Extracting multiscale geometric information from high-dimensional and infinite-dimensional data with application to classification

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Joint work with

Gabriel Chandler

Multiscale feature extraction in multi-dimensions

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Will will use notions of

- depth (Tukey depth)
- FDA

Relations and inspirations

- mass estimation (Ting et al. 2012)
- shorth plot (Einmahl et al. 2010)
- local depth (Agostinelli and Ramanazzi, 2011, Paindaveine and van Bever, 2012, and Dutta et al., 2015)

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  But: Limit cases are not meaningful.

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- Construct a feature map driven by geometric consideration (in contrast to RKHS-type);
- Features are real-valued functions on $[0,1]$ that

thus can be plotted $\rightsquigarrow$ visualization,

contain geometric information $\rightsquigarrow$ interpretability.

Wine data

from UC Irvine Machine Learning Repository.

177 observations in 13 dimensions

3 classes (labeled) [58 in class 1, 70 class 2, 49 class 3]

Feature functions for wine data

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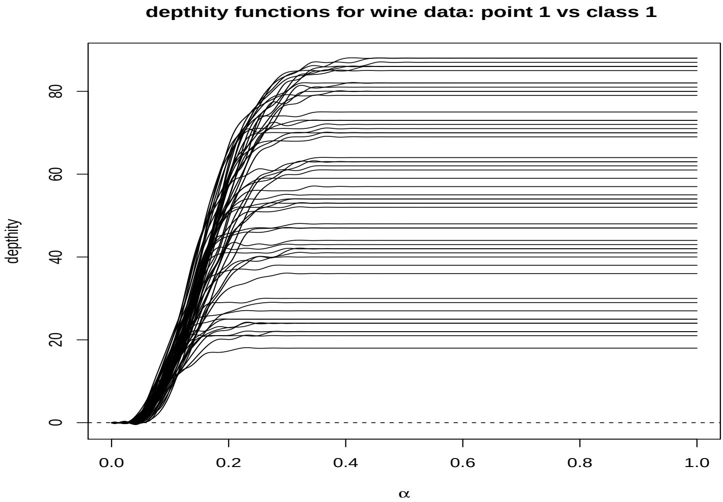

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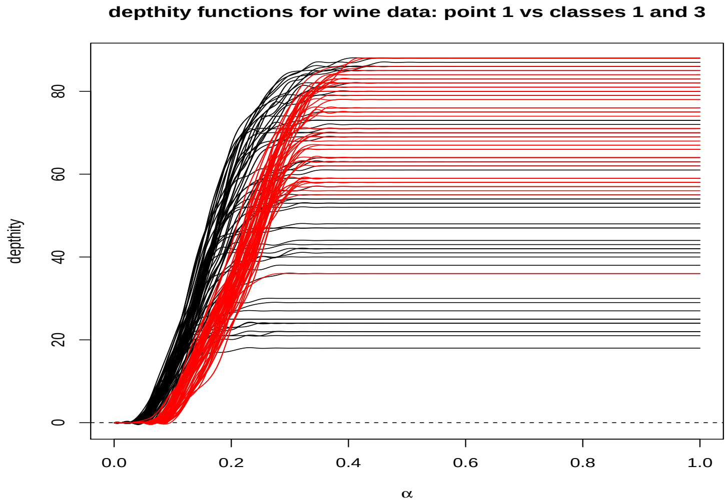

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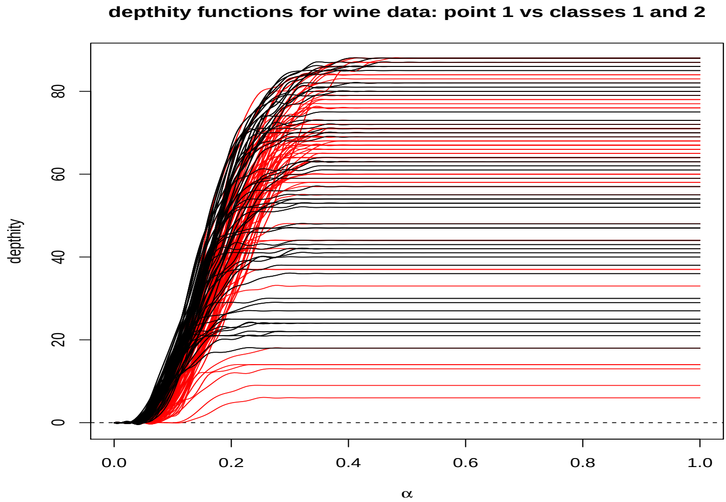

