

BS-MS Thesis

STATISTICAL DEPTH FUNCTIONS

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ABSTRACT

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Chapter 1

INTRODUCTION

1.1 Centrality vs Density

1.2 Nonparametric procedures

Chapter 2

MULTIVARIATE DATA

It is desirable for a depth function $D: \mathbb{R}^d \times \mathcal{F} \rightarrow \mathbb{R}$ to satisfy the following properties, described by Zuo and Serfling (2000).

P1. *Affine invariance.* For any random vector \mathbf{X} in \mathbb{R}^d , any $d \times d$ nonsingular matrix A , and any d -vector \mathbf{b} ,

$$D(A\mathbf{x} + \mathbf{b}, F_{A\mathbf{X}+\mathbf{b}}) = D(\mathbf{x}, F_{\mathbf{X}}). \quad (2.0.1)$$

This makes $D(\mathbf{x}, F_{\mathbf{X}})$ independent of the choice of coordinate system.

P2. *Maximality at center.* For any $F \in \mathcal{F}$ having ‘center’ $\boldsymbol{\theta}$,

$$D(\boldsymbol{\theta}, F) = \sup_{\mathbf{x} \in \mathbb{R}^d} D(\mathbf{x}, F). \quad (2.0.2)$$

This means that the deepest point coincides with some center of symmetry of the distribution F .

P3. *Monotonicity relative to deepest point.* For any $F \in \mathcal{F}$ having deepest point $\boldsymbol{\theta}$ and for $\alpha \in [0, 1]$,

$$D(\mathbf{x}, F) \leq D(\boldsymbol{\theta} + \alpha(\mathbf{x} - \boldsymbol{\theta}), F). \quad (2.0.3)$$

Thus, $D(\cdot, F)$ monotonically decreases along any ray pointing away from the deepest point.

P4. *Vanishing at infinity.* For any $F \in \mathcal{F}$,

$$D(\mathbf{x}, F) \rightarrow 0 \quad \text{as} \quad \|\mathbf{x}\| \rightarrow \infty. \quad (2.0.4)$$

Furthermore, we demand that D be non-negative and bounded. Thus, we may assume hereon that D only takes values in $[0, 1]$.

The notion of a ‘center’ of a distribution in **P2** is typically described in terms of symmetry. We say that a random vector \mathbf{X} is *centrally symmetric* about $\boldsymbol{\theta} \in \mathbb{R}^d$

if $\mathbf{X} - \boldsymbol{\theta} \stackrel{d}{=} \boldsymbol{\theta} - \mathbf{X}$. Similarly, we say that \mathbf{X} is *angularly symmetric* about $\boldsymbol{\theta}$ if $(\mathbf{X} - \boldsymbol{\theta})/\|\mathbf{X} - \boldsymbol{\theta}\|$ is centrally symmetric about $\mathbf{0}$. An even more restrictive notion of symmetry is *spherical symmetry*, where we demand that $U(\mathbf{X} - \boldsymbol{\theta}) \stackrel{d}{=} \mathbf{X} - \boldsymbol{\theta}$ for every orthonormal matrix U . *Elliptical symmetry* requires that $V\mathbf{X}$ is spherically symmetric about $\boldsymbol{\theta}$ for some nonsingular matrix V . Finally, the weakest notions of symmetry discussed here is *halfspace symmetry*, where we impose $P(\mathbf{X} \in H) \geq 1/2$ for every closed halfspace in \mathbb{R}^d containing $\boldsymbol{\theta}$. Thus, the symmetries in decreasing order of strength are $S > E > C > A > H$.

2.1 Multivariate depth functions

Definition 2.1.1 (Halfspace/Tukey depth). Denote the collection of all closed halfspaces in \mathbb{R}^d containing \mathbf{x} by $\mathcal{H}_{\mathbf{x}}$. The halfspace depth, or Tukey depth, is defined as

$$D_H(\mathbf{x}, F) = \inf_{H \in \mathcal{H}_{\mathbf{x}}} P_F(H). \quad (2.1.1)$$

Remark. If $F \in \mathcal{F}$ is supported on a convex region $C \subset \mathbb{R}^d$, then $D(\cdot, F)$ vanishes outside C .

Proposition 2.1.2. *The halfspace depth can be formulated as*

$$D_H(\mathbf{x}, F) = \inf_{\mathbf{v} \in S^{d-1}} P_{\mathbf{X} \sim F}(\langle \mathbf{v}, \mathbf{X} \rangle \leq \langle \mathbf{v}, \mathbf{x} \rangle). \quad (2.1.2)$$

Remark. When $d = 1$, the halfspace depth reduces to

$$D_H(x, F) = \min\{P_F(-\infty, x], P_F[x, \infty)\}. \quad (2.1.3)$$

Struyf and Rousseeuw (1999) showed that halfspace depth fully characterizes empirical distributions.

Theorem 2.1.3 (Struyf and Rousseeuw, 1999). *The empirical distribution of any dataset $\{\mathbf{X}_i\}_{i=1}^n \subset \mathbb{R}^d$ is uniquely determined by its halfspace depth function $D(\cdot, \hat{F}_n)$.*

Nagy (2020) offers a comprehensive overview of this characterization problem. Indeed, Nagy (2021) supplies examples of distinct probability distributions F_1, F_2 such that $D_H(\cdot, F_1) = D_H(\cdot, F_2)$. It can be shown that for an α -symmetric distribution F that $D_H(\mathbf{x}, F) = G(-\|\mathbf{x}\|_{\alpha^*})$, where G is the marginal distribution of the first component of $\mathbf{X} \sim F$ and $1/\alpha + 1/\alpha^* = 1$.

Definition 2.1.4 (Mahalanobis depth). Let $\mathbf{X} \sim F$ have mean $\boldsymbol{\mu}$ and covariance matrix Σ . The Mahalanobis depth is defined as

$$D_M(\mathbf{x}, F) = (1 + (\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}))^{-1}. \quad (2.1.4)$$

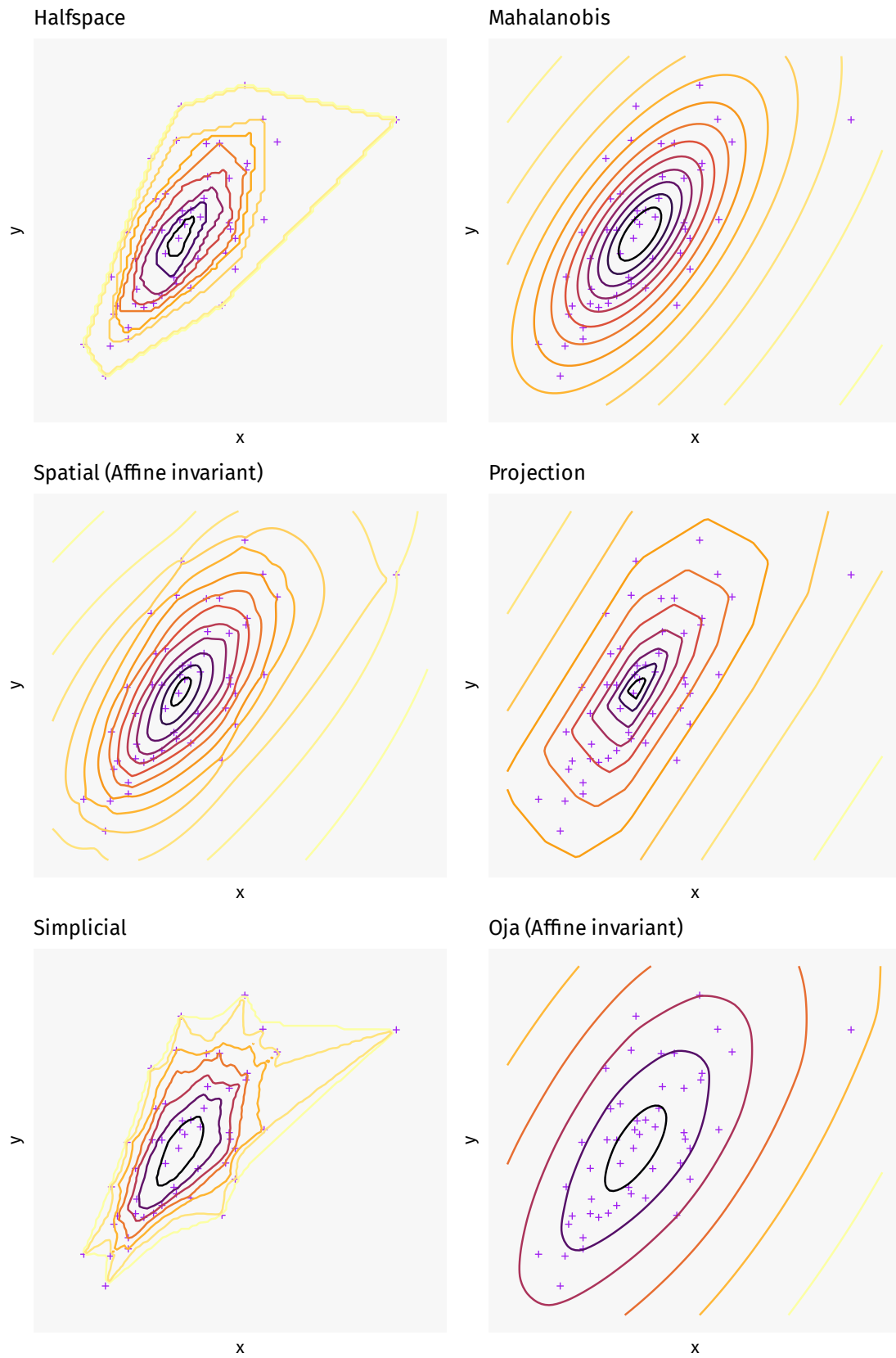


Figure 2.1: Depth contours with respect to purple points.

Remark. The mean and covariance in the above definition may be replaced with more robust estimates $\boldsymbol{\mu}^*$ and Σ^* , for instance using the minimum covariance determinant (MCD) method. The corresponding depth function is called the robust Mahalanobis depth.

Definition 2.1.5 (Spatial depth). The spatial depth is defined as

$$D_{Sp}(\mathbf{x}, F) = 1 - \left\| \mathbb{E}_{\mathbf{X} \sim F} \left[\frac{\mathbf{x} - \mathbf{X}}{\|\mathbf{x} - \mathbf{X}\|} \right] \right\|. \quad (2.1.5)$$

We use the convention $\mathbf{0}/0 = \mathbf{0}$.

