Level Sets Based Distances for Probability Measures and Ensembles with Applications

Alberto Muñoz¹, Gabriel Martos¹ and Javier González²

¹Department of Statistics, University Carlos III of Madrid
Spain. C/ Madrid, 126 - 28903, Getafe (Madrid), Spain.
alberto.munoz@uc3m.es, gabriel.martos@uc3m.es

²Sheffield Institute for Translational Neuroscience,
Department of Computer Science, University of Sheffield.
Glossop Road S10 2HQ, Sheffield, UK.
j.h.gonzalez@sheffield.ac.uk

ABSTRACT

In this paper we study Probability Measures (PM) from a functional point of view: we show that PMs can be considered as functionals (generalized functions) that belong to some functional space endowed with an inner product. This approach allows us to introduce a new family of distances for PMs, based on the action of the PM functionals on ‘interesting’ functions of the sample. We propose a specific (non parametric) metric for PMs belonging to this class, based on the estimation of density level sets. Some real and simulated data sets are used to measure the performance of the proposed distance against a battery of distances widely used in Statistics and related areas.
1 Introduction

Probability metrics, also known as statistical distances, are of fundamental importance in Statistics. In essence, a probability metric is a measure that quantifies how (dis)similar are two random quantities, in particular two probability measures (PM). Typical examples of the use of probability metrics in Statistics are homogeneity, independence and goodness of fit tests. For instance there are some goodness of fit tests based on the use of the $\chi^2$ distance and others that use the Kolmogorov-Smirnoff statistics, which corresponds to the choice of the supremum distance between two PMs. There exist a large literature about probability metrics, for a summary review on interesting probability metrics and theoretical results refer to (Deza and Deza, 2009; Muller, 1997; Zolotarev, 1983) and references therein.

Statistical distances are also extensively used in several applications related to Machine Learning and Pattern Recognition. Several examples can be found, for instance, in Clustering (Nielsen and Boltz, 2011; Banerjee et al., 2005), Image Analysis (Levina and Bickel, 2001; Rubner et al., 2000), Bioinfomatics (Minas et al., 2013; Saez et al., 2013), Time Series Analysis (Ryabko and Mary, 2012; Moon et al., 1995) or Text Mining (Lebanon, 2006), just to name a few.

In practical situations we do not know explicitly the underlying distribution of the data at hand, and we need to compute a distance between probability measures by using a finite data sample. In this context, the computation of a distance between PMs that rely on the use of non-parametric density estimations often is computationally difficult and the rate of convergence of the estimated distance is usually slow (Nguyen et al., 2007; Wang et al., 2005; Stone, 1980). In this work we extend the preliminary idea presented in (Munoz et al., 2012), that consist in considering PMs as points in a functional space endowed with an inner product. We derive then different distances for PMs from the metric structure inherited from the ambient inner product. We propose particular instances of such metrics for PMs based on the estimation of density level sets regions avoiding in this way the difficult task of density estimation.

This article is organized as follows: In Section 2 we review some distances for PMs and represent probability measures as generalized functions; next we define general distances acting on the Schwartz distribution space that contains the PMs. Section 3 presents a new distance built according to this point of view. Section 4 illustrates the theory with some simulated and real data sets. Section 5 concludes.
2 Distances for probability distributions

Several well known statistical distances and divergence measures are special cases of $f$-divergences (Csiszár and Shields, 2004). Consider two PMs, say $P$ and $Q$, defined on a measurable space $(X, \mathcal{F}, \mu)$, where $X$ is a sample space, $\mathcal{F}$ a $\sigma$-algebra of measurable subsets of $X$ and $\mu : \mathcal{F} \rightarrow \mathbb{R}^+$ the Lebesgue measure. For a convex function $f$ and assuming that $P$ is absolutely continuous with respect to $Q$, then the $f$-divergence from $P$ to $Q$ is defined by:

$$d_f(P, Q) = \int_X f \left( \frac{dP}{dQ} \right) dQ.$$  \hfill (2.1)

Some well known particular cases: for $f(t) = \frac{|t-1|}{2}$ we obtain the Total Variation metric; $f(t) = (t - 1)^2$ yields the $\chi^2$-distance; $f(t) = \left(\sqrt{t} - 1\right)^2$ yields the Hellinger distance.

The second important family of dissimilarities between probability distributions is made up of Bregman Divergences: Consider a continuously-differentiable real-valued and strictly convex function $\varphi$ and define:

$$d_\varphi(P, Q) = \int_X (\varphi(p) - \varphi(q) - (p - q)\varphi'(q)) d\mu(x),$$  \hfill (2.2)

where $p$ and $q$ represent the density functions for $P$ and $Q$ respectively and $\varphi'(q)$ is the derivative of $\varphi$ evaluated at $q$ (see (Frigyik at al., 2008; Cichocki and Amari, 2010) for further details). Some examples of Bregman divergences: $\varphi(t) = \frac{t^2}{2}$ yields the Euclidean distance between $p$ and $q$ (in $L_2$); $\varphi(t) = t \log(t)$ yields the Kullback Leibler (KL) Divergence; and for $\varphi(t) = -\log(t)$ we obtain the Itakura-Saito distance. In general $d_f$ and $d_\varphi$ are not metrics because the lack of symmetry and because they do not necessarily satisfy the triangle inequality.

A third interesting family of PM distances are integral probability metrics (IPM) (Zolotarev, 1983; Muller, 1997). Consider a class of real-valued bounded measurable functions on $X$, say $\mathcal{H}$, and define the IPM between $P$ and $Q$ as

$$d_\mathcal{H}(P, Q) = \sup_{f \in \mathcal{H}} \left| \int f dP - \int f dQ \right|.$$  \hfill (2.3)

If we choose $\mathcal{H}$ as the space of bounded functions such that $h \in \mathcal{H}$ if $\|h\|_{\infty} \leq 1$, then $d_\mathcal{H}$ is the Total Variation metric; when $\mathcal{H} = \{\prod_{i=1}^d 1_{[\cdot, x_i]} : x = (x_1, \ldots, x_d) \in \mathbb{R}^d\}$, $d_\mathcal{H}$ is the Kolmogorov distance; if $\mathcal{H} = \{e^{\sqrt{-1} \varphi(\omega \cdot)} : \omega \in \mathbb{R}^d\}$ the metric computes the maximum difference between characteristics functions. In (Sriperumbudur et al., 2010) the authors propose to choose $\mathcal{H}$ as a Reproducing Kernel Hilbert Space and study conditions on $\mathcal{H}$ to obtain proper metrics $d_\mathcal{H}$.
In practice, the obvious problem to implement the above described distance functions is that we do not know the density (or distribution) functions corresponding to the samples under consideration. For instance suppose we want to estimate the KL divergence (a particular case of Eq. (2.1) taking $f(t) = -\log t$) between two continuous distributions $P$ and $Q$ from two given samples. In order to do this we must choose a number of regions, $N$, and then estimate the density functions for $P$ and $Q$ in the $N$ regions to yield the following estimation:

$$\hat{KL}(P, Q) = \sum_{i=1}^{N} \hat{p}_i \log \frac{\hat{p}_i}{\hat{q}_i},$$

(2.4)

see further details in (Boltz et al., 2009).

As it is well known, the estimation of general distribution functions becomes intractable as dimension arises. This motivates the need of metrics for probability distributions that do not explicitly rely on the estimation of the corresponding probability/distribution functions. For further details on the sample versions of the above described distance functions and their computational subtleties see (Scott, 1992; Cha, 2007; Wang et al., 2005; Nguyen et al., 2007; Sriperumbudur et al. 2010; Goria et al. 2005; Székely and Rizzo, 2004) and references therein.

To avoid the problem of explicit density function calculations we will adopt the perspective of the generalized function theory of Schwartz (see (Zemanian, 1965), for instance), where a function is not specified by its values but by its behavior as a functional on some space of testing functions.

### 2.1 Probability measures as Schwartz distributions

Consider a measure space $(X, F, \mu)$, where $X$ is a sample space, here a compact set of a real vector space: $X \subset \mathbb{R}^d$, $F$ a $\sigma$-algebra of measurable subsets of $X$ and $\mu : F \to \mathbb{R}^+$ the ambient $\sigma$-additive measure (here the Lebesgue measure). A probability measure $P$ is a $\sigma$-additive finite measure absolutely continuous w.r.t. $\mu$ that satisfies the three Kolmogorov axioms. By Radon-Nikodym theorem, there exists a measurable function $f : X \to \mathbb{R}^+$ (the density function) such that $P(A) = \int_A f d\mu$, and $f = \frac{dP}{d\mu}$ is the Radon-Nikodym derivative.