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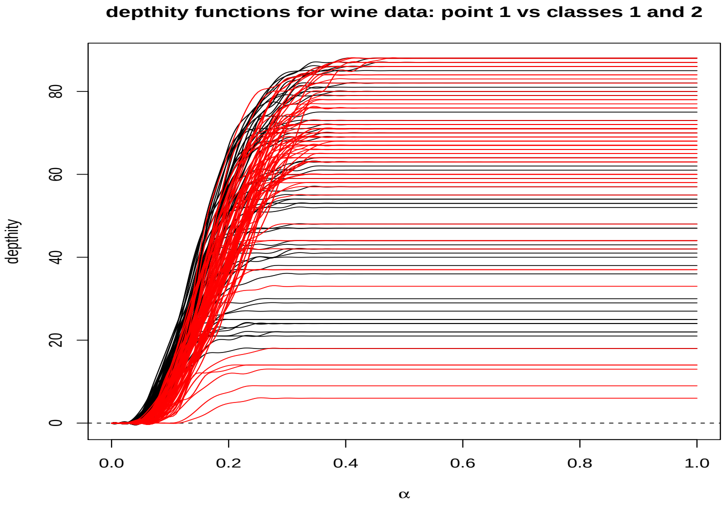

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We propose to use (circular) cones as basic subsets.

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- *small quantiles* $\rightsquigarrow$ *local information (density)*
- *large quantiles* $\rightsquigarrow$ *global information (depth)*
- *intermediate quantiles? (How important are they for high dimensions?)*

  $\rightsquigarrow$ *multiscale (scale given by quantile level)*

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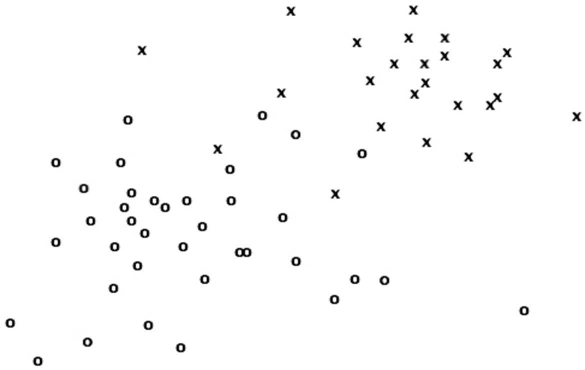
QUESTION: How to find relevant directions?

Construction of depth quantile functions



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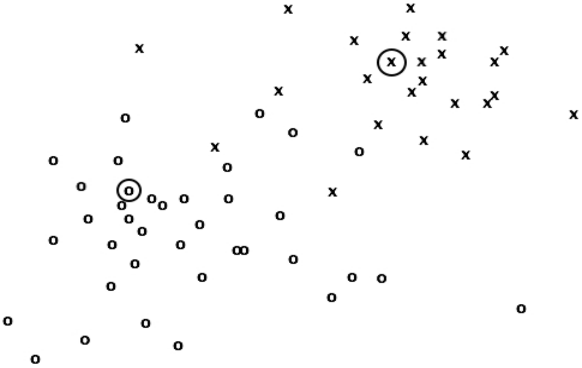