Remark. Spatial depth defined as above does not obey **P1**. Indeed, spatial depth is only invariant under spherical transformations of the form $U\mathbf{X} + \mathbf{b}$ for orthonormal U . We may define an affine invariant version of spatial depth as

$$D_{AISP}(\mathbf{x}, F) = 1 - \left\| \mathbb{E}_{\mathbf{X} \sim F} \left[\frac{\Sigma^{-1/2}(\mathbf{x} - \mathbf{X})}{\sqrt{(\mathbf{x} - \mathbf{X})^\top \Sigma^{-1}(\mathbf{x} - \mathbf{X})}} \right] \right\|. \quad (2.1.6)$$

Remark. Nagy (2017) showed that spatial depth does not obey **P3**.

Lemma 2.1.6. *Spatial depth obeys P4, i.e. $D_{Sp}(\mathbf{x}, F) \rightarrow 0$ as $\|\mathbf{x}\| \rightarrow \infty$.*

Proof. Let $\epsilon > 0$, and let $M > 0$ such that $P_{\mathbf{X} \sim F}(\|\mathbf{X}\| > M) = \epsilon$. Denote $\mathbf{Y} = (\mathbf{x} - \mathbf{X})/\|\mathbf{x} - \mathbf{X}\|$, and observe that

$$\mathbb{E}_{\mathbf{X} \sim F}[\mathbf{Y}] = (1 - \epsilon) \mathbb{E}[\mathbf{Y} \mid \|\mathbf{X}\| \leq M] + \epsilon \mathbb{E}[\mathbf{Y} \mid \|\mathbf{X}\| > M] \quad (2.1.7)$$

Thus, using $\|\mathbf{Y}\| = 1$ and the reverse triangle inequality,

$$\|\mathbb{E}[\mathbf{Y}]\| \geq (1 - \epsilon) \|\mathbb{E}[\mathbf{Y} \mid \|\mathbf{X}\| \leq M]\| - \epsilon. \quad (2.1.8)$$

Let $\alpha = \arccos((1 - 2\epsilon)/(1 - \epsilon))$, and let $r_\alpha = M/\sin \alpha$. It follows that the ball $\{\mathbf{x} \in \mathbb{R}^d : \|\mathbf{x}\| \leq M\}$ subtends an angle of at most 2α from any point \mathbf{x} such that $\|\mathbf{x}\| > r_\alpha$. This gives $\|\mathbb{E}[\mathbf{Y} \mid \|\mathbf{X}\| \leq M]\| \geq \cos \alpha$. Thus, for $\|\mathbf{x}\| > r_\alpha$,

$$\|\mathbb{E}[\mathbf{Y}]\| \geq (1 - \epsilon) \cos \alpha - \epsilon = 1 - 3\epsilon, \quad (2.1.9)$$

whence $D_{Sp}(\mathbf{x}, F) \leq 3\epsilon$. \square

Definition 2.1.7 (Projection depth). The projection depth is defined as

$$D_P(\mathbf{x}, F) = \left(1 + \sup_{\mathbf{v} \in S^{d-1}} \frac{|\langle \mathbf{v}, \mathbf{x} \rangle - \text{med}(\langle \mathbf{v}, \mathbf{X} \rangle)|}{\text{MAD}(\langle \mathbf{v}, \mathbf{X} \rangle)} \right)^{-1}, \quad \mathbf{X} \sim F. \quad (2.1.10)$$

Definition 2.1.8 (Simplicial depth). The simplicial depth is defined as

$$D_{Sim}(\mathbf{x}, F) = P_{\mathbf{X}_i \stackrel{\text{iid}}{\sim} F}(\mathbf{x} \in \text{conv}(\mathbf{X}_1, \dots, \mathbf{X}_{d+1})), \quad (2.1.11)$$

where $\text{conv}(\mathbf{x}_1, \dots, \mathbf{x}_{d+1})$ denotes the convex hull of $\{\mathbf{x}_1, \dots, \mathbf{x}_{d+1}\}$.

Definition 2.1.9 (Oja depth). The simplicial volume depth, or Oja depth, is defined as

$$D_{Oja}(\mathbf{X}, F) = \left(1 + \mathbb{E}_{\mathbf{X}_i \sim F} [\text{vol}(\text{conv}(\mathbf{x}, \mathbf{X}_1, \dots, \mathbf{X}_d))]\right)^{-1}. \quad (2.1.12)$$

Remark. Oja depth does not obey **P1**, since

$$\text{vol}(\text{conv}(A\mathbf{x}_1 + \mathbf{b}, \dots, A\mathbf{x}_{d+1} + \mathbf{b})) = |\det(A)| \text{vol}(\text{conv}(\mathbf{x}_1, \dots, \mathbf{x}_{d+1})). \quad (2.1.13)$$

Instead, we may define an affine invariant version of Oja depth as

$$D_{AIOja}(\mathbf{X}, F) = \left(1 + \mathbb{E}_{\mathbf{X}_i \sim F} \left[\frac{\text{vol}(\text{conv}(\mathbf{x}, \mathbf{X}_1, \dots, \mathbf{X}_d))}{\sqrt{\det(\Sigma)}} \right] \right)^{-1}, \quad (2.1.14)$$

where Σ is the covariance matrix of F .

2.1.1 The projection property

Definition 2.1.10 (Projection property). We say that a depth function D has the projection property if

$$D(\mathbf{x}, F_{\mathbf{X}}) = \inf_{\mathbf{v} \in S^{d-1}} D(\langle \mathbf{v}, \mathbf{x} \rangle, F_{\langle \mathbf{v}, \mathbf{X} \rangle}). \quad (2.1.15)$$

Depths which have this property can be approximated by calculating the univariate depths of the projected data along many directions \mathbf{v} .

Lemma 2.1.11. *The halfspace depth, Mahalanobis depth, and projection depth have the projection property.*

The halfspace depth in particular is often computationally challenging. Thus, the property motivates the definition of the random Tukey depth (Cuesta-Albertos & Nieto-Reyes, 2008a).

Definition 2.1.12 (Random Tukey depth). Let $\mathbf{v}_1, \dots, \mathbf{v}_n$ be a realization of an iid sample from $\mathcal{U}(S^{d-1})$. The random Tukey depth is defined as

$$D_{RT}(\mathbf{x}, F_{\mathbf{X}}) = \min_{1 \leq i \leq n} D_H(\langle \mathbf{v}_i, \mathbf{x} \rangle, F_{\langle \mathbf{v}_i, \mathbf{X} \rangle}). \quad (2.1.16)$$

2.1.2 Continuity properties

It is also desirable for a depth function to obey some notions of continuity.

C1. *Continuity in \mathbf{x} .*

$$D(\mathbf{x}_n, F) \rightarrow D(\mathbf{x}, F) \quad \text{when } \mathbf{x}_n \rightarrow \mathbf{x}. \quad (2.1.17)$$

C2. *Continuity in F .*

$$D(\mathbf{x}, F_n) \rightarrow D(\mathbf{x}, F) \text{ when } F_n \xrightarrow{d} F. \quad (2.1.18)$$

C3. *Uniform continuity.*

$$\sup_{\mathbf{x} \in G} |D(\mathbf{x}, F_n) - D(\mathbf{x}, F)| \rightarrow 0 \text{ when } F_n \xrightarrow{d} F. \quad (2.1.19)$$

Property **C1** is rarely satisfied without imposing some regularity conditions on F , such as absolute continuity. Property **C2** helps bridge the gap between the population and empirical versions of depth. Property **C3** becomes relevant when dealing with the convergence of depth contours.

The Mahalanobis depth is trivially continuous in \mathbf{x} , i.e. obeys **C1**. Furthermore, it also satisfies **C2** as long as F has a regular covariance matrix (Mosler & Mozharovskiy, 2022).

The halfspace depth also enjoys all three notions of continuity, under mild restrictions on F .

Theorem 2.1.13 (Mizera and Volau, 2002). *Let $F \in \mathcal{F}$ be such that the probability of every hyperplane in \mathbb{R}^d is zero, i.e. for all $\alpha \in \mathbb{R}$ and $\mathbf{v} \in S^{d-1}$,*

$$P_{\mathbf{X} \sim F}(\langle \mathbf{v}, \mathbf{X} \rangle = \alpha) = 0. \quad (2.1.20)$$

Then for $\mathbf{x}_n \rightarrow \mathbf{x}$ and $F_n \xrightarrow{d} F$, we have $D_H(\mathbf{x}_n, F_n) \rightarrow D_H(\mathbf{x}, F)$.

Remark. Equation 2.1.20 is satisfied whenever F is absolutely continuous.

Remark. It follows that if $F \in \mathcal{F}$ satisfies Equation 2.1.20, then the map $D_H(\cdot, F)$ is continuous.

Corollary 2.1.14. *Let $F \in \mathcal{F}$ satisfy Equation 2.1.20. Then, for $F_n \xrightarrow{d} F$, and compact $K \subset \mathbb{R}^d$,*

$$\sup_{\mathbf{x} \in K} |D_H(\mathbf{x}, F_n) - D_H(\mathbf{x}, F)| \rightarrow 0. \quad (2.1.21)$$

Proof. Denoting $g = D(\cdot, F)$, $g_n = D_H(\cdot, F_n)$, we have the continuity of g along with $g_n(\mathbf{x}_n) \rightarrow g(\mathbf{x})$ whenever $\mathbf{x}_n \rightarrow \mathbf{x}$ in K . If the given conclusion is false, we may pass to a subsequence of g_n and find $\epsilon > 0$ such that each $\sup_{\mathbf{x} \in K} |g_n(\mathbf{x}) - g(\mathbf{x})| \geq \epsilon$. Using the compactness of K , we pass to a further subsequence and find $\mathbf{x} \in K$ such that $\mathbf{x}_n \rightarrow \mathbf{x}$. This contradicts $|g_n(\mathbf{x}_n) - g(\mathbf{x}_n)| \geq \epsilon$. \square

Theorem 2.1.15. *Let $F \in \mathcal{F}$ satisfy Equation 2.1.20. Then, for $F_n \xrightarrow{d} F$,*

$$\sup_{\mathbf{x} \in \mathbb{R}^d} |D_H(\mathbf{x}, F_n) - D_H(\mathbf{x}, F)| \rightarrow 0. \quad (2.1.22)$$

Proof. Let $K_r = \{\mathbf{x} \in \mathbb{R}^d : \|\mathbf{x}\| \leq r\}$ be a continuity set of F . Observe that $D_H(\mathbf{y}, F) \leq P_F(K_r^c)$ for $\mathbf{y} \in K_r^c$, hence

$$\sup_{\mathbf{y} \in K_r^c} |D_H(\mathbf{y}, F_n) - D_H(\mathbf{y}, F)| \leq P_{F_n}(K_r^c) + P_F(K_r^c). \quad (2.1.23)$$

As $n \rightarrow \infty$, we have $P_{F_n}(K_r^c) \rightarrow P_F(K_r^c) = p_r$ (say). Thus, denoting $\delta_n(X) = \sup_{\mathbf{x} \in X} |D_H(\mathbf{x}, F_n) - D_H(\mathbf{x}, F)|$, we have

$$\limsup_{n \rightarrow \infty} \delta_n(\mathbb{R}^d) \leq \lim_{n \rightarrow \infty} \delta_n(K_r) + \limsup_{n \rightarrow \infty} \delta_n(K_r^c) \quad (2.1.24)$$

$$\leq 0 + 2p_r. \quad (2.1.25)$$

Using $p_r \rightarrow 0$ as $r \rightarrow \infty$ completes the proof. \square

The spatial depth is similarly well behaved.