A PM can be regarded as a Schwartz distribution (a generalized function, see (Strichartz, 1994) for an introduction to Distribution Theory): We consider a vector space $\mathcal{D}$ of test functions. The usual choice for $\mathcal{D}$ is the subset of $C^\infty(X)$ made up of functions with compact support. A distribution (also named generalized function) is a continuous linear functional on $\mathcal{D}$. A probability measure can be regarded as a Schwartz distribution $P : \mathcal{D} \to \mathbb{R}$ by

---

1A not restrictive assumption in real scenarios, see for instance (Moguerza and Muñoz, 2006).
defining \( \mathbb{P}(\phi) = \langle \mathbb{P}, \phi \rangle = \int \phi d\mathbb{P} = \int \phi(x) f(x) d\mu(x) = \langle \phi, f \rangle \). When the density function \( f \in \mathcal{D} \), then \( f \) acts as the representer in the Riesz representation theorem: \( \mathbb{P}(\cdot) = \langle \cdot, f \rangle \).

In particular, the familiar condition \( \mathbb{P}(X) = 1 \) is equivalent to \( \langle \mathbb{P}, 1_{[X]} \rangle = 1 \), where the function \( 1_{[X]} \) belongs to \( \mathcal{D} \), being \( X \) compact. Note that we do not need to impose that \( f \in \mathcal{D} \); only the integral \( \langle \phi, f \rangle \) should be properly defined for every \( \phi \in \mathcal{D} \).

Hence a probability measure/distribution is a continuous linear functional acting on a given function space. Two given linear functionals \( \mathbb{P}_1 \) and \( \mathbb{P}_2 \) will be identical (similar) if they act identically (similarly) on every \( \phi \in \mathcal{D} \). For instance, if we choose \( \phi = \text{Id} \), \( \mathbb{P}_1(\phi) = \langle f_{\mathbb{P}_1}, x \rangle = \int x d\mathbb{P}_1 = \mu_{\mathbb{P}_1} \), and if \( \mathbb{P}_1 \) and \( \mathbb{P}_2 \) are ‘similar’ then \( \mu_{\mathbb{P}_1} \simeq \mu_{\mathbb{P}_2} \) because \( \mathbb{P}_1 \) and \( \mathbb{P}_2 \) are continuous functionals. Similar arguments apply for variance (take \( \phi(x) = (x - \mu)^2 \)) and in general for higher order moments. For \( \phi_\xi(x) = e^{ix\xi}, \xi \in \mathbb{R} \), we obtain the Fourier transform of the probability measure (called characteristic functions in Statistics), given by \( \hat{\mathbb{P}}(\xi) = \langle \mathbb{P}, e^{ix\xi} \rangle = \int e^{ix\xi} d\mathbb{P} \).

Thus, two PMs can be identified with their action as functionals on the test functions if the set of test functions \( \mathcal{D} \) is rich enough and hence, distances between two distributions can be defined from the differences between functional evaluations for appropriately chosen test functions.

**Definition 1. (Identification of PM’s).** Let \( \mathcal{D} \) be a set of test functions and \( \mathbb{P} \) and \( \mathbb{Q} \) two PM’s defined on the measure space \((X, \mathcal{F}, \mu)\), then we say that \( \mathbb{P} = \mathbb{Q} \) on \( \mathcal{D} \) if:

\[
\langle \mathbb{P}, \phi \rangle = \langle \mathbb{Q}, \phi \rangle \quad \forall \phi \in \mathcal{D}.
\]

The key point in our approach is that if we appropriately choose a finite subset of test functions \( \{\phi_i\} \), we can compute the distance between the probability measures by calculating a finite number of functional evaluations. In the next section we demonstrate that when \( \mathcal{D} \) is composed by indicator functions that indicates the regions where the density remains constant, then the set \( \mathcal{D} \) is rich enough to identify PM. In the next section we define a distance based on the use of this set of indicator functions.

### 3 A metric based on the estimation of level sets

We choose \( \mathcal{D} \) as \( C_c(X) \), the space of all compactly supported, piecewise continuous functions on \( X \) (compact), as test functions (remember that \( C_c(X) \) is dense in \( L_p \)). Given two PMs \( \mathbb{P} \) and \( \mathbb{Q} \), we consider a family of test functions \( \{\phi_i\}_{i \in I} \subseteq \mathcal{D} \) and then define distances between \( \mathbb{P} \) and \( \mathbb{Q} \) by weighting terms of the type \( d(\langle \mathbb{P}, \phi_i \rangle, \langle \mathbb{Q}, \phi_i \rangle) \) for \( i \in I \), where \( d \) is some distance function. Our test functions will be indicator functions of \( \alpha \)-level sets, described below.
Given a PM $\mathbb{P}$ with density function $f_{\mathbb{P}}$, minimum volume sets are defined by $S_\alpha(f_{\mathbb{P}}) = \{x \in X | f_{\mathbb{P}}(x) \geq \alpha\}$, such that $P(S_\alpha(f_{\mathbb{P}})) = 1 - \nu$, where $0 < \nu < 1$. If we consider an ordered sequence $0 \leq \alpha_1 < \ldots < \alpha_m$, then $S_{\alpha_i}(f_{\mathbb{P}}) \subseteq S_{\alpha_{i+1}}(f_{\mathbb{P}})$. Let us define the $\alpha_i$-level set: $A_i(\mathbb{P}) = S_{\alpha_i}(f_{\mathbb{P}}) - S_{\alpha_{i+1}}(f_{\mathbb{P}}), i \in \{1, \ldots, m - 1\}$. We can choose $\alpha_1 \simeq 0$ and $\alpha_m \geq \max_{x \in X} f_{\mathbb{P}}(x)$ (which exists, given that $X$ is compact and $f_{\mathbb{P}}$ piecewise continuous); then $\bigcup_i A_i(\mathbb{P}) \simeq \text{Supp}(\mathbb{P}) = \{x \in X | f_{\mathbb{P}}(x) \neq 0\}$ (equality takes place when $m \to \infty$, $\alpha_1 \to 0$ and $\alpha_m \to \max_{x \in X} f_{\mathbb{P}}(x)$). Given the definition of the $A_i$, if $A_i(\mathbb{P}) = A_i(\mathbb{Q})$ for every $i$ when $m \to \infty$, then $\mathbb{P} = \mathbb{Q}$. We formally prove this proposition with the aid of the following theorem.

Definition 2. ($\alpha^m_\mathbb{P}$ sequence). Given a PM $\mathbb{P}$ defined on the measure space $(X, \mathcal{F}, \mu)$, with density function $f_{\mathbb{P}}$ and $m \in \mathbb{N}$, define $\alpha^m_\mathbb{P} = \{\alpha_1, \ldots, \alpha_m\}$ where $0 = \alpha_1 < \ldots < \alpha_m = \max_x f_{\mathbb{P}}(x)$.

Theorem 1. ($\alpha$-level set representation of a PM). Given a PM $\mathbb{P}$ defined on the measure space $(X, \mathcal{F}, \mu)$, with density function $f_{\mathbb{P}}$ and a sequence $\alpha^m_\mathbb{P}$, consider the set of indicator functions $\phi_i(\mathbb{P}) = 1_{[A_i(\mathbb{P})]} : X \to \{0, 1\}$ of the $\alpha$-level sets $A_i(\mathbb{P}) = S_{\alpha_i}(f_{\mathbb{P}}) - S_{\alpha_{i+1}}(f_{\mathbb{P}})$ for $i \in \{1, \ldots, m - 1\}$. Define $f_m(x) = \sum_{i=1}^m \alpha_i \phi_i(\mathbb{P})(x)$. Then:

$$\lim_{m \to \infty} f_m(x) = f_{\mathbb{P}}(x),$$

where the convergence is pointwise almost everywhere. Moreover, as the sequence $f_m$ is monotonically increasing ($f_{m-1} \leq f_m$), by Dini’s Theorem, the convergence is also uniform (converge uniformly almost everywhere).

Corollary 1. ($\alpha$-level sets identification of PMs). If the set of test functions $\mathcal{D}$ contains the indicator functions of the $\alpha$-level sets, then $\mathcal{D}$ is rich enough to discriminate among PMs.