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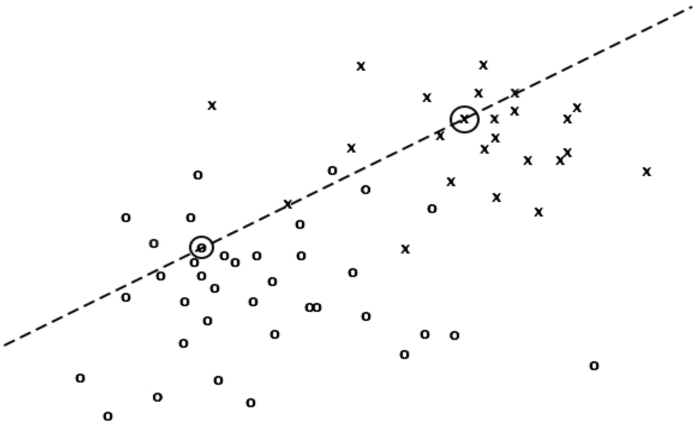

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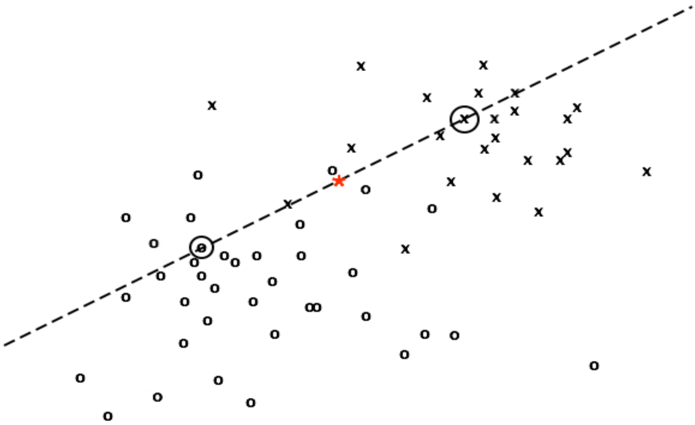

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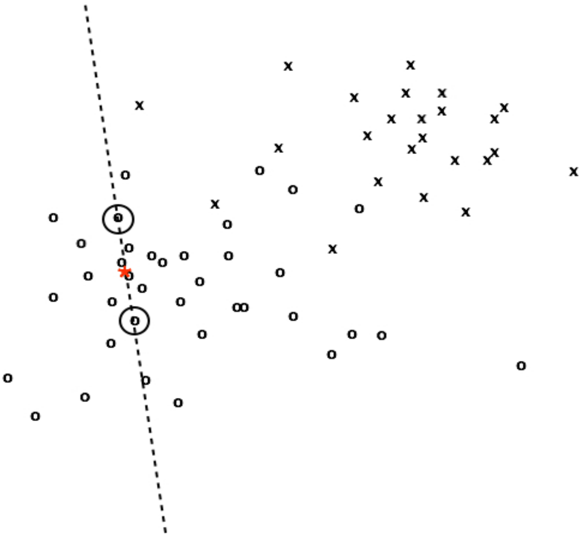

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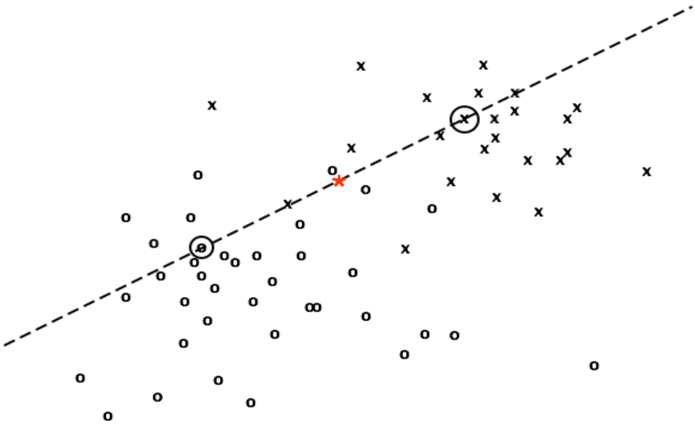