Theorem 2.1.16. *Spatial depth obeys C1 when F is non-atomic, as well as C2.*

Proof. Consider the spatial map

$$S_F: \mathbb{R}^d \rightarrow \mathbb{R}^d, \quad \mathbf{x} \mapsto \mathbb{E}_{\mathbf{X} \sim F} \left[\frac{\mathbf{x} - \mathbf{X}}{\|\mathbf{x} - \mathbf{X}\|} \right]. \quad (2.1.26)$$

The Dominated Convergence Theorem guarantees the continuity of S_F , hence of $D_{Sp}(\cdot, F) = 1 - \|S_F(\cdot)\|$. Furthermore, if $F_n \xrightarrow{d} F$, we have $S_{F_n}(\mathbf{x}) \rightarrow S_F(\mathbf{x})$ by the Portmanteau Lemma for all $\mathbf{x} \in \mathbb{R}^d$. \square

Theorem 2.1.17 (Serfling, 2002). *For $F \in \mathcal{F}$ and compact $K \subset \mathbb{R}^d$,*

$$\sup_{\mathbf{x} \in K} |D_{Sp}(\mathbf{x}, \hat{F}_n) - D_{Sp}(\mathbf{x}, F)| \xrightarrow{a.s.} 0. \quad (2.1.27)$$

Remark. This result can be generalized from compact subsets K to the whole of \mathbb{R}^d , using Lemma 2.1.6 and arguments similar to the proof of Theorem 2.1.15.

2.2 Depth contours

The following definitions are adapted from Liu et al., 1999.

Definition 2.2.1. The contour of depth t is the set $\{\mathbf{x} \in \mathbb{R}^d : D(\mathbf{x}, F) = t\}$.

Definition 2.2.2. The region enclosed by the contour of depth t is the set

$$R_F(t) = \{\mathbf{x} \in \mathbb{R}^d : D(\mathbf{x}, F) > t\}. \quad (2.2.1)$$

Definition 2.2.3. The p -th central region is the set

$$C_F(p) = \bigcap_t \{R_F(t) : P_F(R_F(t)) \geq p\}. \quad (2.2.2)$$

Definition 2.2.4. The p -th level contour, or center-outward contour surface, is the set $Q_F(p) = \partial C_F(p)$.

Example 2.2.5. Consider $\mathcal{U}(B^d)$, i.e. the uniform distribution on the unit ball in \mathbb{R}^d . While there are no proper density contours to speak of, halfspace depth contours are concentric spheres centered at the origin, the deepest point. This illustrates how depth contours are more suited to indicating centrality than density contours.

Definition 2.2.6. Let $\mathbf{X}_1, \dots, \mathbf{X}_n \stackrel{\text{iid}}{\sim} F$. We introduce depth based order statistics $\mathbf{X}_{[1]}, \dots, \mathbf{X}_{[n]}$, which are a reordering of the sample in decreasing order of depth, i.e. $D(\mathbf{X}_{[1]}, F) \geq \dots \geq D(\mathbf{X}_{[n]}, F)$.

With this, given $\mathbf{X}_1, \dots, \mathbf{X}_n \stackrel{\text{iid}}{\sim} F$, the sample p -th central region is given by

$$C_{\hat{F}_n}(p) = \text{conv}(\mathbf{X}_{[1]}, \dots, \mathbf{X}_{[np]}). \quad (2.2.3)$$

2.3 Depth-Depth plots

Definition 2.3.1 (DD plot). Let F, G be two distributions on \mathbb{R}^d , and let D be a depth function. The Depth-Depth plot, also known as the DD plot, of F and G is given by

$$\text{DD}(F, G) = \{(D(\mathbf{z}, F), D(\mathbf{z}, G)) : \mathbf{z} \in \mathbb{R}^d\}. \quad (2.3.1)$$

Remark. The above definition generalizes naturally to involve more than two distributions on \mathbb{R}^d .

When the depth function D only takes values in $[0, 1]$, the DD plot is a subset of $[0, 1]^2$ and hence easily visualized. Clearly when $F = G$, the corresponding DD plot is confined to the diagonal $\{(t, t) : t \in [0, 1]\}$. However, when $d \geq 2$ and F, G are absolutely continuous, $\text{DD}(F, G)$ has non-zero area (Lebesgue measure) when $F \neq G$. Assuming that D is affine invariant, Liu et al. (1999) propose this area as an affine invariant measure of the discrepancy between F and G .

If the distributions F, G are unknown, we may use data samples $\mathcal{D}_F = \{\mathbf{X}_i\}$ and $\mathcal{D}_G = \{\mathbf{Y}_j\}$ where $\mathbf{X}_1, \dots, \mathbf{X}_n \stackrel{\text{iid}}{\sim} F$ and $\mathbf{Y}_1, \dots, \mathbf{Y}_m \stackrel{\text{iid}}{\sim} G$, then construct empirical distributions \hat{F}_n, \hat{G}_m . With this, we may examine the empirical DD plot

$$\text{DD}(\hat{F}_n, \hat{G}_m) = \{(D(\mathbf{z}, \hat{F}_n), D(\mathbf{z}, \hat{G}_m)) : \mathbf{z} \in \mathcal{D}_F \cup \mathcal{D}_G\}. \quad (2.3.2)$$

DD plots can be used as a diagnostic tool to detect differences in location and scale between two multivariate distributions.

1. If $F = G$, the points in $\text{DD}(\hat{F}_n, \hat{G}_m)$ stay close to the diagonal. See Figure 2.2.



Figure 2.2: Empirical DD plot using spatial depth, where both underlying distributions (bivariate normal) are identical. Observe how the points in the DD plot stay close to the diagonal black line.

2. If the same point \mathbf{z}_0 achieves maximum depths with respect to both distributions F and G , this indicates that \mathbf{z}_0 is their common center. See Figure 2.3.
3. Suppose that F and G have the same center. If the points in $\text{DD}(\hat{F}_n, \hat{G}_m)$ arch above the diagonal, i.e. the bulk of points are deeper in G than in F , this indicates that F has a greater spread than G . See Figure 2.4a.

Liu et al. (1999) also demonstrate the use of DD plots to detect differences in skewness and kurtosis. This tool is especially convenient since the DD plot is always two dimensional regardless of the dimension d of the sample points.

2.4 Testing

We are mainly interested in the two sample homogeneity test. Given samples from F and G , we wish to test the null hypothesis $H_0 : F = G$ against an alternate hypothesis that F and G differ in location or scale.

When F, G are distributions on \mathbb{R} , rank based tests such as the Wilcoxon rank-sum test or the Siegel-Tukey test are readily available. A very useful tool in this setting is the probability integral transform.

Proposition 2.4.1. *Let $\mathbf{X} \sim F$, and let the distribution F be continuous. Then, $F(\mathbf{X}) \sim \mathcal{U}[0, 1]$.*

Since $F(\mathbf{X}_j)$ has the same rank within $\{F(\mathbf{X}_i)\}$ as does \mathbf{X}_j within $\{\mathbf{X}_i\}$, the above result is the key towards establishing many distribution-free tests and procedures.

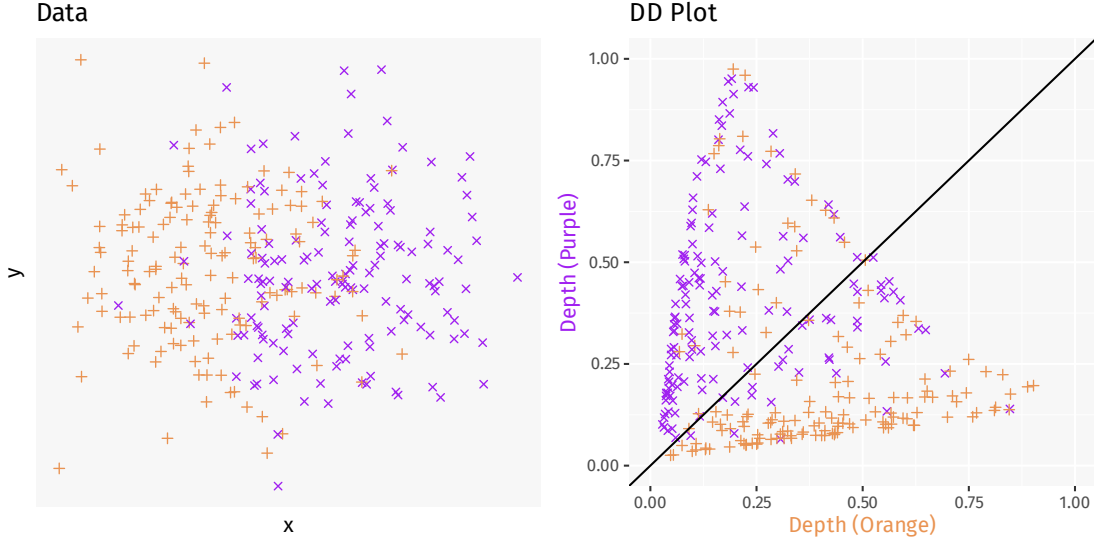


Figure 2.3: Empirical DD plot using spatial depth, where both underlying distributions (bivariate normal) differ only in location. Observe how most of the orange points fall in the lower triangle, while the purple ones fall in the upper triangle. The deepest point with respect to the orange distribution has fairly low depth with respect to the purple one, and vice versa.

In the multivariate setting, Liu and Singh (1993) use the following depth based analogue.

Definition 2.4.2. Denote

$$R(\mathbf{z}, F) = P_{\mathbf{X} \sim F}(D(\mathbf{X}, F) \leq D(\mathbf{z}, F)). \quad (2.4.1)$$

Note that in the empirical setting, $R(\mathbf{z}, \hat{F}_n)$ is simply the proportion of sample points $\{\mathbf{X}_i\}$ which are deeper in F than \mathbf{z} .