Now we elaborate on the construction of a metric that is able to identify PM. Denote by $\mathcal{D}_X$ to the set of probability distributions on $X$ and given a suitable sequence of non-decreasing values $\{\alpha_i\}_{i=1}^m$, define: $\mathcal{D}_X \xrightarrow{\phi_i} \mathcal{D} : \phi_i(\mathbb{P}) = 1_{[A_i(\mathbb{P})]}$. We propose distances of the form $\sum_{i=1}^{m-1} \omega_i d(\phi_i(\mathbb{P}), \phi_i(\mathbb{Q}))$. Consider, as an example, the measure of the standardized symmetric difference:

$$d(\phi_i(\mathbb{P}), \phi_i(\mathbb{Q})) = \frac{\mu(A_i(\mathbb{P}) \triangle A_i(\mathbb{Q}))}{\mu(A_i(\mathbb{P}) \cup A_i(\mathbb{Q}))}.$$

This motivates the definition of the $\alpha$-level set semi-metric as follows.

Definition 3. (Weighted $\alpha$-level set semi-metric). Given $m \in \mathbb{N}$, consider two sequences: $\alpha^m_{\mathbb{P}}$ and $\alpha^m_{\mathbb{Q}}$, for $\mathbb{P}$ and $\mathbb{Q}$ respectively. Then define a family of weighted $\alpha$-level set
where \( w \) is the ambient measure.

Equation (3.1) can be interpreted as a weighted sum of Jaccard distances between the \( A_i(\mathbb{P}) \) and \( A_i(\mathbb{Q}) \) sets. For \( m \gg 0 \), when \( \mathbb{P} \approx \mathbb{Q} \), then \( d_{\alpha,\beta}(\mathbb{P}, \mathbb{Q}) \approx 0 \) since \( \mu(A_i(\mathbb{P}) \triangle A_i(\mathbb{Q})) \approx 0 \) for all \( i \in \{1, \ldots, m\} \) (assume \( |f_\mathbb{P}(x) - f_\mathbb{Q}(x)| \leq \varepsilon \) for all \( x \), since \( f_\mathbb{P} \approxeq f_\mathbb{Q} \) then \( \mu(A_i(\mathbb{P}) \triangle A_i(\mathbb{Q})) \approx 0 \) \( \forall i \), because otherwise contradicts the fact that \( f_\mathbb{P} \approxeq f_\mathbb{Q} \).

**Proposition 1. (Convergence of the \( \alpha \)-level set semi-metric to a metric).** \( d_{\alpha,\beta}(\mathbb{P}, \mathbb{Q}) \) converges to a metric when \( m \to \infty \).

The semi-metric proposed in Eq. (3.1) obeys the following properties: is non-negative, that is \( d_{\alpha,\beta}(\mathbb{P}, \mathbb{Q}) \geq 0 \) and \( \lim_{m \to \infty} d_{\alpha,\beta}(\mathbb{P}, \mathbb{Q}) = 0 \) if and only if \( \mathbb{P} = \mathbb{Q} \). For fixed pairs \((\alpha, \mathbb{P})\) and \((\beta, \mathbb{Q})\) it is symmetric \( d_{\alpha,\beta}(\mathbb{P}, \mathbb{Q}) = d_{\beta,\alpha}(\mathbb{Q}, \mathbb{P}) \). Therefore constitutes a proper metric when \( m \to \infty \). The semi-metric proposed in Eq. (3.1) is invariant under affine transformations (see the Appendix B for a formal proof). In section 3.2, we will propose a weighting scheme for setting the weights \( \{w_i\}_{i=1}^{m-1} \).

Of course, we can calculate \( d_{\alpha,\beta} \) in Eq. (3.1) only when we know the distribution function for both PMs \( \mathbb{P} \) and \( \mathbb{Q} \). In practice there will be available two data samples generated from \( \mathbb{P} \) and \( \mathbb{Q} \), and we need to define some plug estimator: Consider estimators \( \hat{A}_i(\mathbb{P}) = \hat{S}_{\alpha_i}(f_\mathbb{P}) - \hat{S}_{\alpha_{i+1}}(f_\mathbb{P}) \) (details in subsection 3.1), then we can estimate \( d_{\alpha,\beta}(\mathbb{P}, \mathbb{Q}) \) by

\[
\hat{d}_{\alpha,\beta}(\mathbb{P}, \mathbb{Q}) = \sum_{i=1}^{m-1} w_i \frac{\mu(\hat{A}_i(\mathbb{P}) \triangle \hat{A}_i(\mathbb{Q}))}{\mu(\hat{A}_i(\mathbb{P}) \cup \hat{A}_i(\mathbb{Q}))}.
\] (3.2)

It is clear that \( \mu(\hat{A}_i(\mathbb{P}) \cup \hat{A}_i(\mathbb{Q})) \) equals the total number of points in \( \hat{A}_i(\mathbb{P}) \cup \hat{A}_i(\mathbb{Q}) \), say \( \#(\hat{A}_i(\mathbb{P}) \cup \hat{A}_i(\mathbb{Q})) \). Regarding the numerator in Eq. (3.2), given two level sets, say \( A \) and \( B \) to facilitate the notation, and the corresponding sample estimates \( \hat{A} \) and \( \hat{B} \), one is tempted to estimate \( \mu(A \triangle B) \), the area of region \( A \triangle B \), by \( \mu(A \triangle B) = \#(\hat{A} \setminus \hat{B}) \cup \#(\hat{B} \setminus \hat{A}) = \#(A \cup B) - \#(A \cap B) \). However this is incorrect since probably there will be no points in common between \( \hat{A} \) and \( \hat{B} \) (which implies \( \hat{A} \triangle \hat{B} \)).

In our particular case, the algorithm in Table 1 shows that \( \hat{A}_i(\mathbb{P}) \) is always a subset of the sample \( s_\mathbb{P} \) drawn from the density function \( f_\mathbb{P} \), and we will denote this estimation by
Figure 1: Set estimate of the symmetric difference. (a) Data samples $s_A$ (red) and $s_B$ (blue).
(b) $s_B$ - Covering $\hat{A}$: blue points. (c) $s_A$ - Covering $\hat{B}$: red points. Blue points in (b) plus red points in (c) are the estimate of $A \triangle B$.

$s_{\hat{A}_i(P)}$ from now on. We will reserve the notation $\hat{A}_i(P)$ for the covering estimation of $A_i(P)$ defined by $\bigcup_j^n B(x_j, r_A)$ where $x_j \in s_{\hat{A}_i(P)}$, $B(x_j, r_A)$ are closed balls with centres at $x_j$ and (fixed) radius $r_A$ (Devroye and Wise 1980). The radius is chosen to be constant (for data points in $\hat{A}_i(P)$) because we can assume that density is approximately constant inside region $\hat{A}_i(P)$, if the partition $\{\alpha_i\}_{i=1}^m$ of the set is fine enough. For example, in the experimental section, we fix $r_A$ as the median distance between the points that belongs to the set $s_{\hat{A}_i(P)}$.

To illustrate this notation we include Figure 1. In Figure 1 (a) we show two data different samples from $\alpha$-level sets $A$ and $B$: $s_A$ (red points) and $s_B$ (blue points), respectively. In Figure 1 (b) $\hat{A}$ is the covering estimation of set $A$ made up of the union of balls centered in the data red points $s_A$. That is $\hat{A} = \bigcup_j^n B(x_j, r_A) \xrightarrow{n \to \infty} A$. Figure 1 (c) can be interpreted equivalently regarding the covering of the sample $s_B$. The problem of calculating $\mu(A \triangle B)$ thus reduces to estimate the number points in $\hat{B}$ not belonging to the covering estimate of $A$, plus the number points in $\hat{A}$ not belonging to the covering estimate of $B$. To make the computation explicit consider $x \in A, y \in B$ and define

$$I_{r_A, r_B}(x, y) = \mathbb{1}_{B(x, r_A)}(y) + \mathbb{1}_{B(y, r_B)}(x) - \mathbb{1}_{B(x, r_A)}(y) \mathbb{1}_{B(y, r_B)}(x),$$

where $I_{r_A, r_B}(x, y) = 1$ when $y$ belongs to the covering $\hat{A}$, $x$ belongs to the covering $\hat{B}$ or both events happen. Thus if we define

$$I(A, B) = \sum_{x \in A} \sum_{y \in B} I_{r_A, r_B}(x, y),$$
Estimation of $R_n = \hat{S}_\alpha(f)$:

1. Choose a constant $\nu \in [0, 1]$.
2. Consider the order induced in the sample $s_n$ by the sparsity measure $g_n(x)$, that is, $g_n(x_{(1)}) \leq \cdots \leq g_n(x_{(n)})$, where $x_{(i)}$ denotes the $i^{th}$ sample, ordered after $g$.
3. Consider the value $\rho_n^* = g(x(\nu n))$ if $\nu n \in \mathbb{N}$, $\rho_n^* = g_n(x_{[\nu n]+1})$ otherwise, where $[x]$ stands for the largest integer not greater than $x$.
4. Define $h_n(x) = \text{sign}(\rho_n^* - g_n(x))$.