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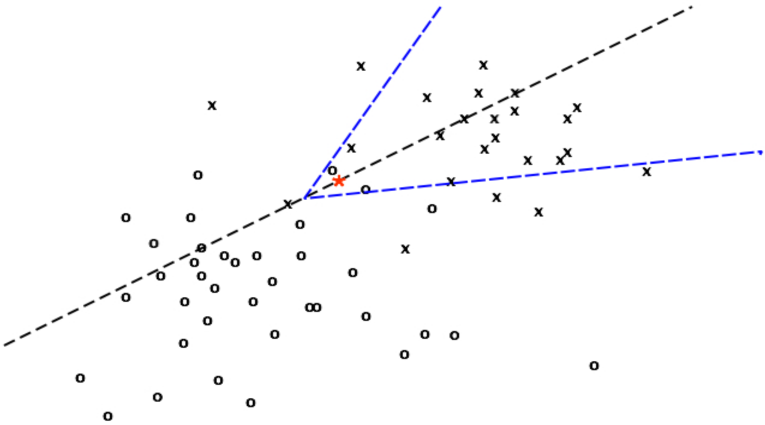

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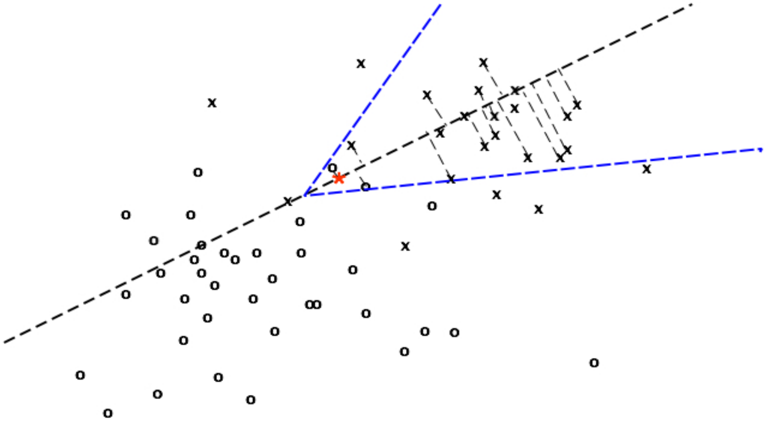

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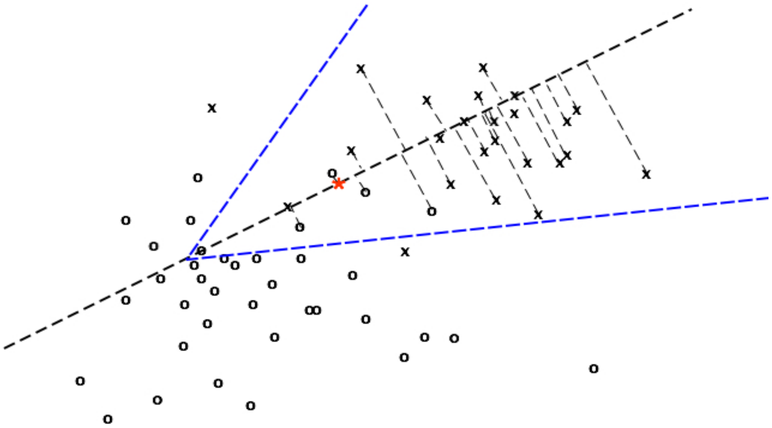

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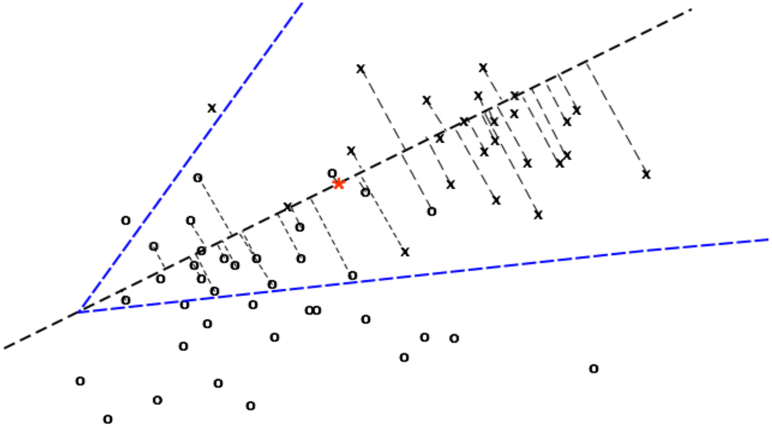