Proposition 2.4.3 (Liu and Singh, 1993). *Let $\mathbf{X} \sim F$, and let the distribution of $D(\mathbf{X}, F)$ be continuous. Then, $R(\mathbf{X}, F) \sim \mathcal{U}[0, 1]$.*

Definition 2.4.4. Denote the quality index

$$Q(F, G) = P(D(\mathbf{X}, F) \leq D(\mathbf{Y}, F) \mid \mathbf{X} \sim F, \mathbf{Y} \sim G). \quad (2.4.2)$$

Note that $Q(F, G)$ and $Q(G, F)$ are not necessarily the same. We may also write

$$Q(F, G) = \mathbb{E}_{\mathbf{Y} \sim G}[R(\mathbf{Y}, F)]. \quad (2.4.3)$$

It is clear that $Q(F, G) = 1/2$ when $F = G$. It can be shown under special circumstances that $Q(F, G) < 1/2$ if F, G differ in terms of location or scale. This will form the basis of our testing scheme, with $H_0 : F = G$ versus $H_A : Q(F, G) < 1/2$.

Here, we restrict our attention to elliptical distributions on \mathbb{R}^d .



Figure 2.4: Empirical DD plot using spatial depth, where both underlying distributions (bivariate normal) differ only in scale. In (a), observe how the points remain in the upper triangle in the DD plot. In (b), observe how there are more orange points in the lower triangle, and more purple points in the upper triangle in the DD plot, especially in the region close to the origin.

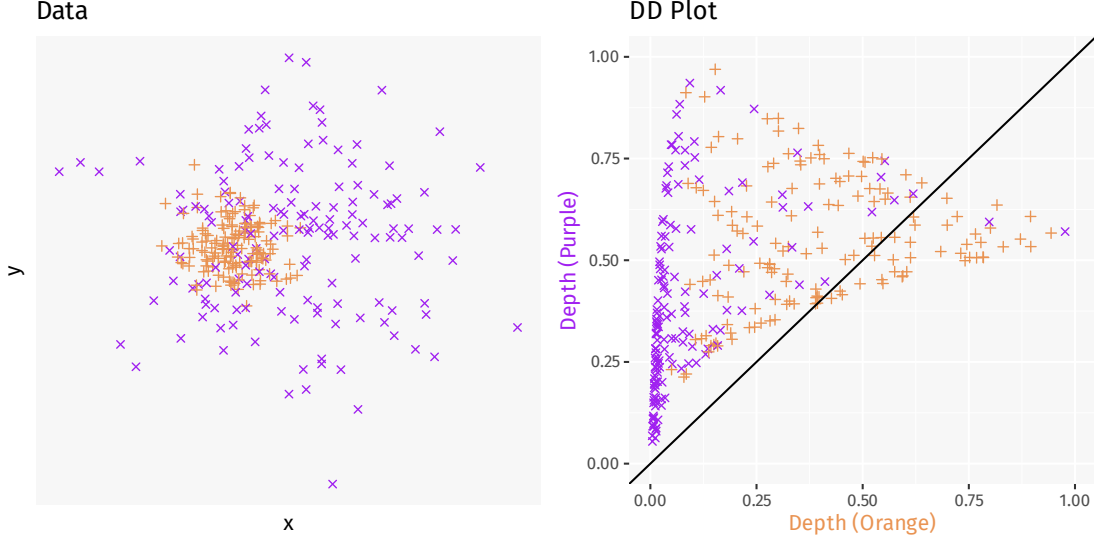


Figure 2.5: Empirical DD plot using spatial depth, where both underlying distributions (bivariate normal) differ in both location and scale. Observe that there is a clear separation between the orange and purple points in the DD plot, although not about the diagonal line.

Definition 2.4.5 (Elliptical distributions). We say that a distribution is elliptical if it has a density of the form

$$f(\mathbf{x}) = c |\Sigma|^{-1/2} h((\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu})) \quad (2.4.4)$$

for some non-increasing function h . This is denoted by $\text{Ell}(h; \boldsymbol{\mu}, \Sigma)$.

The quality index obeys the following properties.

Proposition 2.4.6 (Liu and Singh, 1993). Let $F \sim \text{Ell}(h; \boldsymbol{\mu}_1, \Sigma_1)$ and $G \sim \text{Ell}(h; \boldsymbol{\mu}_2, \Sigma_2)$ where $\Sigma_1 - \Sigma_2$ is positive definite. Further suppose that $D(\cdot, F)$ has the affine invariance and monotonicity properties. Then, $Q(F, G) \leq 1/2$ decreases monotonically as $\boldsymbol{\mu}_2$ is moved away from $\boldsymbol{\mu}_1$ along any line.

Proposition 2.4.7 (Liu and Singh, 1993). Let $F \sim \text{Ell}(h; \boldsymbol{\mu}, \Sigma_1)$ and $G \sim \text{Ell}(h; \boldsymbol{\mu}, \Sigma_2)$ where $\Sigma_1 - \Sigma_2$ is positive definite. Consider Huber's contamination of the form

$$G_\alpha = (1 - \alpha)F + \alpha G \quad (2.4.5)$$

where $0 \leq \alpha \leq 1$. Then, $Q(F, G_\alpha)$ decreases monotonically as α increases.

This motivates a modified Wilcoxon rank-sum test in the multivariate setting, using the quality index $Q(F, G)$. Let $\mathbf{X}_1, \dots, \mathbf{X}_n \stackrel{\text{iid}}{\sim} F$, and $\mathbf{Y}_1, \dots, \mathbf{Y}_m \stackrel{\text{iid}}{\sim} G$. Since $R(\cdot, F), Q(F, \cdot)$ depend on $D(\cdot, F)$, the latter has to be approximated using $D(\cdot, \hat{F}_{n_0})$, where \hat{F}_{n_0} is based on a (fairly large) additional sample $\mathbf{Z}_1, \dots, \mathbf{Z}_{n_0} \stackrel{\text{iid}}{\sim} F$, with $n_0 \gg n, m$. With this, we compute

$$R(\cdot, \hat{F}_{n_0}) = \frac{1}{n_0} \sum_{i=1}^{n_0} \mathbf{1}(D(\mathbf{Z}_i, \hat{F}_{n_0}) \leq D(\cdot, \hat{F}_{n_0})). \quad (2.4.6)$$

Assign ranks $1, \dots, n+m$ to the arranged values $R(\mathbf{X}_i, \hat{F}_{n_0}), R(\mathbf{Y}_j, \hat{F}_{n_0})$ (ascending order), and define W to be the sum of ranks of the $R(\mathbf{Y}_j, \hat{F}_{n_0})$. If necessary, break ties at random. Under the null hypothesis $F = G$, it is clear that W has the same distribution as the sum of m numbers drawn without replacement from $\{1, \dots, n+m\}$. Under the alternate hypothesis $Q(F, G) < 1/2$, the ranks of $R(\mathbf{Y}_j, \hat{F}_{n_0})$ will tend to be lower on average, making W smaller.

Theorem 2.4.8 (Liu and Singh, 1993). *Let $H_{n,m}$ be the distribution of the sum of m numbers drawn randomly without replacement from $\{1, \dots, n+m\}$. Suppose that F admits a density function f . Under the null hypothesis $F = G$, we have $W \sim H_{n,m}$.*

It is also possible to approximate $Q(F, G)$ more directly via $Q(\hat{F}_n, \hat{G}_m)$ and perform our test this way. This sidesteps the need for the ‘reference’ sample $\mathbf{Z}_1, \dots, \mathbf{Z}_{n_0} \stackrel{\text{iid}}{\sim} F$. Note that

$$Q(\hat{F}_n, \hat{G}_m) = \frac{1}{m} \sum_{j=1}^m R(\mathbf{Y}_j, \hat{F}_n) = \frac{1}{nm} \sum_{i,j} \mathbf{1}(D(\mathbf{X}_i, \hat{F}_n) \leq D(\mathbf{Y}_j, \hat{F}_n)). \quad (2.4.7)$$

This estimate is indeed consistent under mild assumptions.

Theorem 2.4.9 (Liu and Singh, 1993). *Suppose that the distribution of $D(\mathbf{Y}, F)$ is continuous where $\mathbf{Y} \sim G$, and that*

$$\sup_{\mathbf{z} \in \mathbb{R}^d} |D(\mathbf{z}, \hat{F}_n) - D(\mathbf{z}, F)| \xrightarrow{a.s.} 0. \quad (2.4.8)$$

Then, $Q(\hat{F}_n, \hat{G}_n) \xrightarrow{a.s.} Q(F, G)$ as $\min\{n, m\} \rightarrow \infty$.

This allows us to determine the asymptotic null distribution of $Q(\hat{F}_n, \hat{G}_m)$.

Theorem 2.4.10 (Liu and Singh, 1993). *Let F be absolutely continuous, such that $\mathbb{E}_{\mathbf{X} \sim F} \|\mathbf{X}\|^4 < \infty$. Using Mahalanobis depth to define Q , we have*

$$S(\hat{F}_n, \hat{G}_m) = \left[\frac{1}{12} \left(\frac{1}{n} + \frac{1}{m} \right) \right]^{-1/2} \left[Q(\hat{F}_n, \hat{G}_m) - \frac{1}{2} \right] \xrightarrow{d} \mathcal{N}(0, 1) \quad (2.4.9)$$

as $\min\{n, m\} \rightarrow \infty$, under the null hypothesis $F = G$.

Later, Zuo and He (2006) show that under certain mild regularity conditions, the above asymptotic convergence can be extended to a broader class of depth functions, without the assumption $F = G$. They demonstrate that

$$\left[\frac{\sigma_{GF}^2}{n} + \frac{\sigma_{FG}^2}{m} \right]^{-1/2} \left[Q(\hat{F}_n, \hat{G}_m) - Q(F, G) \right] \xrightarrow{d} \mathcal{N}(0, 1), \quad (2.4.10)$$

where

$$\sigma_{FG}^2 = \int P_{\mathbf{X} \sim F}^2(D(\mathbf{X}, F) \leq D(\mathbf{y}, F)) dG(\mathbf{y}) - Q^2(F, G), \quad (2.4.11)$$

$$\sigma_{GF}^2 = \int P_{\mathbf{Y} \sim G}^2(D(\mathbf{x}, F) \leq D(\mathbf{Y}, F)) dF(\mathbf{x}) - Q^2(F, G). \quad (2.4.12)$$

Observe that given two samples, we have a choice between using $Q(\hat{F}_n, \hat{G}_m)$ or $Q(\hat{G}_m, \hat{F}_n)$. It may be advantageous to use the sample with a greater number of observations as the reference distribution. Shi et al. (2023) propose a weighted combination of the form

$$W_{n,m}^\alpha = \alpha S(\hat{F}_n, \hat{G}_m)^2 + (1 - \alpha) S(\hat{G}_m, \hat{F}_n)^2 \quad (2.4.13)$$

for $\alpha \in [0, 1]$, or a maximum

$$M_{n,m} = \max\{S(\hat{F}_n, \hat{G}_m)^2, S(\hat{G}_m, \hat{F}_n)^2\}. \quad (2.4.14)$$

Under similar assumptions, they show that both $W_{n,m}^\alpha \xrightarrow{d} \chi_1^2$ and $M_{n,m} \xrightarrow{d} \chi_1^2$ as $\min\{n, m\} \rightarrow \infty$ and n/m converges to a positive constant, under the null hypothesis $F = G$.