Table 1: Algorithm to estimate minimum volume sets $(S_\alpha(f))$ of a density $f$.

---

we are able to estimate the symmetric difference by

$$\mu(A \Delta B) = \mu(A \cup B) - \mu(A \cap B) = \#\mu(A \cup B) - I(A, B).$$

3.1 Estimation of level sets

To estimate the set denoted as $s_{A_i(P)}$ we implement a One-Class Neighbor Machine approach (Muñoz and Moguerza 2006, 2005). The One-Class Neighbor Machine solves the following optimization problem:

$$\max_{\rho, \xi} \nu n \rho - \sum_{i=1}^{n} \xi_i$$

s.t. $g(x_i) \geq \rho - \xi_i$, $\xi_i \geq 0$, $i = 1, \ldots, n$,

where $g(x) = M(x, s_n)$ is a sparsity measure (see the Appendix C for further details), $\nu \in [0, 1]$ such that $P(S_\alpha) = 1 - \nu$, $\xi_i$ with $i = 1, \ldots, n$ are slack variables and $\rho$ is a predefined constant. With the aid of the Support Neighbor Machine, we estimate a density contour cluster $S_{\alpha_i}(f)$ around the mode for a suitable sequence of values $\{\nu_i\}_{i=1}^m$ (note that the sequence $0 \geq \nu_1, \ldots, \nu_m = 1$ it is in a one-to-one correspondence with the sequence $0 \leq \alpha_1 < \cdots < \alpha_m = \max_{x \in X} f_P(x)$). In Table 1 we present the algorithm to estimate $S_\alpha(f)$ of a density function $f$. Hence, we take $s_{A_i(P)} = \hat{S}_{\alpha_i}(f_P) - \hat{S}_{\alpha_{i+1}}(f_P)$, where $\hat{S}_{\alpha_i}(f_P)$ is estimated by $R_n$ defined in Table 1 (the same estimation procedure applies for $s_{A_i(Q)}$).

The computational complexity of the algorithm of Table 1 and more details on the estimation of the regions $\hat{S}_\alpha(f)$ are contained in (Muñoz and Moguerza 2004, 2005, 2006). The execution time required to compute $\hat{S}_\alpha(f)$ grows at a rate of order $O(dn^2)$, where $d$ represent the dimension and $n$ the sample size of the data at hand.
3.2 Choice of weights for $\alpha$-level set distances

In this section we define a weighting scheme for the family of distances defined by Eq. (3.1). Denote by $s_P$ and $s_Q$ the data samples corresponding to PMs $\mathbb{P}$ and $\mathbb{Q}$ respectively, and denote by $s_{\hat{A}_i}(\mathbb{P})$ and $s_{\hat{A}_i}(\mathbb{Q})$ the data samples that estimate $A_i(\mathbb{P})$ and $A_i(\mathbb{Q})$, respectively. Remember that we can estimate these sets by coverings $\hat{A}_i(\mathbb{P}) = \bigcup_{x \in s_{\hat{A}_i}(\mathbb{P})} B(x, r_{\hat{A}_i}(\mathbb{P}))$, $\hat{A}_i(\mathbb{Q}) = \bigcup_{x \in s_{\hat{A}_i}(\mathbb{Q})} B(x, r_{\hat{A}_i}(\mathbb{Q}))$.

Let $m$ denote the size of the $\alpha^m_P$ and $\beta^m_Q$ sequences. Denote by $n_{\hat{A}_i}(\mathbb{P})$ the number of data points in $s_{\hat{A}_i}(\mathbb{P})$, $n_{\hat{A}_i}(\mathbb{Q})$ the number of data points in $s_{\hat{A}_i}(\mathbb{Q})$, $r_{\hat{A}_i}(\mathbb{P})$ the (fixed) radius for the covering $\hat{A}_i(\mathbb{P})$ and $r_{\hat{A}_i}(\mathbb{Q})$ the (fixed) radius for the covering $\hat{A}_i(\mathbb{Q})$, usually the mean or the median distance inside the region $\hat{A}_i(\mathbb{P})$ and $\hat{A}_i(\mathbb{Q})$ respectively. We define the following weighting scheme:

$$w_i = \frac{1}{m} \sum_{x \in s_{\hat{A}_i}(\mathbb{P})} \sum_{y \in s_{\hat{A}_i}(\mathbb{Q})} \left( 1 - I_{r_{\hat{A}_i}(\mathbb{P}), r_{\hat{A}_i}(\mathbb{Q})} (x, y) \right) \cdot \frac{\| x - y \|_2}{(s_{\hat{A}_i}(\mathbb{Q}) - s_{\hat{A}_i}(\mathbb{P})) \cup (s_{\hat{A}_i}(\mathbb{P}) - s_{\hat{A}_i}(\mathbb{Q}))}.$$  \hspace{1cm} (3.4)

The weight $w_i$ is a weighted average of distances between a point of $s_{\hat{A}_i}(\mathbb{P})$ and a point of $s_{\hat{A}_i}(\mathbb{Q})$ where $\| x - y \|_2$ is taken into account only when $I_{r_{\hat{A}_i}(\mathbb{P}), r_{\hat{A}_i}(\mathbb{Q})} (x, y) = 0$. More details about the weighting scheme and its extension can be seen in the Appendix D.

4 Experimental work

Since the proposed distance is intrinsically nonparametric, there are no simple parameters on which we can concentrate our attention to do exhaustive benchmarking. The strategy will be to compare the proposed distance to other classical PM distances for some well known (and parametrized) distributions and for real data problems. Here we consider distances belonging to the main types of PMs metrics: Kullback-Leibler (KL) divergence (Boltz et al., 2009; Nguyen et al., 2007) ($f$-divergence and also Bregman divergence), t-test (T) measure (Hotelling test in the multivariate case), Maximum Mean Discrepancy (MMD) distance (Gretton et al., 2012; Sriperumbudur et al., 2010) and Energy distance (Székely and Rizzo, 2004; Sejdinovic et al., 2012) (an Integral Probability Metric, as it is demonstrated in Sejdinovic et al., 2012).
Table 2: $\delta^* \sqrt{d}$ for a 5% type I and 10% type II errors.

| Metric | d: 1 2 3 4 5 10 15 20 50 100 |
|--------|-------------------------------|
| KL     | 0.870 0.636 0.433 0.430 0.402 0.474 0.542 0.536 0.495 0.470 |
| T      | 0.490 0.297 0.286 0.256 0.246 0.231 0.201 0.182 0.153 0.110 |
| Energy | 0.460 0.287 0.284 0.256 0.250 0.234 0.203 0.183 0.158 0.121 |
| MMD    | 0.980 0.850 0.650 0.630 0.590 0.500 0.250 0.210 0.170 0.130 |
| LS(0)  | 0.490 0.298 0.289 0.252 0.241 0.237 0.220 0.215 0.179 0.131 |
| LS(1)  | **0.455 0.283 0.268 0.240 0.224 0.221 0.174 0.178 0.134 0.106** |

4.1 Artificial data

4.1.1 Discrimination between normal distributions

In this experiment we quantify the ability of the considered PM distances to test the null hypothesis $H_0: P = Q$ when $P$ and $Q$ are multivariate normal distributions. To this end, we generate a data sample of size 100$d$ from a normal distribution $N(0, I_d) = P$, where $d$ stands for dimension and then we generate 1000 iid data samples of size 100$d$ from the same $N(0, I_d)$ distribution. Next we calculate the distances between each of these 1000 iid data samples and the first data sample to obtain the 95% distance percentile denoted as $d_{H_0}^{95\%}$. Now define $\delta = \delta \mathbf{1} = \delta(1, \ldots, 1) \in \mathbb{R}^d$ and increase $\delta$ by small amounts (starting from 0). For each $\delta$ we generate a data sample of size 100$d$ from a $N(0 + \delta, I_d) = Q$ distribution. If $d(P, Q) > d_{H_0}^{95\%}$ we conclude that the present distance is able to discriminate between both populations (we reject $H_0$) and this is the value $\delta^*$ referenced in Table 4.1.1. To track the power of the test, we repeat this process 1000 times and fix $\delta^*$ to the present $\delta$ value if the distance is above the percentile in 90% of the cases. Thus we are calculating the minimal value $\delta^*$ required for each metric in order to discriminate between populations with a 95% confidence level (type I error = 5%) and a 90% sensitivity level (type II error = 10%). In Table 4.1.1 we report the minimum distance ($\delta^* \sqrt{d}$) between distributions centers required to discriminate for each metric in several alternative dimensions, where small values implies better results. In the particular case of the $T$-distance for normal distributions we can use the Hotelling test to compute a $p$-value to fix the $\delta^*$ value.