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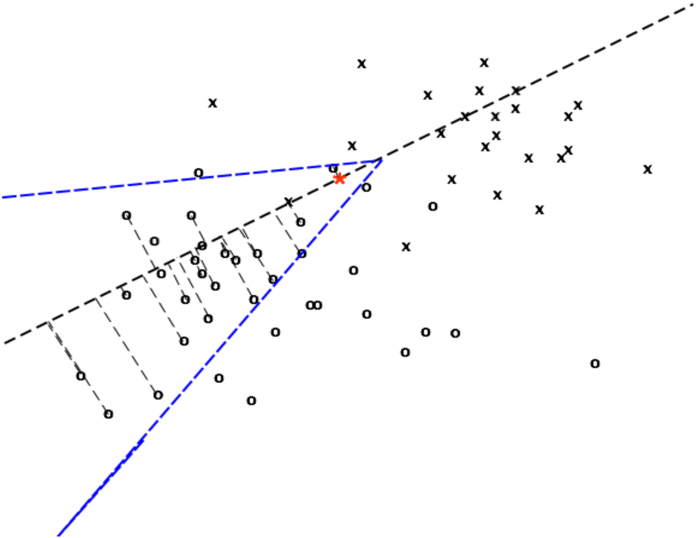

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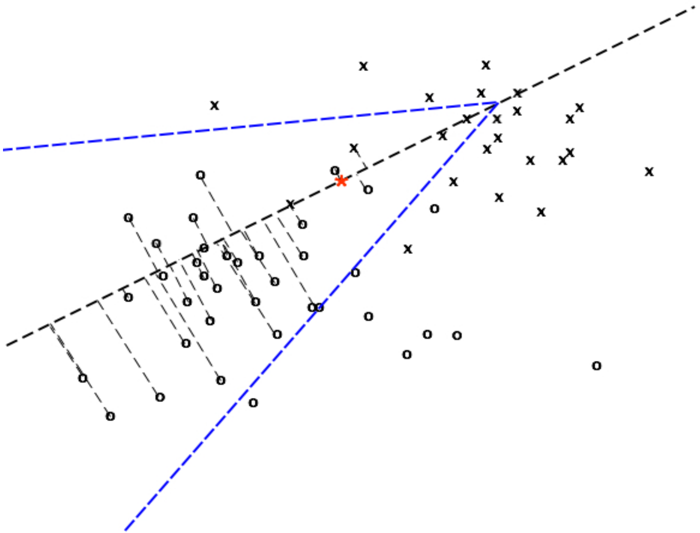

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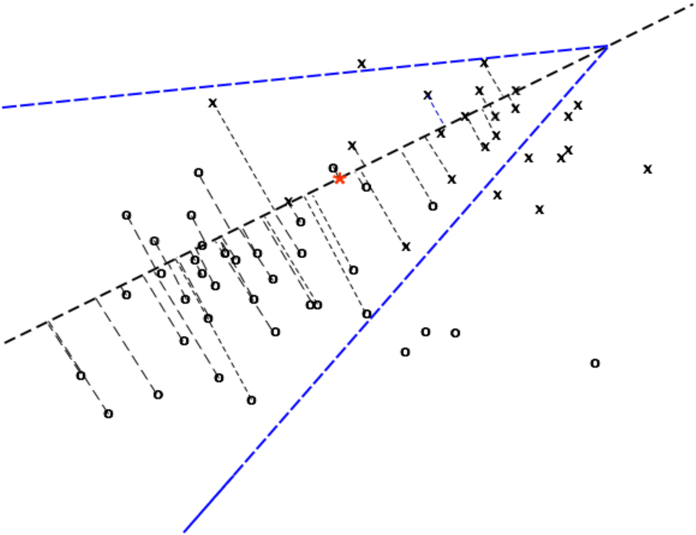