2.5 Classification

The k -class classification task involves assigning an observation \mathbf{x} to one of k populations, described by distributions F_i for $1 \leq i \leq k$. The populations may also be associated with prior probabilities π_i .

Definition 2.5.1 (Classifier). A classifier is a map $\hat{t}: \mathbb{R}^d \rightarrow \{1, \dots, k\}$.

Example 2.5.2 (Bayes classifier). Suppose that the population densities f_i for each $1 \leq i \leq k$ are known. The Bayes classifier assigns \mathbf{x} to the \hat{t}_B -th population where

$$\hat{t}_B(\mathbf{x}) = \arg \max_{1 \leq i \leq k} \pi_i f_i(\mathbf{x}). \quad (2.5.1)$$

One way of measuring the performance of a classifier (given the population distributions and their priors) is by measuring its average misclassification rate.

Definition 2.5.3 (Average misclassification rate). The average misclassification rate of a classifier \hat{t} is given by

$$\Delta(\hat{t}) = \sum_{i=1}^k \pi_i P_{\mathbf{X} \sim F_i}(\hat{t}(\mathbf{X}) \neq i). \quad (2.5.2)$$

Proposition 2.5.4. *The Bayes classifier has the lowest possible average misclassification rate. This is known as the optimal Bayes risk, denoted Δ_B .*

The simplest depth based classifier is the maximum depth classifier (Ghosh & Chaudhuri, 2005).

Example 2.5.5 (Maximum depth classifier). Suppose that the prior probabilities π_i are equal. The maximum depth classifier \hat{t}_D for a choice of depth function D is described by

$$\hat{t}_D(\mathbf{x}) = \arg \max_{1 \leq i \leq k} D(\mathbf{x}, F_i). \quad (2.5.3)$$

In practice, instead of having direct access to the population distributions F_i , we have typically deal with labeled training data

$$\mathcal{D} = \{(\mathbf{x}_{ij}, i)\} \subset \mathbb{R}^d \times \{1, \dots, k\}, \quad (2.5.4)$$

where $\mathbf{x}_{i1}, \dots, \mathbf{x}_{in_i}$ is an instance of an iid sample from F_i for each $1 \leq i \leq k$. The empirical maximum depth classifier simply replaces the population distributions F_i with their empirical counterparts \hat{F}_i determined by $\mathbf{x}_{i1}, \dots, \mathbf{x}_{in_i}$. Thus, it is given by

$$\hat{l}_D(\mathbf{x}) = \arg \max_{1 \leq i \leq k} D(\mathbf{x}, \hat{F}_i). \quad (2.5.5)$$

Under certain restrictions, this classifier becomes asymptotically optimal in the following sense.

Theorem 2.5.6 (Ghosh and Chaudhuri, 2005). *Suppose that the population density functions f_i are elliptically symmetric, with $f_i(\mathbf{x}) = g(\mathbf{x} - \boldsymbol{\mu}_i)$ for parameters $\boldsymbol{\mu}_i$ and a density function g such that $g(k\mathbf{x}) \leq g(\mathbf{x})$ for every \mathbf{x} and $k > 1$. Further suppose that the priors on the populations are equal, and the depth function D is one of HD, SD, MJD, PD. Then, $\Delta(\hat{l}_D) \rightarrow \Delta_B$ as $\min\{n_1, \dots, n_k\} \rightarrow \infty$.*

Note that this result deals with elliptic population densities differing only in location. Relax this assumption, and instead suppose that $f_i \sim \text{Ell}(h_i; \boldsymbol{\mu}_i, \Sigma)$, i.e.

$$f_i(\mathbf{x}) = c_i |\Sigma|^{-1/2} h_i((\mathbf{x} - \boldsymbol{\mu}_i)^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}_i)) \quad (2.5.6)$$

for strictly decreasing h_i , and that the depths can be expressed as $D(\cdot, F_i) = l_i(f_i(\cdot))$ for strictly increasing functions l_i . It follows that the Bayes decision rule can be reformulated as

$$\pi_i f_i(\mathbf{x}) > \pi_j f_j(\mathbf{x}) \iff D(\mathbf{x}, F_i) > r_{ij}(D(\mathbf{x}, F_j)) \quad (2.5.7)$$

for some real increasing function r_{ij} . Using this observation, the DD classifier (Li et al., 2012) picks separating functions r_{ij} which best classify the training data \mathcal{D} .

Definition 2.5.7 (Empirical misclassification rate). The empirical misclassification rate of a classifier \hat{l} , with respect to data \mathcal{D} , is given by

$$\hat{\Delta}(\hat{l}) = \sum_{i=1}^k \frac{\pi_i}{n_i} \sum_{j=1}^{n_i} \mathbf{1}(\hat{l}(\mathbf{x}_{ij}) \neq i). \quad (2.5.8)$$

Definition 2.5.8 (DD classifier). Suppose that $k = 2$, that D is a depth function, and that $r: [0, 1] \rightarrow [0, 1]$ is an increasing function. The DD classifier $\hat{l}_{D,r}$ is given by

$$\hat{l}_{D,r}(\mathbf{x}) = \begin{cases} 1, & \text{if } D(\mathbf{x}, F_2) \leq r(D(\mathbf{x}, F_1)), \\ 2, & \text{if } D(\mathbf{x}, F_2) > r(D(\mathbf{x}, F_1)). \end{cases} \quad (2.5.9)$$

The empirical DD classifier $\hat{l}_{D,\hat{r}}$ replaces F_i by their empirical counterparts \hat{F}_i . Here, the separating curve \hat{r} is chosen from a family Γ so as to minimize the empirical misclassification rate, i.e.

$$\hat{r} = \arg \min_{r \in \Gamma} \hat{\Delta}(\hat{l}_{D,r}). \quad (2.5.10)$$

Remark. The maximum depth classifier $\hat{\iota}_D$ is simply the DD classifier $\hat{\iota}_{D,\text{id}}$, where $\text{id}(x) = x$. Figure 2.5 clearly illustrates how this choice of separating function may not always be appropriate.

Li et al. (2012) show that under certain restrictions, the empirical DD classifier is asymptotically equivalent to the Bayes rule. We give one such instance below.

Lemma 2.5.9. *Suppose that the following conditions hold.*

1. Γ is the class of polynomial functions on $[0, 1]$.
2. The depth functions $D(\cdot, F_i)$ are continuous.
3. As $\min\{n_1, n_2\} \rightarrow \infty$, we have for each $i \in \{1, 2\}$,

$$\sup_{\mathbf{z} \in \mathbb{R}^d} |D(\mathbf{z}, \hat{F}_i) - D(\mathbf{z}, F_i)| \xrightarrow{a.s.} 0. \quad (2.5.11)$$

4. The distributions F_i are elliptical and satisfy for all $\delta \in \mathbb{R}$

$$P_{\mathbf{Z} \sim F_i}(D(\mathbf{Z}, F_i) = \delta) = 0. \quad (2.5.12)$$

Then, $\Delta(\hat{\iota}_{D,\hat{r}}) \rightarrow \Delta_B$ as $\min\{n_1, n_2\} \rightarrow \infty$.

In all the depth based classifiers we have seen so far, the classification rule depends on the observation \mathbf{x} only through the depths $D(\mathbf{x}, F_i)$. Thus, we are motivated to define the following transformation from \mathbb{R}^d to a depth feature space.

Definition 2.5.10. The depth feature vector \mathbf{x}^D of an observation \mathbf{x} , with respect to the population distributions F_i and a choice of depth function D , is defined as

$$\mathbf{x}^D = (D(\mathbf{x}, F_1), \dots, D(\mathbf{x}, F_k)). \quad (2.5.13)$$

Remark. The graph

$$\text{DD}(F_1, \dots, F_k) = \{\mathbf{x}^D : \mathbf{x} \in \mathbb{R}^d\} \quad (2.5.14)$$

is the analogue of the **DD plot**, with k distributions.

Assuming that the depth function D only takes values in $[0, 1]$, the map $\mathbf{x} \mapsto \mathbf{x}^D$ takes values in $[0, 1]^k$, regardless of the dimensionality of the original vector \mathbf{x} . With this, the maximum depth classification rule can be expressed as

$$\hat{\iota}_D(\mathbf{x}) = i \iff \mathbf{x}^D \in R_i^D = \{\mathbf{y} \in [0, 1]^k : y_i = \max_j y_j\}. \quad (2.5.15)$$

Indeed, any partition of the unit cube $[0, 1]^k$ into k decision regions R_i^D gives rise to a depth based classifier. The DD classifier achieves this by using an increasing separating function r to partition $[0, 1]^2$. Furthermore, $r \in \Gamma$ is chosen so as to best separate the training data \mathcal{D} transformed into the depth feature space. However, we can in principle use the transformed training data

$$\mathcal{D}^D = \{(\mathbf{x}_{ij}^D, i)\} \subset [0, 1]^k \times \{1, \dots, k\} \quad (2.5.16)$$

along with any multivariate classification algorithm (LDA, QDA, k NN, GLM, etc) to devise suitable decision regions. This is the basis of the DD^G classifier (Cuesta-Albertos et al., 2017).

2.6 Clustering

The unsupervised clustering grouping a collection of observations, such that points within the same group are more similar to each other than those from different groups.

Definition 2.6.1 (Clustering). Given observations $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^d$, a clustering assignment is a choice of a partition I_1, \dots, I_K of $\{1, \dots, N\}$.