The data chosen for this experiment are ideal for the use of the $T$ statistics that, in fact, outperforms KL and MMD. However, Energy distance works even better than $T$ distance in dimensions 1 to 4. The LS(0) distance work similarly to $T$ and Energy until dimension 10. The LS(1) distance outperform to all the competitor metrics in all the considered dimensions.
Table 3: \((1 + \sigma^*)\) for a 5% type I and 10% type II errors.

| Metric | dim: 1 | 2 | 3 | 4 | 5 | 10 | 15 | 20 | 50 | 100 |
|--------|--------|---|---|---|---|----|----|----|----|-----|
| KL     | 3.000  | 1.700 | 1.250 | 1.180 | 1.175 | 1.075 | 1.055 | 1.045 | 1.030 | 1.014 |
| T      | –      | –      | –      | –      | –      | –      | –      | –      | –      | –    |
| Energy | 1.900  | 1.600  | 1.450  | 1.320  | 1.300  | 1.160  | 1.150  | 1.110  | 1.090  | 1.030 |
| MMD    | 6.000  | 4.500  | 3.500  | 2.900  | 2.400  | 1.800  | 1.500  | 1.320  | 1.270  | 1.150 |
| LS(0)  | 1.850  | 1.450  | 1.300  | 1.220  | 1.180  | 1.118  | 1.065  | 1.040  | 1.030  | 1.012 |
| LS(1)  | 1.700  | 1.350  | 1.150  | 1.120  | 1.080  | 1.050  | 1.033  | 1.025  | 1.015  | 1.009 |

In a second experiment we consider again normal populations but different variance-covariance matrices. Define as an expansion factor \(\sigma \in \mathbb{R}\) and increase \(\sigma\) by small amounts (starting from 0) in order to determine the smallest \(\sigma^*\) required for each metric in order to discriminate between the 100\(d\) sampled data points generated for the two distributions: \(N(0, I_d) = P\) and \(N(0, (1 + \sigma)I_d) = Q\). If \(d(P, Q) > d_P^{95}\%\) we conclude that the present distance is able to discriminate between both populations and this is the value \((1 + \sigma^*)\) reported in Table 4.1.1. To make the process as independent as possible from randomness we repeat this process 1000 times and fix \(\sigma^*\) to the present \(\sigma\) value if the distance is above the 90\% percentile of the cases, as it was done in the previous experiment.

There are no entries in Table 4.1.1 for the T distance because it was not able to distinguish between the considered populations in none of the considered dimensions. The MMD distance do not show a good discrimination power in this experiment. We can see here again that the proposed LS(1) distance is better than the competitors in all the dimensions considered, having the LS(0) and the KL similar performance in the second place among the metrics with best discrimination power.

4.1.2 Homogeneity tests

This experiment concerns a homogeneity test between two populations: a mixture between a Normal and a Uniform distribution \((P = \alpha N(\mu = 1, \sigma = 1) + (1 - \alpha)U(a = 1, b = 8)\) where \(\alpha = 0.7\)) and a Gamma distribution \((Q = \gamma(shape = 1, scale = 2))\). To test the null hypothesis: \(H_0 : P = Q\) we generate two random i.i.d. samples of size 100 from \(P\) and \(Q\), respectively. Figure 2 shows the corresponding density functions for \(P\) and \(Q\). In the cases of KL-divergence, T, Energy MMD and LS distances we proceed as in the previous experiment, we run a permutation test based on 1000 random permutation of the original
data in order to compute the \( p \)-value. In the case of Kolmogorov-Smirnov, \( \chi^2 \) and Wilcoxon test we report the \( p \)-value given by these tests. Results are displayed in Table 4. Only the LS distances are able to distinguish between both distributions. Notice that first and second order moments for both distribution are quite similar in this case (\( \mu_P = 2.05 \approx \mu_Q = 2 \) and \( \sigma_P = 4.5 \approx \sigma_Q = 4 \)) and additionally both distributions are strongly asymmetric, which also contributes to explain the failure of those metrics strongly based on the use of the first order moments.

Table 4: Hypothesis test between a mixture of Normal and Uniform distributions and a Gamma distribution.

| Metric             | Parameters | \( p \)-value | Reject? |
|--------------------|------------|---------------|---------|
| Kolmogorov-Smirnov |            | 0.281         | No.     |
| \( \chi^2 \) test |            | 0.993         | No.     |
| Wilcoxon test      |            | 0.992         | No.     |
| KL                 | \( k = 10 \) | 0.248         | No.     |
| T                  |            | 0.342         | No.     |
| Energy             |            | 0.259         | No.     |
| MMD                |            | 0.177         | No.     |
| LS (0)             | \( m = 10 \) | **0.092**     | Yes.    |
| LS (1)             | \( m = 10 \) | **0.050**     | Yes.    |

Figure 2: Mixture of a Normal and a Uniform Distribution and a Gamma distribution.
Figure 3: Real image (a) and sampled image (b) of a hart in the MPEG7 CE-Shape-1 database.

4.2 Two real case-studies

4.2.1 Shape classification

As an application of the preceding theory to the field of pattern recognition problem we consider the MPEG7 CE-Shape-1 (Latecki et al., 2000), a well known shape database. We select four different classes of objects/shapes from the database: hearts, coups, hammers and bones. For each object class we choose 3 images in the following way: 2 standard images plus an extra image that exhibit some distortion or rotation (12 images in total). In order to represent each shape we do not follow the usual approach in pattern recognition that consists in representing each image by a feature vector catching its relevant shape aspects; instead we will look at the image as a cloud of points in $\mathbb{R}^2$, according to the following procedure: Each image is transformed to a binary image where each pixel assumes the value 1 (white points region) or 0 (black points region) as in Figure 3 (a). For each image $i$ of size $N_i \times M_i$ we generate a uniform sample of size $N_i M_i$ allocated in each position of the shape image $i$. To obtain the cloud of points as in Figure 3 (b) we retain only those points which fall into the white region (image body) whose intensity gray level are larger than a variable threshold fixed at 0.99 so as to yield around one thousand and two thousand points image representation depending on the image as can be seen in Figure 3 (b). After rescaling and centering, we compute the $12 \times 12$ image distance matrices, using the LS(1) distance and the KL divergence, and then compute Euclidean coordinates for the images via MDS (results in Figure 4). It is apparent that the LS distance produces a MDS map coherent with human image perception (fig. 3 (a)). This does not happen for the rest of tested metrics, in particular for the KL divergence as it is shown in Figure 3 (b)).
4.2.2 Testing statistical significance in Microarray experiments

Here we present an application of the proposed LS distance in the field of Bioinformatics. The data set we analyze comes from an experiment in which the time to respiratory recovery in ventilated post trauma patients is studied. Affymetrix U133+2 micro-arrays were prepared at days 0, 1, 4, 7, 14, 21 and 28. In this analysis, we focus on a subset of 46 patients which were originally divided into two groups: “early recovery patients” (group $G_1$) that recovered ventilation prior to day seven and “late recovery patients” (group $G_2$), those who recovered ventilation after day seven. The size of the groups is 22 and 26 respectively.

It is of clinical interest to find differences between the two groups of patients. In particular, the originally goal of this study was to test the association of inflammation on day one and subsequent respiratory recovery. In this experiment we will show how the proposed distance can be used in this context to test statistical differences between the groups and also to identify the genes with the largest effect in the post trauma recovery.

From the original data set we select the sample of 675 probe sets corresponding to those genes whose GO annotation include the term “inflamatory”. To do so we use a query (July 2012) on the Affymetrix web site (affymetrix.com). The idea of this search is to obtain a pre-selection of the genes involved in post trauma recovery in order to avoid working with the whole human genome.