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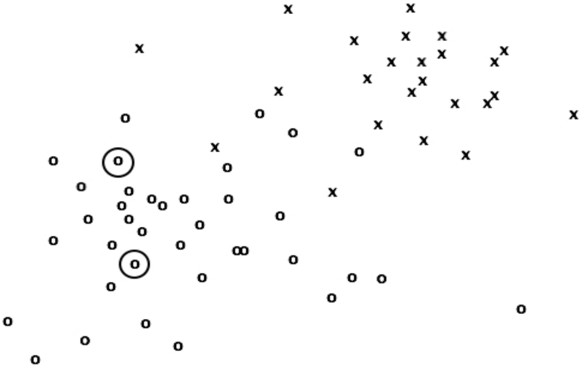

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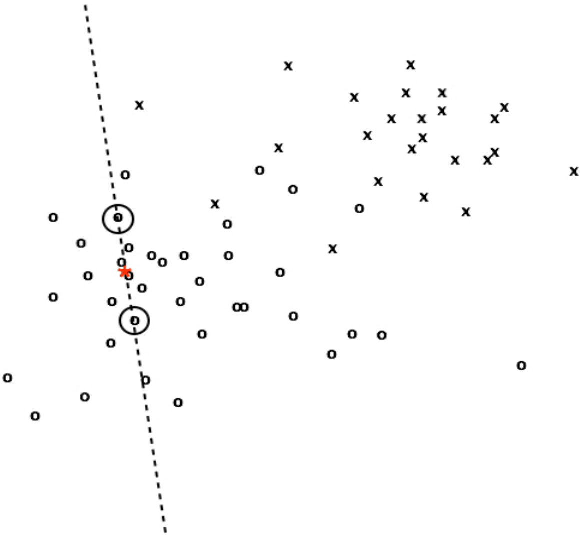

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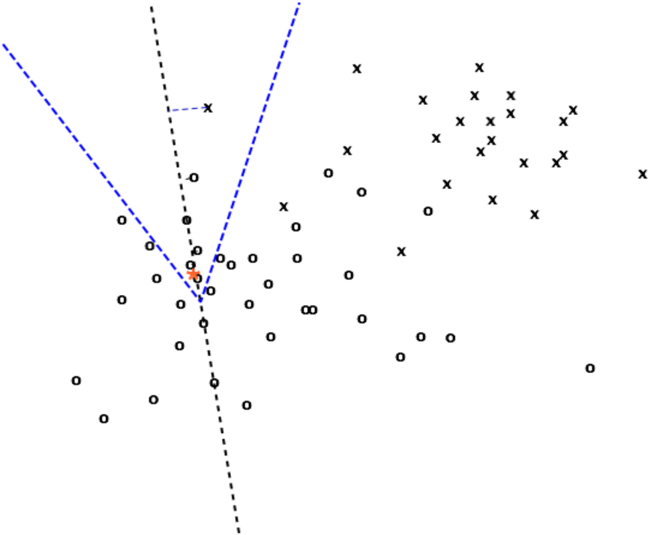

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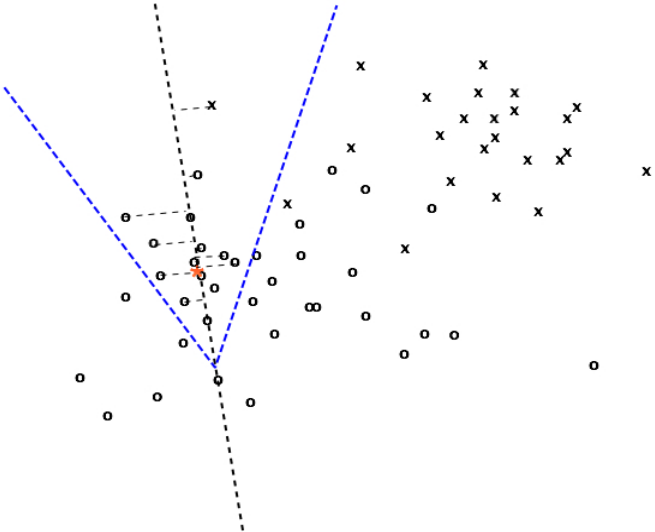