With this notation, the k -th cluster consists of the points $\{\mathbf{x}_i\}_{i \in I_k}$. A good cluster assignment is one that maximizes similarity within clusters, as well as dissimilarity between clusters. Thus, the problem of clustering can be framed as the optimization of some objective function which combines these notions of similarity and dissimilarity. A simple algorithm such as the K -means clustering seeks to minimize

$$\{I_1, \dots, I_K\} \mapsto \frac{1}{N} \sum_{k=1}^K \sum_{i \in I_k} \|\mathbf{x}_i - \boldsymbol{\mu}_k\|^2, \quad (2.6.1)$$

the average sum of square distances between each point and its cluster mean

$$\boldsymbol{\mu}_k = \frac{1}{|I_k|} \sum_{i \in I_k} \mathbf{x}_i = \arg \min_{\boldsymbol{\mu} \in \mathbb{R}^d} \sum_{i \in I_k} \|\mathbf{x}_i - \boldsymbol{\mu}\|^2. \quad (2.6.2)$$

Jörnsten (2004) proposes a depth based approach to this problem, by examining the depth of a point within its cluster, relative to its depth within the best competing cluster.

In this section, we will abbreviate $D_k(\mathbf{x}) = D(\mathbf{x}, \hat{F}_{I_k})$, i.e. the empirical depth of \mathbf{x} with respect to the points in the k -th cluster. Jörnsten (2004) chooses L_1 depth, the empirical version of spatial depth.

Definition 2.6.2. The within cluster depth of \mathbf{x}_i is $D_i^w = D_k(\mathbf{x}_i)$, where $i \in I_k$.

To deal with dissimilarity between clusters, we represent each cluster by its L_1 -median.

Definition 2.6.3 (L_1 -median). The L_1 -median of the k -th cluster is given by

$$\boldsymbol{\theta}_k = \arg \min_{\boldsymbol{\theta} \in \mathbb{R}^d} \sum_{i \in I_k} \|\mathbf{x}_i - \boldsymbol{\theta}\|. \quad (2.6.3)$$

Definition 2.6.4. The between cluster depth of \mathbf{x}_i is $D_i^b = D_\ell(\mathbf{x}_i)$, where

$$\ell = \arg \min_{k: i \notin I_k} \|\mathbf{x}_i - \boldsymbol{\theta}_k\|. \quad (2.6.4)$$

In other words, the between cluster depth of \mathbf{x}_i is its depth within the best competing cluster.

Definition 2.6.5 (Relative depth). The relative depth of \mathbf{x}_i is $\text{ReD}_i = D_i^w - D_i^b$.

A point \mathbf{x}_i is *well clustered* if ReD_i is very high, i.e. it is deep within its own cluster, and has low depth with respect to its next best competing cluster. Thus, to obtain a good clustering, we may choose to maximize the objective function

$$\{I_1, \dots, I_K\} \mapsto \frac{1}{N} \sum_{k=1}^K \sum_{i \in I_k} \text{ReD}_i, \quad (2.6.5)$$

which is simply the average relative depth. This maximization can be achieved iteratively, starting with a random cluster assignment and reassigning a subset of observations with low ReD_i to their nearest competing clusters. The reassignment is accepted if the objective function increases, and the process is repeated. Jörnsten (2004) also suggests the use of simulated annealing to overcome the problem of getting trapped in local maxima. Here, the reassignment is accepted with some probability $P(\beta, \delta)$ where δ is the change in the objective function value, even if the objective function decreases at that step. $P(\beta, \delta)$ is chosen to decrease with increasing β and δ . The tuning parameter β can be increased every iteration so that the probability of accepting poorer clustering assignments drops to zero eventually.

Another notion of similarity and dissimilarity involves *silhouette width*.

Definition 2.6.6 (Silhouette width). Denote the average distance of \mathbf{z} from points in the k -th cluster not equal to \mathbf{z} by

$$\bar{d}_k(\mathbf{z}) = \frac{1}{|\{i \in I_k : \mathbf{x}_i \neq \mathbf{z}\}|} \sum_{\substack{i \in I_k \\ \mathbf{x}_i \neq \mathbf{z}}} \|\mathbf{x}_i - \mathbf{z}\|. \quad (2.6.6)$$

The silhouette width of \mathbf{x}_i where $i \in I_k$ is given by

$$\text{Sil}_i = \frac{b_i - a_i}{\max\{a_i, b_i\}}, \quad a_i = \bar{d}_k(\mathbf{x}_i), \quad b_i = \min_{\ell \neq k} \bar{d}_\ell(\mathbf{x}_i). \quad (2.6.7)$$

It has been observed that the silhouette width is greatly affected by differences in scale between clusters, while the relative depth is not. An objective function of the form

$$\{I_1, \dots, I_K\} \mapsto \frac{1}{N} \sum_{k=1}^K \sum_{i \in I_k} (1 - \lambda) \text{Sil}_i + \lambda \text{ReD}_i \quad (2.6.8)$$

may be used to combine both notions. Here, $\lambda \in [0, 1]$ controls the influence of the relative depth. It seems that small values of λ encourages equal scale clusters, while large values of λ allows unequal scale clusters. Thus, λ may be tuned accordingly to favour these different kinds of clustering assignments.

Chapter 3

FUNCTIONAL DATA

Consider a class of functions \mathcal{X} of the form $\mathbf{x}: [0, 1] \rightarrow \mathbb{R}^d$, and let \mathcal{F} be a suitable class of distributions on \mathcal{X} .

It is desirable for a depth function $D: \mathcal{X} \times \mathcal{F} \rightarrow \mathbb{R}$ to satisfy the following properties (Gijbels & Nagy, 2017).

P0. *Non-degeneracy.* For $F \in \mathcal{F}$,

$$\inf_{\mathbf{x} \in \mathcal{X}} D(\mathbf{x}, F) < \sup_{\mathbf{x} \in \mathcal{X}} D(\mathbf{x}, F). \quad (3.0.1)$$

The property **P0** requires some care; the natural functional analogue to half-space/Tukey depth when \mathcal{X} is a Hilbert space,

$$D_H(\mathbf{x}, F) = \inf_{\mathbf{v} \in \mathcal{X}} P_{\mathbf{X} \sim F}(\langle \mathbf{v}, \mathbf{X} \rangle \leq \langle \mathbf{v}, \mathbf{x} \rangle), \quad (3.0.2)$$

turns out to be degenerate for a wide class of distributions \mathcal{F} (Chakraborty & Chaudhuri, 2014a).

3.1 Functional depth functions

Let D be a multivariate depth function. We can use this to define functional depths as follows.

Definition 3.1.1 (Fraiman-Muniz depth). The integrated depth, or Fraiman-Muniz depth, is defined as

$$D_F(\mathbf{x}, F_{\mathbf{X}}) = \int_{[0,1]} D(\mathbf{x}(t), F_{\mathbf{X}(t)}) w(t) dt. \quad (3.1.1)$$

Here, w is a weight function.

Definition 3.1.2 (Infimal depth). The infimal depth is defined as

$$D_{Inf}(\mathbf{x}, F_{\mathbf{X}}) = \inf_{t \in [0,1]} D(\mathbf{x}(t), F_{\mathbf{X}(t)}). \quad (3.1.2)$$

For $\mathcal{X} = L_2$, the spatial depth has its natural functional analogue.

Definition 3.1.3 (Functional spatial depth). The spatial depth for $\mathcal{X} = L_2$ is defined as

$$D_S(\mathbf{x}, F_{\mathbf{X}}) = 1 - \left\| \mathbb{E}_{\mathbf{X} \sim F} \left[\frac{\mathbf{x} - \mathbf{X}}{\|\mathbf{x} - \mathbf{X}\|_2} \right] \right\|_2, \quad (3.1.3)$$

where $\|\cdot\|_2$ denotes the standard L_2 norm.

López-Pintado and Romo (2009) later introduced the notion of band depth for univariate functional data.

Definition 3.1.4 (Band depth). The band depth, for some index $J \geq 2$, is defined as

$$D_B^J(\mathbf{x}, F_{\mathbf{X}}) = \sum_{j=2}^J P_{\mathbf{X}_i \stackrel{\text{iid}}{\sim} F_{\mathbf{X}}}(\mathbf{x} \in \text{conv}(\mathbf{X}_1, \dots, \mathbf{X}_j)). \quad (3.1.4)$$

The empirical version of band depth is defined as

$$D_B^J(\mathbf{x}, \hat{F}_n) = \sum_{j=2}^J \binom{n}{j}^{-1} \sum_{1 \leq i_1 < \dots < i_j \leq n} \mathbf{1}(\mathbf{x} \in \text{conv}(\mathbf{x}_{i_1}, \dots, \mathbf{x}_{i_j})). \quad (3.1.5)$$

This is simply the proportion of j -tuples of curves (for $2 \leq j \leq J$) which envelope \mathbf{x} .

Definition 3.1.5 (Modified band depth). Define the enveloping time

$$ET(\mathbf{x}; \mathbf{x}_1, \dots, \mathbf{x}_j) = m_1(\{t \in [0, 1] : \mathbf{x} \in \text{conv}(\mathbf{x}_1, \dots, \mathbf{x}_j)\}), \quad (3.1.6)$$

where m_1 is the Lebesgue measure on \mathbb{R} . The modified band depth is defined as

$$D_{MB}^J(\mathbf{x}, F_{\mathbf{X}}) = \sum_{j=2}^J \mathbb{E}_{\mathbf{X}_i \stackrel{\text{iid}}{\sim} F_{\mathbf{X}}} [ET(\mathbf{x}; \mathbf{X}_1, \dots, \mathbf{X}_j)]. \quad (3.1.7)$$

The empirical version of modified band depth is defined as

$$D_{MB}^J(\mathbf{x}, \hat{F}_n) = \sum_{j=2}^J \binom{n}{j}^{-1} \sum_{1 \leq i_1 < \dots < i_j \leq n} ET(\mathbf{x}; \mathbf{x}_{i_1}, \dots, \mathbf{x}_{i_j}). \quad (3.1.8)$$

Definition 3.1.6. We say that \mathbf{y} is in the hypograph of \mathbf{x} , denoted, $\mathbf{y} \in H_{\mathbf{x}}$, if $\mathbf{y}(t) \leq \mathbf{x}(t)$ for all $t \in [0, 1]$. Similarly, we say that \mathbf{y} is in the epigraph of \mathbf{x} , denoted, $\mathbf{y} \in E_{\mathbf{x}}$, if $\mathbf{y}(t) \geq \mathbf{x}(t)$ for all $t \in [0, 1]$.

Definition 3.1.7 (Half-region depth). The half-region depth is defined as

$$D_{HR}(\mathbf{x}, F) = \min\{P_F(H_{\mathbf{x}}), P_F(E_{\mathbf{x}})\}. \quad (3.1.9)$$

3.2 Classification

Observe that the classification procedures for multivariate data described in Section 2.5 (the maximum depth classifier, the DD classifier, and the DD^G classifier) only depend on the data through the depth feature vectors

$$\mathbf{x}^D = (D(\mathbf{x}, F_1), \dots, D(\mathbf{x}, F_k)) \in \mathbb{R}^k. \quad (3.2.1)$$

By simply choosing an appropriate functional data depth D , all of these classification procedures naturally generalize to the functional setting.

