males insects from the Palaeartic, from three 442 different species : Heptapotamica, Concinna, Heikertingeri. The variables correspond to 443 measurements on the tarsus, the aedeagus and the head. We normalized data so that the 444 mean and variance of each of the 6 variables are respectively 0 and 1. In Table 2, we computed 445 the NMI between the true species and the clustering returned by different methods. We ran 446 each algorithm 10 times with at most 100 iterations. For every k-nearest-neighbours-based 447 algorithm, we set k = 10. For ToMATo, we set r = 1.9 so that the graph is connected ; 448 for the c-PLM and the c-PDTM, c = 50 and for dbscan, eps = 1.5 and minPts = 10. The 449 3-PDTM and 3-PLM methods consists in clustering data according to the weighted Voronoi 450 cells given by the optimal centers and covariance matrices. 451

| 453 | Without | k-means | tclust | DBSCAN | Spectral clustering | 3-PLM | 3-PDTM |
|-----|-------------|---------|-----------|--------|---------------------|---------------------|----------------------|
| 454 | Algorithm 1 | 0.825 | 0.848 | 0.647 | 1 | 1 | 1 |
| 455 | With | ToMATo | Witnessed | power | DTM-filtration | <i>c</i> -PLM hier. | <i>c</i> -PDTM hier. |
| 456 | Algorithm 1 | 0.628 | 0.906 | 1 | 1 | 1 | 1 |

452 **Table 2** NMI between clustering of fleas and their true specie

The methods based on the decomposition of \mathbb{R}^6 into 3 (weighted and/or curved) Voronoi 457 cells are efficient: at most 3 bad labels for k-means and tclust and all labels correct for their 458 "robust" versions, the 3-PDTM and the 3-PLM. The perfect performance of these two last 459 functions is due to the weights that force the centers of cells to lie in massive areas for X. The 460 bad performance of ToMATo is due to the difficulty to select the parameter r for the Rips 461 graph, the small number of points, and the fact that the inverse of the DTM should be used 462 instead of the DTM, as recommended by the authors. Nonetheless, we made the choice to 463 use the DTM since the other methods (witnessed distance, power function, DTM-filtration, 464 c-PLM and c-PDTM) are based on filtrations from approximations of the DTM, and almost 465 all of these methods perform perfectly. The method dbscan performs poorly since labels 14 466 points as outliers. Nonetheless, the points considered as signal are well clustered. 467

468 4.3.2 Clustering a earthquake dataset

We consider a set of 12790 points representing the longitude and latitude of measured earth-469 quakes of magnitude non smaller than 5.0, between the 01/01/1970 and the 01/01/2010. This 470 dataset was picked from the website http://earthquake.usgs.gov/earthquakes/eqarchives/epic/. 471 We used Algorithm 1 with an approximation of the c-PLM based on a sub-sample of 472 2000 points from the dataset, with parameters c = 200, k = 10 and for it = 50 iterations. 473 We restricted matrices Σ to have eigenvalues smaller than 50 by thresholding them. The 474 persistence diagram in Figure 4 suggests that the dataset has 4 or 10 clusters. Moreover, the 475 curve of the sorted values of the c-PLM approximation on the pointset in Figure 4 suggests 476

to keep sig = 12250 points as signal points. See Figure 5 for the corresponding clustering.



⁴⁷⁸ **Figure 4** Parameters selection heuristics.

⁴⁸⁰ —— References

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⁵⁶² A Proof of Theorem 1

For ease of exposition, we set i = 1 and j = 2, with the assumption that $\omega_1 \leq \omega_2$. In order to make the problem simpler, we first transform ellipsoid \mathcal{E}_1^t into a sphere by noting that

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$$||x-m_1||_{\Sigma_1^{-1}}^2 = (x-m_1)^T P_1 D_1^{-1} P_1^T (x-m_1) = \left(\sqrt{D_1^{-1}} P_1^T (x-m_1)\right)^T \left(\sqrt{D_1^{-1}} P_1^T (x-m_1)\right).$$

Therefore, we set $m'_1 = \sqrt{D_1^{-1}} P_1^T m_1$ and $y = \sqrt{D_1^{-1}} P_1^T x - m'_1$. With this notation, it comes that $y^T y \leq t - \omega_1$ is the new equation of \mathcal{E}_1^t , and $(y - m'_2)^T \tilde{\Sigma}(y - m'_2) \leq t - \omega_2$ the new equation of \mathcal{E}_2^t , with $\tilde{\Sigma} = \sqrt{D_1} P_1^T \Sigma_2^{-1} P_1 \sqrt{D_1}$ and $m'_2 = \sqrt{D_1^{-1}} P_1^T m_2 - m'_1$. Set $\tilde{m} = \tilde{P}^T m'_2$ and $z = \tilde{P}^T y$, for \tilde{P} orthogonal and \tilde{D} diagonal matrices such that $\tilde{\Sigma} = \tilde{P} \tilde{D} \tilde{P}^T$. With these notations, \mathcal{E}_1^t has equation $z^T z \leq t - \omega_1$ and \mathcal{E}_2^t has equation $(z - \tilde{m})^T \tilde{D}(z - \tilde{m}) \leq t - \omega_2$ in some coordinate system.

The ellipsoid \mathcal{E}_1^t appears at time $t = \omega_1$, this is before \mathcal{E}_2^t that appears at time $t = \omega_2$. Consequently, when $\|\tilde{m}\| \leq \sqrt{\omega_2 - \omega_1}$, the first time t for which \mathcal{E}_1^t and \mathcal{E}_2^t intersect is given by $t_{1,2} = \omega_2$.