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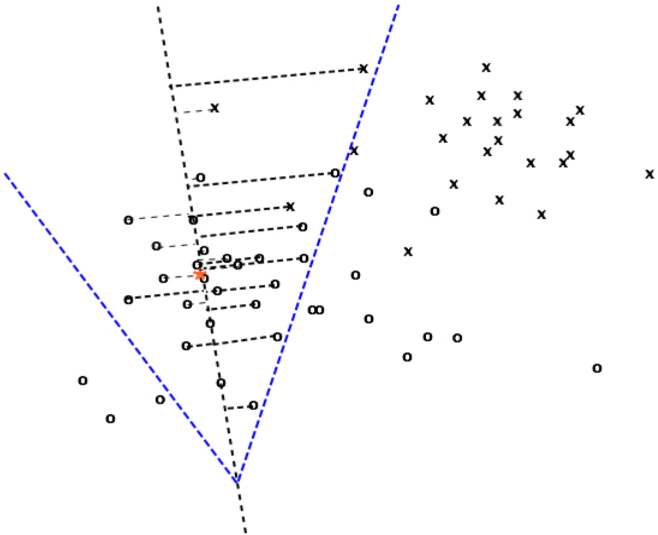

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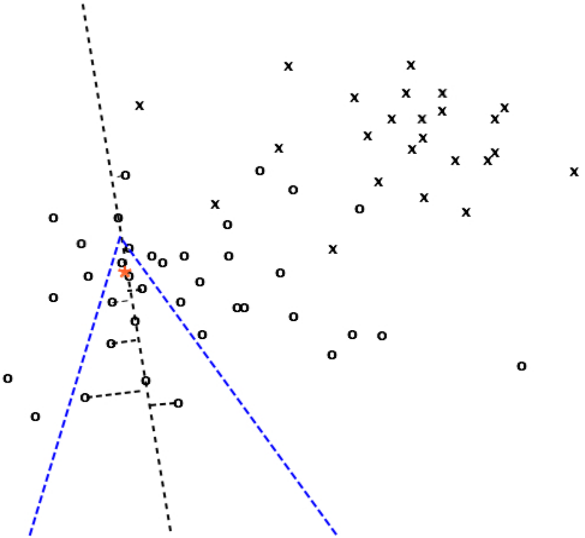

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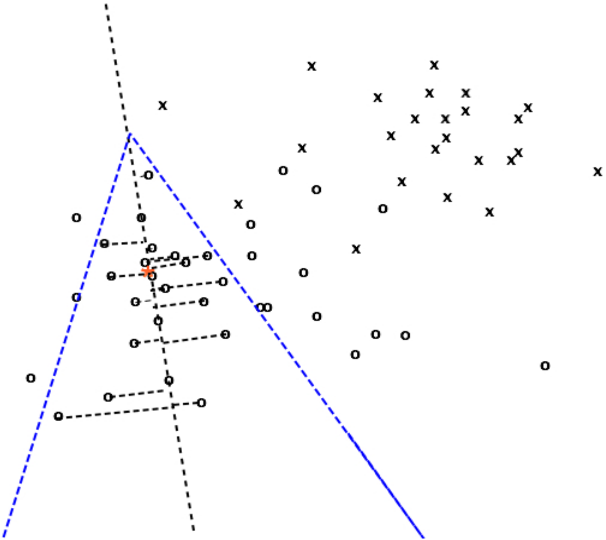