Dai and Genton (2018) proposed a method which measures the outlyingness of \mathbf{x} with respect to a population via depth as follows.

Definition 3.2.1. Let \mathbf{X} be a d -variate stochastic process of continuous functions. At each time point $t \in [0, 1]$, the directional outlyingness is defined as

$$\mathbf{O}(t) = \mathbf{O}(\mathbf{X}(t), F_{\mathbf{X}(t)}) = \left(\frac{1}{D(\mathbf{X}(t), F_{\mathbf{X}(t)})} - 1 \right) \mathbf{v}(t), \quad (3.2.2)$$

where $\mathbf{v}(t)$ is the unit vector pointing from the median of $F_{\mathbf{X}(t)}$ to $\mathbf{X}(t)$.

Definition 3.2.2. The functional directional outlyingness is defined as

$$\text{FO}(\mathbf{X}, F_{\mathbf{X}}) = \int_{[0,1]} \|\mathbf{O}(t)\|^2 w(t) dt. \quad (3.2.3)$$

Definition 3.2.3. The mean directional outlyingness is defined as

$$\mathbf{MO}(\mathbf{X}, F_{\mathbf{X}}) = \int_{[0,1]} \mathbf{O}(t) w(t) dt. \quad (3.2.4)$$

Definition 3.2.4. The variation of directional outlyingness is defined as

$$\text{VO}(\mathbf{X}, F_{\mathbf{X}}) = \int_{[0,1]} \|\mathbf{O}(t) - \mathbf{MO}(t)\|^2 w(t) dt. \quad (3.2.5)$$

Here, w is a weight function on $[0, 1]$. In our discussion, we set $w = 1$.

It is easily verified that

$$\text{FO}^2 = \|\mathbf{MO}\|^2 + \text{VO}. \quad (3.2.6)$$

Dai and Genton (2018) propose using the $(d + 1)$ -variate feature vectors

$$\mathbf{Y}(\mathbf{X}, F_{\mathbf{X}}) = (\mathbf{MO}^\top, \text{VO})^\top \quad (3.2.7)$$

corresponding to the curve \mathbf{X} for the purposes of classification. For instance, one may define the classifier

$$\hat{i}(\mathbf{X}) = \hat{i}_{D'}(\mathbf{Y}(\mathbf{X}, F_i)) = \arg \max_{1 \leq i \leq k} D'(\mathbf{Y}(\mathbf{X}, F_i), F_{\mathbf{Y}(\mathbf{X}, F_i)}), \quad (3.2.8)$$

where D' is a multivariate depth function. This is simply a maximum depth classifier applied on the feature vectors \mathbf{Y} . When D' is chosen to be the robust Mahalanobis depth, we have the classifier

$$\hat{l}_{RM}(\mathbf{X}) = \arg \max_{1 \leq i \leq k} D_{RM}(\mathbf{Y}(\mathbf{X}, F_i), F_{\mathbf{Y}(\mathbf{X}, F_i)}). \quad (3.2.9)$$

Definition 3.2.5. The functional directional outlyingness matrix is defined as

$$\text{FOM}(\mathbf{X}, F_{\mathbf{X}}) = \int_{[0,1]} \mathbf{O}(t) \mathbf{O}(t)^\top w(t) dt. \quad (3.2.10)$$

Definition 3.2.6. The functional directional outlyingness matrix is defined as

$$\text{VOM}(\mathbf{X}, F_{\mathbf{X}}) = \int_{[0,1]} (\mathbf{O}(t) - \mathbf{MO}(t)) (\mathbf{O}(t) - \mathbf{MO}(t))^\top w(t) dt. \quad (3.2.11)$$

Again, it is easily verified that

$$\text{FOM} = \mathbf{MO} \mathbf{MO}^\top + \text{VOM}, \quad (3.2.12)$$

and that

$$\text{FO} = \text{trace}(\text{FOM}), \quad \text{VO} = \text{trace}(\text{VOM}). \quad (3.2.13)$$

We may also use the feature matrix VOM, or its matrix norm $\|\text{VOM}\|_F$ corresponding to the curve \mathbf{X} for the purposes of classification. Here, $\|\cdot\|_F$ denotes the Frobenius norm. For instance, a VOM based classifier may be defined as

$$\hat{l}_{\text{VOM}}(\mathbf{X}) = \arg \min_{1 \leq i \leq k} \|\text{VOM}(\mathbf{X}, F_i)\|_F. \quad (3.2.14)$$

Another approach is to use a feature vector consisting of multiple projections of \mathbf{X} . Given functions $\mathbf{v}_1, \dots, \mathbf{v}_d$ chosen at random, we examine the d -variate feature vectors

$$\mathbf{Z}(\mathbf{X}) = (\langle \mathbf{v}_1, \mathbf{X} \rangle, \dots, \langle \mathbf{v}_d, \mathbf{X} \rangle) \quad (3.2.15)$$

and apply a depth based multivariate classifier.

3.3 Outlier detection

3.4 Partially observed functional data

Consider the setting where the stochastic process \mathbf{X} of continuous functions is not observed on the entire interval $[0, 1]$, but rather on a random subset $O \subseteq [0, 1]$. Then, a dataset of partially observed curves is of the form $\mathcal{D} = \{(\mathbf{X}_i, O_i)\}_{i=1}^n$, where $\mathbf{X}_i \stackrel{\text{iid}}{\sim} F_{\mathbf{X}}$, $O_i \stackrel{\text{iid}}{\sim} Q$ where Q generates random compact subsets of $[0, 1]$,

independent of \mathbf{X}_i . In other words, $(\mathbf{X}_i, O_i) \stackrel{\text{iid}}{\sim} F_{\mathbf{X}} \times Q$. This setup is known as the ‘Missing Completely at Random’ assumption.

We set $\mathcal{J}(t) = \{j: t \in O_j\}$ to keep track of which curves \mathbf{X}_i have been observed at time t . Furthermore, denote $q(t) = |\mathcal{J}(t)|$ as the number of curves \mathbf{X}_i observed at time t .

Elías, Jiménez, Paganoni, and Sangalli (2023) propose the following.

Definition 3.4.1 (Partially observed integrated functional depth). Let D be a d -variate depth function. The Partially Observed Integrated Functional Depth (POIFD) is defined as

$$D_{POIFD}((\mathbf{x}, o), F_{\mathbf{X}} \times Q) = \int_o D(\mathbf{x}(t), F_{\mathbf{X}(t)}) w_o(t) dt, \quad (3.4.1)$$

where $w_o(t) = q(t) / \int_o q(t) dt$.

We can now proceed with tasks such as classification, outlier detection, etc. on our partially observed dataset, via depth based procedures using POIFD values. Another natural problem is one of curve reconstruction: given a partially observed curve (\mathbf{X}, O) , can we estimate \mathbf{X} on $M = [0, 1] \setminus O$? For instance, we may search for a reconstruction operator $\mathcal{R}: L_2(O) \rightarrow L_2(M)$ that minimizes the mean integrated prediction squared error $\mathbb{E}[\|\mathbf{X}_M - \mathcal{R}(\mathbf{X}_O)\|^2]$. Here, \mathbf{X}_O denotes the curve \mathbf{X} restricted to O , and similarly for \mathbf{X}_M . The best predictor in this sense is the conditional expectation $\mathbb{E}[\mathbf{X}_M | \mathbf{X}_O]$, which is in general a non-linear operator. Thus, Kraus (2015) and Kneip and Liebl (2020) search for continuous linear operators \mathcal{A} , using methods based on estimating terms of the Karhunen-Loève expansion of \mathbf{X} .

Elías, Jiménez, and Shang (2023) offer a depth based solution to the reconstruction problem, adapted from a similar algorithm for time-series forecasting (Elías et al., 2022). The main idea involves selecting a collection of curves, with indices \mathcal{J} , which best envelope (\mathbf{X}, O) , then taking a weighted linear combination. In particular, they suggest

$$\hat{\mathbf{X}}(t) = \frac{\sum_{i \in \mathcal{J}(t)} w_i \mathbf{X}_i(t)}{\sum_{i \in \mathcal{J}(t)} w_i}, \quad w_i = \exp\left(-\theta \frac{\|(\mathbf{X}, O) - (\mathbf{X}_i, O_i)\|}{\delta}\right), \quad (3.4.2)$$

where $\mathcal{J}(t) = \mathcal{J} \cap \mathcal{J}(t) = \{i \in \mathcal{J}: t \in O_i\}$ and $\delta = \min_{i \in \mathcal{J}} \|(\mathbf{X}, O) - (\mathbf{X}_i, O_i)\|$. Here, θ is a tuning parameter, perhaps chosen by minimizing the mean squared error on (\mathbf{X}, O) . Furthermore, we have denoted

$$\|(\mathbf{X}, O) - (\mathbf{X}', O')\| = \frac{1}{m(O \cap O')} \left(\int_{O \cap O'} \|\mathbf{X}(t) - \mathbf{X}'(t)\|^2 dt \right)^{1/2}. \quad (3.4.3)$$

Choosing the best envelope \mathcal{J} involves both depth and distance. Elías, Jiménez, and Shang (2023) use the following three criteria to devise an algorithm that iteratively selects \mathcal{J} .

1. (\mathbf{X}, O) should be as deep as possible in the collection of curves $\{(\mathbf{X}, O)\} \cup \{(\mathbf{X}_i, O_i)\}_{i \in \mathcal{I}}$, in the sense of POIFD.
2. (\mathbf{X}, O) should be enveloped by $\{(\mathbf{X}_i, O_i)\}_{i \in \mathcal{I}}$ as much as possible, i.e. we want to maximize the enveloping time $ET((\mathbf{X}, O); \{\mathbf{X}_i, O_i\}_{i \in \mathcal{I}})$.
3. $\{(\mathbf{X}_i, O_i)\}_{i \in \mathcal{I}}$ should contain as many near curves to (\mathbf{X}, O) as possible, in the sense of the distance 3.4.3.