Figure 5 shows the heat map of day one gene expression for the 46 patients (columns) over the 675 probe-sets. By using a hierarchical procedure, it is apparent that the two

\[\text{http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSE13488}\]
main clusters we find do not correspond to the two groups of patients of the experiment. However, the first cluster (on the left hand of the plot) contains mainly patients form the “early recovery” group (approx. 65 %) whereas the second cluster (on the right) is mainly made up of patients from the “late recovery” group (approx 60%). This lack of balance suggests a different pattern of gene expression between the two groups of patients.

In order to test if statistical differences exists between the groups $G_1$ and $G_2$ we define, inspired by [Hayden et al., 2009], an statistical test based on the LS distance proposed
in this work. To this end, we identify each patient $i$ with a probability distribution $P_i$. The expression of the 675 genes across the probe-sets are assumed to be samples of such distributions. Ideally, if the genes expression does not have any effect on the recovery speed then all distributions $P_i$ should be equal ($H_0$). On the other hand, assume that expression of a gene or a group of genes effectively change between “early” and “late” recovery patients. Then, the distributions $P_i$ will be different between patients belonging to groups $G_1$ and $G_2$ ($H_1$).

To validate or reject the previous hypothesis, consider the proposed LS distance $\hat{d}_\alpha(P_i, P_j)$ defined in (3.2) for two patients $i$ and $j$. Denote by

$$\Delta_1 = \frac{1}{22(22 - 1)} \sum_{i,j \in G_1} \hat{d}_\alpha(P_i, P_j),$$

$$\Delta_2 = \frac{1}{26(26 - 1)} \sum_{i,j \in G_2} \hat{d}_\alpha(P_i, P_j)$$

and

$$\Delta_{12} = \frac{1}{22 \cdot 26} \sum_{i \in G_1, j \in G_2} \hat{d}_\alpha(P_i, P_j),$$

the averaged $\alpha$-level set distances within and between the groups of patients. Using the previous quantities we define a distance between the groups $G_1$ and $G_2$ as

$$\Delta^* = \Delta_{12} - \frac{\Delta_1 + \Delta_2}{2}. \quad (4.1)$$
Figure 7: Heat-map of the 50-top ranked genes and p-values for different samples.

Notice that if the distributions are equal between the groups then $\Delta^*$ will be close to zero. On the other hand, if the distributions are similar within the groups and different between them, then $\Delta^*$ will be large. To test if $\Delta^*$ is large enough to consider it statistically significant we need the distribution of $\Delta^*$ under the null hypothesis. Unfortunately, this distribution is unknown and some re-sampling technique must be used. In this work we approximate it by calculating a sequence of distances $\Delta^*_1, \ldots, \Delta^*_N$ where each $\Delta^*_k$ is the distance between the groups $G_1$ and $G_2$ under a random permutation of the patients. For a total of $N$ permutations, then

$$p-value = \frac{\#[\Delta^*_k \geq \Delta^*: k = 1, \ldots, N]}{N},$$

where $\#[\Theta]$ refers to the number of times the condition $\Theta$ is satisfied, is a one-side p-value of the test.

We apply the previous LS distance based test (weighting scheme 1 with 10000 permutations) using the values of the 675 probe-sets and we obtain a p-value = 0.1893. This result suggests that none differences exists between the groups exist. The test for micro-arrays proposed in (Hayden et al., 2009) also confirms this result with a p-value of 0.2016. The
reason to explain this -a priori- unexpected result is that, if differences between the groups exist, they are probably hidden by a main group of genes with similar behavior between the groups. To validate this hypothesis, we first rank the set of 675 genes in terms of their individual variation between groups \( G_1 \) and \( G_2 \). To do so, we use the p-values of individual difference mean T-tests. Then, we consider the top-50 ranked genes and we apply the \( \alpha \)-level set distance test. The obtained p-value is 0.010, indicating a significant difference in gene expression of the top-50 ranked genes. In Figure 6 we show the estimated density profiles of the patients using a kernel estimator. It is apparent that the profiles between groups are different as it is reflected in the obtained results. In Figure 7 we show the heat-map calculated using the selection of 50 genes. Note that a hierarchical cluster using the Euclidean distance, which is the most used technique to study the existence of groups in micro-array data, is not able to accurately reflect the existence of the two groups even for the most influential genes.

To conclude the analysis we go further from the initial 50-genes analysis. We aim to obtain the whole set of genes in the original sample for which differences between groups remain significant. To do so, we sequentially include in the first 50-genes sample the next-highest ranked genes and we apply to the augmented data sets the LS distance based test. The p-values of such analysis are shown in Figure 7. Their value increases as soon as more genes are included in the sample. With a type-I error of 5\%, statistical differences are found for the 75 first genes. For a 10\% type-I error, with the first 110 genes we still are able to find differences between groups. This result shows that differences between “early” and “late” recovery trauma patients exist and they are caused by the top-110 ranked genes of the Affymetrix U133+2 micro-arrays (filtered by the query “inflammatory”). By considering each patient as a probability distribution the LS distance has been used to test differences between groups and to identify the most influential genes of the sample. This shows the ability of the new proposed distance to provide new insights in the analysis of biological data.

5 Conclusions

In this paper we presented probability measures as generalized functions, acting on appropriate function spaces. In this way we were able to introduce a new family of distances for probability measures, based on the evaluation of the PM functionals on a finite number of well chosen functions of the sample. The calculation of these PM distances does not require the use of either parametric assumptions or explicit probability estimations which makes a clear advantage over most well established PM distances, such as Bregman divergences, which makes a clear advantage over most well established PM distances and divergences.
A battery of artificial and real data experiments have been used to study the performance of the new family of distances. Using synthetically generated data, we have shown their performance in the task of discriminating normally distributed data. Although the generated data sets are ideal for the use of T-statistics the new distances shows superior discrimination results than classical methods. Similar conclusions have been obtained when the proposed distances are used in homogeneity test scenarios. Regarding the practical applications, the new PM distances have been proven to be competitive in shape recognition problems. Also they represent a novel way to identify genes and discriminate between groups of patients in micro-arrays.

In the near future we will afford the study of the geometry induced by the proposed measure and its asymptotic properties. It is also interesting to investigate in the relationship there may be exist between the proposed distance and other probability metrics.

Acknowledgements This work was partially supported by projects MIC 2012/00084/00, ECO2012-38442, SEJ2007-64500, MTM2012-36163-C06-06, DGUCM 2008/00058/002 and MEC 2007/04438/001.

Appendix

A) Proof for Theorems of Section 3

of Theorem 1. Consider \( x \in \text{Supp}(\mathbb{P}) \); given \( m \) and a sequence \( \alpha_m \), \( x \in A_i(\mathbb{P}) = S_{\alpha_i}(f_\mathbb{P}) - S_{\alpha_{i+1}}(f_\mathbb{P}) \) for one (and only one) \( i \in \{1, \ldots, m-1\} \), that is \( \alpha_i \leq f_\mathbb{P}(x) \leq \alpha_{i+1} \). Then \( \phi_i(x) = 1_{[A_i(\mathbb{P})]}(x) = 1 \) in the region \( A_i(\mathbb{P}) \) and zero elsewhere. Given \( \varepsilon > 0 \), choose \( m > \frac{1}{\varepsilon} \) and \( \alpha_{i+1} = \alpha_i + \frac{1}{m} \). Given that \( \alpha_i \leq f_\mathbb{P}(x) \leq \alpha_{i+1} \), then \( |\alpha_i - f_\mathbb{P}(x)| \leq \frac{1}{m} \), and thus:

\[
|f_{m-1}(x) - f_\mathbb{P}(x)| = \left| \sum_{j=1}^{m-1} \alpha_j \phi_j(x) - f_\mathbb{P}(x) \right| \\
= |\alpha_i - f_\mathbb{P}(x)| \leq \frac{1}{m} < \varepsilon. 
\]

That is \( \lim_{m \to \infty} f_{m-1}(x) = f_\mathbb{P}(x) \) pointwise and also uniformly by Dini’s Theorem. Therefore we can approximate (by fixing \( m \gg 0 \)) the density function as a simple function, made up of linear combination of indicator functions weighted by coefficients that represents the density value of the \( \alpha \)-level sets of the density at hand.
of Corollary 1. By Theorem 1 we can approximate (by fixing $m \gg 0$) the density function as:

$$f_P(x) \approx \sum_{j=1}^{m-1} \alpha_j \phi_j(x),$$

where $\alpha_j = \langle \phi_j, f_P \rangle$ and $\phi_j$ is the indicator function of the $\alpha_j$-level set of $\mathbb{P}$. Then if $\langle \phi_j, f_P \rangle \xrightarrow{m \to \infty} \langle \phi_j, f_Q \rangle$, for all the indicator functions $\phi_j$, then $f_P = f_Q$. \qed

of Proposition 1. If $\lim_{m \to \infty} d_{\alpha,\beta}(\mathbb{P}, \mathbb{Q}) = 0$, then $A_i(\mathbb{P}) \xrightarrow{m \to \infty} A_i(\mathbb{Q}) \forall i$. Thus $f_{P_m}^* = \sum_{j=1}^{m} \alpha_j \phi_j(x) = f_{Q_m}^* \forall m$, and by Theorem 1 $f_P = f_Q$. In the other way around if $\mathbb{P} = \mathbb{Q}$ ($f_P = f_Q$) then it is certain that $\lim_{m \to \infty} d_{\alpha,\beta}(\mathbb{P}, \mathbb{Q}) = 0$. \qed

B) Invariance under affine transformations

Lemma 1. Lebesgue measure is equivalent under affine transformations.