From now on, we may assume that $\|\tilde{m}\| > \sqrt{\omega_2 - \omega_1}$. Ellipsoids \mathcal{E}_1^t and \mathcal{E}_2^t merge at a time $t_{1,2} > \omega_2$, and their intersection is given by some point $z \in \mathbb{R}^d$ that satisfies:

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$$\sum_{i} (z_i - \tilde{m}_i)^2 \lambda_i = t_{1,2} - \omega_2$$
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$$\sum_{i} z_i^2 = t_{1,2} - \omega_1$$

 $\begin{array}{rcl} & & & \sum_i z_i^2 = t_{1,2} - \omega_1 \\ & & & \exists \lambda > 0, \ \lambda z = -\tilde{D}(z-\tilde{m}). \end{array}$

The last assumption comes from the fact that $\mathcal{E}_1^{t_{1,2}}$ and $\mathcal{E}_2^{t_{1,2}}$ are tangent at their intersection point z. Moreover, the tangent space of $\mathcal{E}_1^{t_{1,2}}$ at z is orthogonal to 2z, the gradient of $\tilde{z} \mapsto \tilde{z}^T \tilde{z}$ at z; and the tangent space of $\mathcal{E}_2^{t_{1,2}}$ at z is orthogonal to $2\tilde{D}(z-\tilde{m})$. Then, necessarily, λ satisfies the following equation (c.f. Equation (2)):

$$\sum_{i=1}^{d} \frac{\lambda_i - \lambda^2}{(\lambda + \lambda_i)^2} \lambda_i \tilde{m}_i^2 = \omega_2 - \omega_1.$$

The eigenvalues of $\tilde{\Sigma}$, $(\lambda_i)_{i \in [\![1,d]\!]}$ are positive. For every a > 0, $f_a : \lambda \mapsto \frac{a-\lambda^2}{(\lambda+a)^2}a$ is decreasing, with $\sum_{i=1}^d f_{\lambda_i}(0)\tilde{m}_i^2 = \|\tilde{m}\|^2 > \omega_2 - \omega_1$ and $\lim_{\lambda \to +\infty} \sum_{i=1}^d f_{\lambda_i}(\lambda)\tilde{m}_i^2 = -\sum_{i=1}^d \lambda_i \tilde{m}_i^2 < 0$. Consequently, Equation (2) has a unique solution λ . It comes that the ellipsoids \mathcal{E}_1^t and \mathcal{E}_2^t intersect at time $t_{1,2} = \omega_2 + \sum_{i=1}^d \left(\frac{\lambda \tilde{m}_i}{\lambda + \lambda_i}\right)^2 \lambda_i$ for this unique λ .

B Proof of Proposition 2

Since the anisotropic weighted Vietoris-Rips complex $\operatorname{VR}_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}(t)$ is the flag complex of the 1-skeleton of the weighted anisotropic Čech complex $\operatorname{Cech}_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}(t)$, $\mathcal{G}_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}^{t}$, the second inclusion of (3) is trivially satisfied. We now focus on the first inclusion of (3). For every $i \in I$ and t > 0, we have that

⁵⁹⁴
$$\overline{\mathrm{B}}\left(m_i, \sqrt{\lambda_{\min}}\sqrt{t-\omega_i}\right) \subset \overline{\mathrm{B}}_{\Sigma_i}\left(m_i, \sqrt{t-\omega_i}\right) \subset \overline{\mathrm{B}}\left(m_i, \sqrt{\lambda_{\max}}\sqrt{t-\omega_i}\right).$$
 (5)

Set t > 0 and $0 < t' \leq \frac{\lambda_{\min}}{\lambda_{\max}} \frac{d+1}{2d} t$. If $\sigma \in VR_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}(t')$, then, for every $i, j \in \sigma$, the intersection $B_{\Sigma_i}(m_i, \sqrt{t'-\omega_i}) \cap B_{\Sigma_j}(m_j, \sqrt{t'-\omega_j})$ is nonempty and according to (5), $B(m_i, \sqrt{\lambda_{\max}}\sqrt{t'-\omega_i}) \cap B(m_j, \sqrt{\lambda_{\max}}\sqrt{t'-\omega_j})$ is nonempty. According to the Vietoris-Rips theorem of [3, Theorem 3.2], $\bigcap_{i \in \sigma} B(m_i, \sqrt{\lambda_{\max}}\sqrt{\frac{2d}{d+1}}\sqrt{t'-\omega_i})$ is nonempty and since the weights are non-negative and $\sqrt{\frac{\lambda_{\max}}{\lambda_{\min}} \frac{2d}{d+1}} \geq 1$, it comes that $\bigcap_{i \in \sigma} B(m_i, \sqrt{\lambda_{\min}}\sqrt{t-\omega_i})$ is nonempty, and finally, according to (5), $\sigma \in \operatorname{Cech}_{\mathbf{m},\boldsymbol{\omega},\boldsymbol{\Sigma}}(t)$.

C Sketch of proof for the q-tameness of power functions

⁶⁰² Any function f of this type is both continuous and proper (the pre-image of any compact set ⁶⁰³ is included in a union of ellipsoids and thus compact).

Since \mathbb{R}^d is triangulable, there is some homeomorphism h between \mathbb{R}^d and some locally finite simplicial complex C, then for any fixed t, we can define a complex C_t that contains $f^{-1}((-\infty, t])$, and $f \circ h_{|C_t}$ is continuous. Just as [7, Proposition 3.5], the conclusion follows from [11, Theorem 2.22] that states that the filtration of the sublevel sets of a continuous function defined on a finite polyhedron is q-tame.