Chapter 4

LOCAL DEPTH

4.1 Local depth regions

Given a distribution $F_{\mathbf{X}}$, we may define a symmetrized distribution about a point $\mathbf{x} \in \mathcal{X}$ as

$$F_{\mathbf{X}}^{\mathbf{x}} = \frac{1}{2}F_{\mathbf{X}} + \frac{1}{2}F_{2\mathbf{x}-\mathbf{X}}. \quad (4.1.1)$$

With this, \mathbf{x} becomes the point of central symmetry, hence the deepest point in $F_{\mathbf{X}}^{\mathbf{x}}$ with respect to a depth function D that obeys **P2**. Thus, the β -th central regions of $F_{\mathbf{X}}^{\mathbf{x}}$ behave like neighbourhoods of \mathbf{x} .

Definition 4.1.1 (Paindaveine and Van Bever, 2013). The probability- β depth-based neighbourhood of \mathbf{x} with respect to the distribution F is defined as

$$N_{\beta}^{\mathbf{x}}(F) = C_{F^{\mathbf{x}}}(\beta), \quad (4.1.2)$$

i.e. the β -th central region of F symmetrized about \mathbf{x} .

When working with a sample $\mathcal{D} = \{\mathbf{X}_i\}_{i=1}^n$ from F , we may obtain the β depth-based neighbourhood of \mathbf{x} by first computing the reflected sample $\mathcal{D}' = \{2\mathbf{x} - \mathbf{X}_i\}_{i=1}^n$, then arranging the elements of the symmetrized sample $\mathcal{D}^{\mathbf{x}} = \mathcal{D} \cup \mathcal{D}'$ in descending order by their empirical depth values and choosing the first β proportion of elements. The neighbourhood $N_{\beta}^{\mathbf{x}}(\hat{F}_n)$ is the convex hull of these elements.

Definition 4.1.2 (Paindaveine and Van Bever, 2013). Let D be a depth function, and let $F_{\beta}^{\mathbf{x}}$ denote the distribution F conditional on the neighbourhood $N_{\beta}^{\mathbf{x}}(F)$. The corresponding local depth function at locality level $\beta \in (0, 1]$ is defined as

$$LD_{\beta}(\mathbf{x}, F) = D(\mathbf{x}, F_{\beta}^{\mathbf{x}}) \quad (4.1.3)$$

Again, when working with a sample $\mathcal{D} = \{\mathbf{X}_i\}_{i=1}^n$, we obtain $LD_{\beta}(\mathbf{x}, \hat{F}_n)$ by arranging the elements of \mathcal{D} in descending order by their empirical depth values in the symmetrized sample $\mathcal{D}^{\mathbf{x}}$, choosing the first β proportion of elements, and computing the depth of \mathbf{x} with respect to these elements.

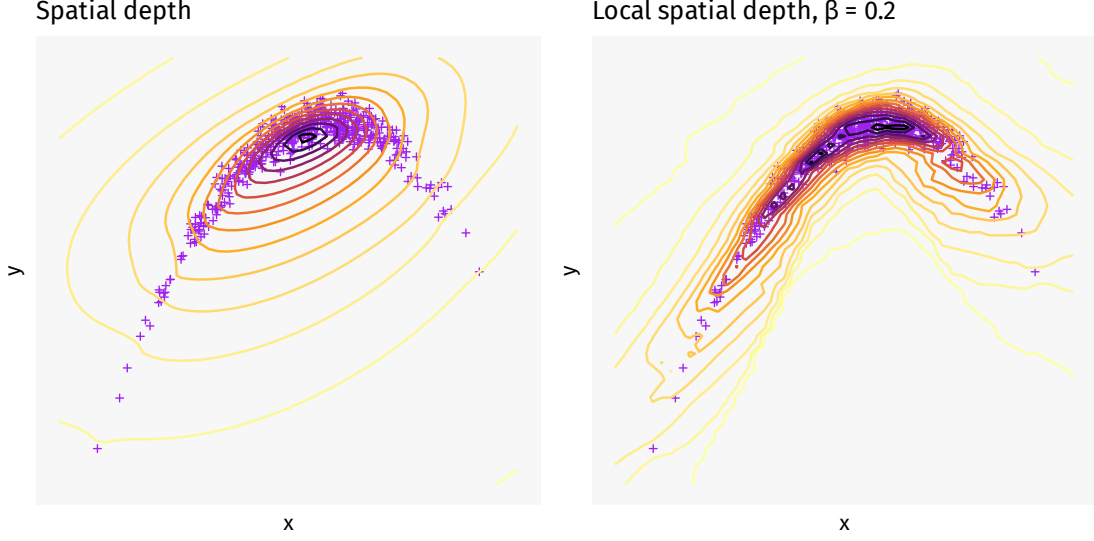


Figure 4.1: Depth contours with respect to a ‘banana-shaped’ distribution. Observe that the spatial depth contours fail to adequately capture the curved shape of the data cloud, in contrast with the local spatial depth (with $\beta = 0.2$) contours.

Remark. When $\beta = 1$, the local depth LD_1 reduces to the original global depth D .

Remark. The notions of depth based neighbourhoods and local depth make sense for any distribution F on a space \mathcal{X} as long as the process of symmetrization around $\mathbf{x} \in \mathcal{X}$ can be achieved.

4.2 Regression based on local depth

Definition 4.2.1. Let D be a depth function, and let $\tilde{F}_\beta^\mathbf{x}$ denote the symmetrized distribution $F^\mathbf{x}$ conditional on the neighbourhood $N_\beta^\mathbf{x}(F)$. Given $\mathbf{x} \in \mathcal{X}$, we may define a local depth kernel at locality level β centered at \mathbf{x} as

$$K_\beta^\mathbf{x}: N_\beta^\mathbf{x}(F) \rightarrow \mathbb{R}, \quad \mathbf{z} \mapsto D(\mathbf{z}, \tilde{F}_\beta^\mathbf{x}). \quad (4.2.1)$$

This naturally extends to a map $\mathcal{X} \rightarrow \mathbb{R}$ as $K_\beta^\mathbf{x}(\mathbf{z}) = 0$ for $\mathbf{z} \notin N_\beta^\mathbf{x}(F)$.

Note that $\tilde{F}_\beta^\mathbf{x}$ is angularly symmetric about \mathbf{x} . As a result, $K_\beta^\mathbf{x}$ is maximized at and decreases away from \mathbf{x} , for reasonably well behaved depth functions (**P2** and **P3** for multivariate depth functions).

With this, we propose the (linear) estimator

$$\hat{\mathbf{y}}_\beta(\mathbf{x}) = \sum_i w_i(\mathbf{x}) \mathbf{y}_i, \quad w_i(\mathbf{x}) = \frac{K_\beta^\mathbf{x}(\mathbf{x}_i)}{\sum_j K_\beta^\mathbf{x}(\mathbf{x}_j)}. \quad (4.2.2)$$

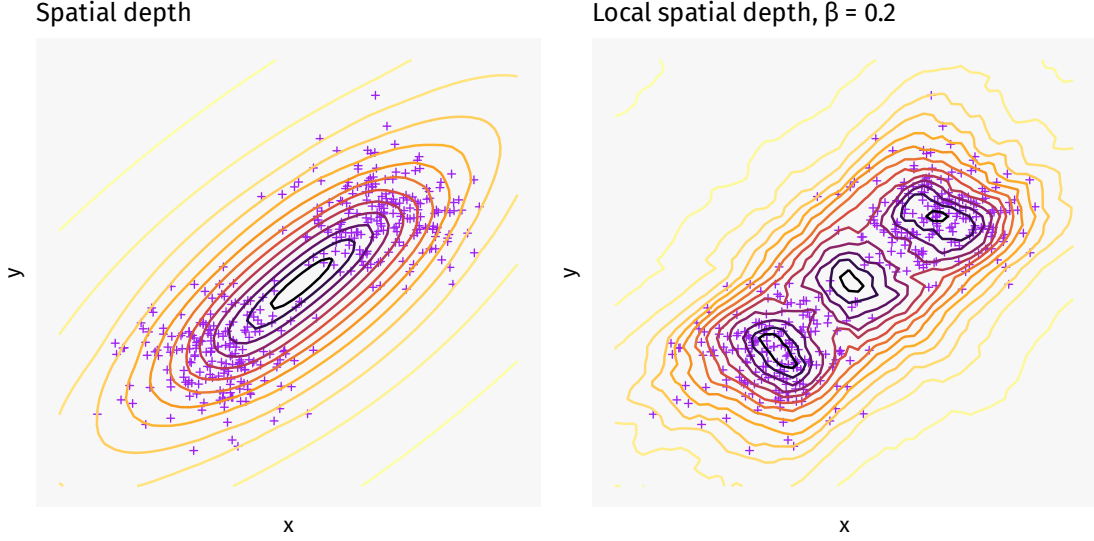


Figure 4.2: Depth contours with respect to a bimodal distribution. Although the local spatial depth contours capture the two modes correctly, it erroneously ascribes high depth values to a region in between them.

The locality level $\beta \in (0, 1]$ is a tuning parameter which may be chosen via methods such as cross-validation.

The kernel function $K_\beta^{\mathbf{x}}$ is supported on the neighbourhood $N_\beta^{\mathbf{x}}(F)$, whose shape may vary with changing $\mathbf{x} \in \mathcal{X}$. Indeed, since $N_\beta^{\mathbf{x}}(\hat{F}_n)$ contains the β proportion of points from $\{\mathbf{x}_i\}$ ‘closest’ to \mathbf{x} (in the sense of being more central in the symmetrized dataset $\mathcal{D}^{\mathbf{x}}$), this neighbourhood ought to be smaller when \mathbf{x} is more central, and larger when \mathbf{x} has fewer points nearby. Thus, $K_\beta^{\mathbf{x}}$ behaves somewhat like a variable bandwidth kernel, whose shape adjusts to the dataset. Furthermore, the ‘bandwidth’ of $K_\beta^{\mathbf{x}}$ is controlled solely by the parameter β regardless of the dimensionality or nature of \mathcal{X} . This stands in contrast with more traditional kernels which often require a selection of multiple bandwidths. For instance, a Gaussian kernel of the form

$$\mathbf{z} \mapsto \exp \left(- \sum_i \frac{(x_i - z_i)^2}{2h_i^2} \right) \quad (4.2.3)$$

needs d parameters $\{h_i\}_{i=1}^d$ to be determined.

Equation 4.2.2 may also be thought of as a weighted KNN estimator, since $N_\beta^{\mathbf{x}}(\hat{F}_n)$ always captures the same number of points.

When the depth function D is chosen to be affine invariant, the estimator 4.2.2 is also affine invariant, in the sense that it is unchanged by an affine transformation of \mathcal{X} . This is because $N_\beta^{A\mathbf{x}+\mathbf{b}}(F_{A\mathbf{X}+\mathbf{b}})$ will simply be the affine image of $N_\beta^{\mathbf{x}}(F_{\mathbf{X}})$.

Chapter 5

CONCLUSION

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