Proof. Let $X$ be a random variable that take values in $\mathbb{R}^d$ distributed according to $\mathbb{P}$, and let $f_P$ be its density function. Let $T : \mathbb{R}^d \to \mathbb{R}^d$ be an affine transformation, define the r.v. $X^* = T(X) = a + bRX$, where $a \in \mathbb{R}^d$, $b \in \mathbb{R}^+$ and $R \in \mathbb{R}^{d \times d}$ is an orthogonal matrix with $\det(R) = 1$ (therefore $R^{-1}$ exist and $R^{-1} = R^T$). Then $X^*$ is distributed according to $f_{P^*}$. Define $E^* = \{x^*|x^* = T(x) \text{ and } x \in E\}$, then:

$$\mu^*(E^*) = \int_{E^*} d\mathbb{P}^* = \int_{E^*} f_{P^*}(x^*) dx^*$$

$$= \int_{E^*} f_P(T^{-1}(x^*)) \left| \frac{\partial T^{-1}(x^*)}{\partial x^*} \right| dx^*$$

$$= \int_{E^*} f_P \left( R^{-1} \left( \frac{x^* - a}{b} \right) \right) \frac{1}{b} dx^*$$

$$= \int_{E} f_P(y) dy = \int_{E} d\mathbb{P} = \mu(E).$$

\qed

Theorem 2. (Invariance under affine transformation) The metric proposed in Eq. (3.1) is invariant under affine transformations.
Proof. Let $T$ be an affine transformation, we prove that the measure of the symmetric difference of any two $\alpha$-level sets is invariant under affine transformation, that is: $\mu(A_i(\mathbb{P}) \triangle A_i(\mathbb{Q})) = \mu^*(T(A_i(\mathbb{P})) \triangle T(A_i(\mathbb{Q}))) = \mu^*(A_i(\mathbb{P}^*) \triangle A_i(\mathbb{Q}^*))$. By Lemma 1:

$$
\mu^*(A_i(\mathbb{P}^*) \triangle A_i(\mathbb{Q}^*)) = \int_{A_i(\mathbb{P}^*) - A_i(\mathbb{Q}^*)} d\mathbb{P}^* + \int_{A_i(\mathbb{Q}^*) - A_i(\mathbb{P}^*)} d\mathbb{Q}^*
$$

$$
= \int_{A_i(\mathbb{P}) - A_i(\mathbb{Q})} d\mathbb{P} + \int_{A_i(\mathbb{Q}) - A_i(\mathbb{P})} d\mathbb{Q}
$$

$$
= \mu(A_i(\mathbb{P}) \triangle A_i(\mathbb{Q})).
$$

The same argument can be applied to the denominator in the expression given in Eq. (3.1), thus

$$
\frac{\mu^*(A_i(\mathbb{P}^*) \cup A_i(\mathbb{Q}^*))}{\mu(A_i(\mathbb{P}) \cup A_i(\mathbb{Q}))} = \frac{\mu^*(A_i(\mathbb{P}^*) \cup A_i(\mathbb{Q}^*))}{\mu(A_i(\mathbb{P}) \cup A_i(\mathbb{Q}))}
$$

for $i = 1, \ldots, m - 1$. Therefore as this is true for all the $\alpha$-level sets, then the distance proposed in Eq. (3.1) is invariant under affine transformations:

$$
d_{\alpha,\beta}(\mathbb{P}^*, \mathbb{Q}^*) = \sum_{i=1}^{m-1} w_i \int d(\phi_i(\mathbb{P}^*), \phi_i(\mathbb{Q}^*))
$$

$$
= \sum_{i=1}^{m-1} \lambda_i d(\phi_i(\mathbb{P}), \phi_i(\mathbb{Q}))
$$

$$
= d_{\alpha,\beta}(\mathbb{P}, \mathbb{Q}).
$$

\[\square\]

C) Details about the estimation of level sets

Definition 4 (Neighbourhood Measures). Consider a random variable $X$ with density function $f(x)$ defined on $\mathbb{R}^d$. Let $S_n$ denote the set of random independent identically distributed samples of size $n$ (drawn from $f$). The elements of $S_n$ take the form $s_n = (x_1, \ldots, x_n)$, where $x_i \in \mathbb{R}^d$. Let $M : \mathbb{R}^d \times S_n \rightarrow \mathbb{R}$ be a real-valued function defined for all $n \in \mathbb{N}$. (a) If $f(x) < f(y)$ implies $\lim_{n \rightarrow \infty} P(M(x, s_n) > M(y, s_n)) = 1$, then $M$ is a sparsity measure. (b) If $f(x) < f(y)$ implies $\lim_{n \rightarrow \infty} P(M(x, s_n) < M(y, s_n)) = 1$, then $M$ is a concentration measure.

Example 1. Consider the distance from a point $x \in \mathbb{R}^d$ to its $k^{th}$-nearest neighbour in $s_n$, $x^{(k)}: M(x, s_n) = d_k(x, s_n) = d(x, x^{(k)}):$ it is a sparsity measure.

Theorem 3. The set $R_\alpha = \{x : h_n(x) = \text{sign}(\rho_n^* - g_n(x)) \geq 0\}$ converges to a region of the form $S_\alpha(f) = \{x \mid f(x) \geq \alpha\}$, such that $P(S_\alpha(f)) = 1 - \nu$. Therefore, the Support Neighbour Machine estimates a density contour cluster $S_\alpha(f)$ (around the mode).
Theorem 3 (see details in [Muñoz and Moguerza 2006, 2005]) ensures the convergence of the empirical estimation of the proposed distance. When the sample size increases, we are able to determine with more precision the sets $A_i(P)$ and $A_i(Q)$ and therefore $\hat{d}_{\alpha,\beta}(P, Q) \xrightarrow{n} d_{\alpha,\beta}(P, Q)$.

D) Extensions of the weighting scheme

We present in this appendix alternative weighting schemes to LS(1):

1. Radius of the set $A_i(P) \triangle A_i(Q)$: Choose $w_i$ in Eq. (3.1) by:
   \[
   w_i = \frac{1}{m} \max_{x \in s_{A_i(P)}, y \in s_{A_i(Q)}} \left\{ (1 - I_{r_{A_i(P)}, r_{A_i(Q)}}(x, y)) \| x - y \|_2 \right\}.
   \]

2. Hausdorff distance between the sets $A_i(P) - A_i(Q)$ and $A_i(Q) - A_i(P)$:
   \[
   \hat{H}(\hat{X}, \hat{Y})
   \]
   Choose $w_i$ in Eq. (3.1) by:
   \[
   w_i = \frac{1}{m} \hat{H}\left(s_{A_i(Q)} - \hat{A_i}(P), s_{A_i(P)} - \hat{A_i}(Q)\right),
   \]
   where $\hat{H}(\hat{X}, \hat{Y})$ denotes the Hausdorff distance (finite size version) between finite sets $\hat{X}$ and $\hat{Y}$ (which estimates the ‘theoretical’ Hausdorff distance between space regions $X$ and $Y$). In this case $X = A_i(P) - A_i(Q)$ and $Y = A_i(Q) - A_i(P)$.

References

Amari, S.-I., Barndorff-Nielsen, O. E., Kass, R. E., Lauritzen, S. L. and Rao, C. R.: Differential Geometry in Statistical Inference. Lecture Notes-Monograph Series 10, (1987)

Amari, S. and Nagaoka, H.: Methods of Information Geometry. American Mathematical Society. (2007)

Atkinson, C. and Mitchell, A. F. S.: Rao’s Distance Measure. The Indian Journal of Statistics, Series A. 43, 345-365, (1981)
Banerjee, A., Merugu, S., Dhillon, I. and Ghosh, J.: Clustering whit Bregman Divergences. Journal of Machine Learning Research 6, 1705:1749, (2005)

Boltz, S., Debreuve, E. and Barlaud, M.: High-dimensional statistical measure for region-of-interest tracking. Transactions in Image Processing, vol. 18, no. 6, pp 1266:1283, (2009)

Burbea, J. and Rao, C. R.: Entropy differential metric, distance and divergence measures in probability spaces: A unified approach. Journal of Multivariate Analysis 12, 575-596, (1982)

Cha, S.H: Comprehensive survey on distance/similarity measures between probability density functions. International Journal of Mathematical Models and Methods in Applied Sciences 1(4), pp.300-307, (2007)

Cichocki, A. and Amari, S.: Families of Alpha- Beta- and Gamma- Divergences: Flexible and Robust Measures of Similarities. Entropy 12, 1532-1568, (2010)

Csiszár, I. and Shields, P.: Information Theory and Statistics: A Tutorial. Foundations and Trends in Communications and Information Theory, (2004)

Devroye, L. and Wise, G.L.: Detection of abnormal behavior via nonparametric estimation of the support. SIAM J. Appl. Math. 38, 480-488 (1980)

Deza, M.M. and Deza, E.: Encyclopedea of Distances. Springer, (2009)

Dryden, I.L., Koloydenko, A. and Zhou, D.: Non-Euclidean statistics for covariance matrices, with applications to diffusion tensor imaging. The Annals of Applied Statistics 3, 1102-1123, (2009)

Frigyik, B.A., Srivastava, S. and Gupta, M. R.: Functional Bregman Divergences and Bayesian Estimation of Distributions. IEEE Transactions on Information Theory 54(11), 51305139, (2008)

Goria, M. N., Leonenko, N. N., Mergel, V. V. and Novi Inverardi, P. L.: A new class of random vector entropy estimators and its applications in testing statistical hypotheses. Journal of Nonparametric Statistics, vol. 13, No. 3, pp. 277-297, (2005)

Gretton, A., Borgwardt, K. M., Rasch, M. J., Schölkopf, B. and Smola, A.: A kernel two-sample test The Journal of Machine Learning Research, 13(1), 723-773, (2012).
Gretton, A., Borgwardt, K., Rasch, M., Schlkopf, B. and Smola, A.: A kernel method for the two sample problem. Advances in Neural Information Processing Systems, 513-520, (2007)

Hastie, T., Tibshirani, R. and Friedman, J.: The elements of statistical learning. 2nd Ed. Springer, (2009)

Hayden, D., Lazar, P. and Schoenfeld, D.: Assessing Statistical Significance in Microarray Experiments Using the Distance Between Microarrays. PLoS ONE 4(6): e5838., (2009)

Institute of Information Theory and Automation ASCR.LEAF - Tree Leaf Database. Prague, Czech Republic. http://zoi.utia.cas.cz/tree_leaves

Kylberg, G.: The Kylberg Texture Dataset v. 1.0. Centre for Image Analysis, Swedish University of Agricultural Sciences and Uppsala University, Uppsala, Sweden. http://www.cb.uu.se/~gustaf/texture/

Latecki, L. J., Lakamper, R. and Eckhardt, U.: Shape Descriptors for Non-rigid Shapes with a Single Closed Contour. IEEE Conference on Computer Vision and Pattern Recognition, 424-429, (2000)

Lebanon, G.: Metric Learning for Text Documents. IEEE Trans on Pattern Analysis and Machine Intelligence, 28(40), 497-508, (2006)

Levina, E. and Bickel, P.: The earth mover’s distance is the Mallows distance: some insights from statistics. Proceedings. Eighth IEEE International Conference on Computer Vision, 2001. ICCV 2001, 2, 251?256, (2001).

Marriot, P. and Salmon, M.: Aplication of Differential Geometry to Econometrics. Cambridge University Press, (2000)

Minas, C., Curry, E. and Montana, G.: A distance-based test of association between paired heterogeneous genomic data Bioinformatics, (2013).

Moon, Y., Rajagopalan, B. and Lall, U.: Estimation of mutual information using kernel density estimators. Physical Review E 52(3), 2318-2321, (1995)

Müller, A.: Integral Probability Metrics and Their Generating Classes of Functions. Advances in Applied Probability, 29(2), 429-443, (1997)
Muñoz, A. and Moguerza, J.M.: One-Class Support Vector Machines and density estimation: the precise relation. Progress in Pattern Recognition, Image Analysis and Applications, 216-223, (2004)

Muñoz, A. and Moguerza, J.M.: Estimation of High-Density Regions using One-Class Neighbor Machines. IEEE Trans. on Pattern Analysis and Machine Intelligence, 28(3), 476-480, (2006)

Moguerza, J. M. and Muñoz, A. Support vector machines with applications Statistical Science, 322-336, (2006).

Muñoz, A., Martos, G., Arriero, J. and Gonzalez, J. A new distance for probability measures based on the estimation of level sets Artificial Neural Networks and Machine Learning–ICANN 2012, 271?278, (2012).

Muñoz, A. and Moguerza, J.M.: A Naive Solution to the One-Class Problem and its Extension to Kernel Methods. LNCS 3773, 193204, (2005)

Nguyen, X., Wainwright, M. J. and Jordan, M. I.: Nonparametric Estimation of the Likelihood and Divergence Functionals. IEEE International Symposium on Information Theory, (2007)

Nielsen, F. and Boltz, S.: The burbea-rao and bhattacharyya centroids. IEEE Transactions on Information Theory, 57(8), 5455?5466, (2006).

Pennec, X.: Statistics on Riemannian Manifolds: Basic Tools for Geometric Measurements. Journal of Mathematical Imaging and Vision, 25, 127-154, (2006)

Ramsay, J. O. and Silverman, B. W.: Applied Functional Data Analysis. New York: Springer, (2005)

Råström, H. R.: An Embeding Theorem for Spaces of Convex Sets. Proceding of the American Mathematical Society 3, No. 1. (1952)

Rubner, Y., Tomasi, C. and Guibas, L. J.: The earth mover’s distance as a metric for image retrieval. International Journal of Computer Vision, 40(2), 99?121, (2000).

Ryabko, D. and Mary, J.: Reducing statistical time-series problems to binary classification Advances in Neural Information Processing Systems, 2060?2068, (2012)
Saez, C., Robles, M. and Garcia-Gomez, J. M.: Comparative study of probability distribution
distances to define a metric for the stability of multi-source biomedical research data
Engineering in Medicine and Biology Society (EMBC), 2013 35th Annual International
Conference of the IEEE, 3226?3229, (2013).

Scott, D.: Multivariate Density Estimation: Theory Practice and Visualization. Wiley, (1992)

Sejdinovic, D., Sriperumbudur, B., Gretton, A. and Fukumizu K.: Equivalence of Distance-
Based and RKHS-Based Statistics in Hypothesis Testing. arXiv, (2012)

Sriperumbudur, B. K., Gretton, A., Fukumizu, K. and Scholkopf, B.: Hilbert Space Embed-
dings and Metrics on Probability Measures. Journal of Machine Learning Research 11,
1297-1322, (2010)

Sriperumbudur, B. K., Fukumizu, K., Gretton, A., Scholkopf, B. and Lanckriet, G. R. G.: Non-parametric estimation of integral probability metrics. International Symposium on
Information Theory, (2010)

Stone, C. J.: Optimal rates of convergence for nonparametric estimators The annals of
Statistics, 1348?1360, (1980).

Strichartz, R.S.: A Guide to Distribution Theory and Fourier Transforms. World Scientific,
(1994)

Székely, G.J., Rizzo, M.L.: Testing for Equal Distributions in High Dimension. InterStat,
(2004)

Wang, Q., Kulkarni, S. R. and Verdú, S.: Divergence estimation of continuous distributions
based on data-dependent partitions IEEE Transactions on Information Theory, 51(9),
3064?3074, (2005).

Zemanian, A.H.: Distribution Theory and Transform Analysis. Dover, (1965)

Zolotarev, V. M.: Probability metrics. Teor. Veroyatnost. i Primenen, 28(2), 264287, (1983)