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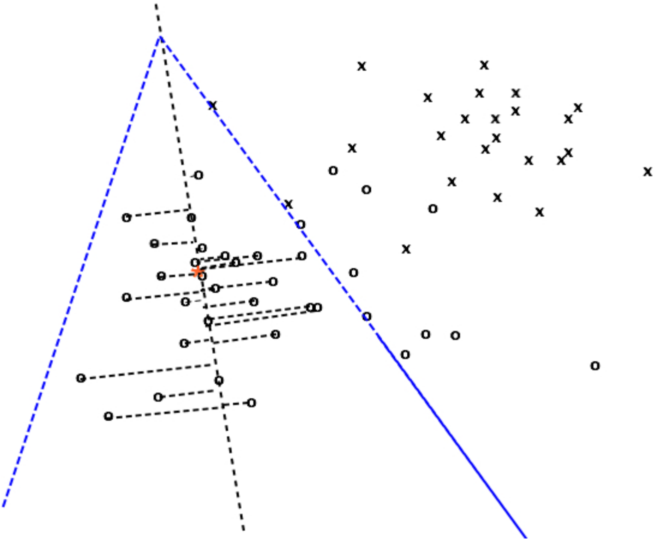

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Given a line $\ell \in \mathbb{R}^d$ and $s, x \in \ell$, let $C_x(s)$ denote a cone with

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Let

$$d_{x,\ell}(s) = \min\left\{F(A_x(s)), F(B_x(s))\right\}.$$

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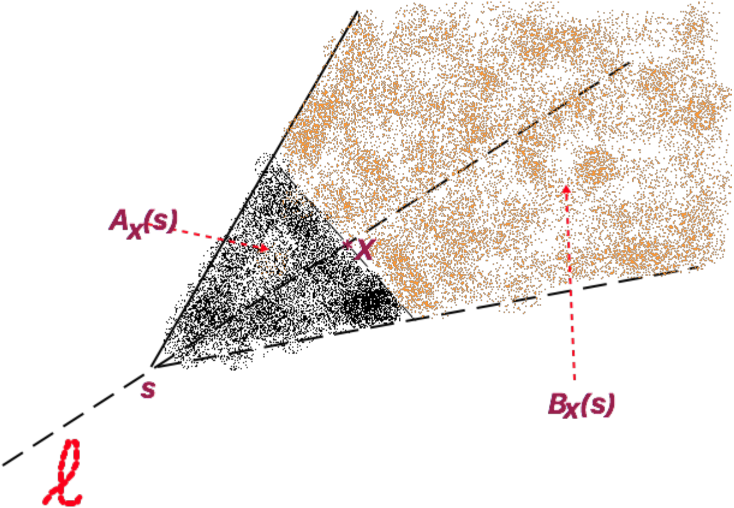
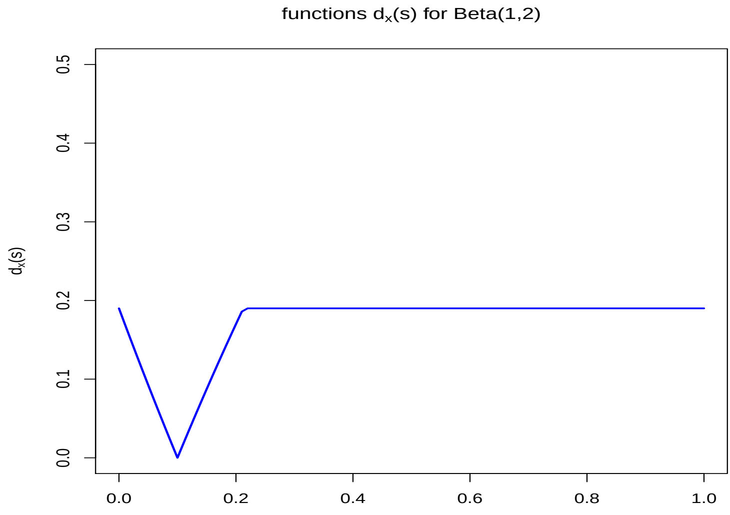


How do these depth functions look like as a function of s?

Examples



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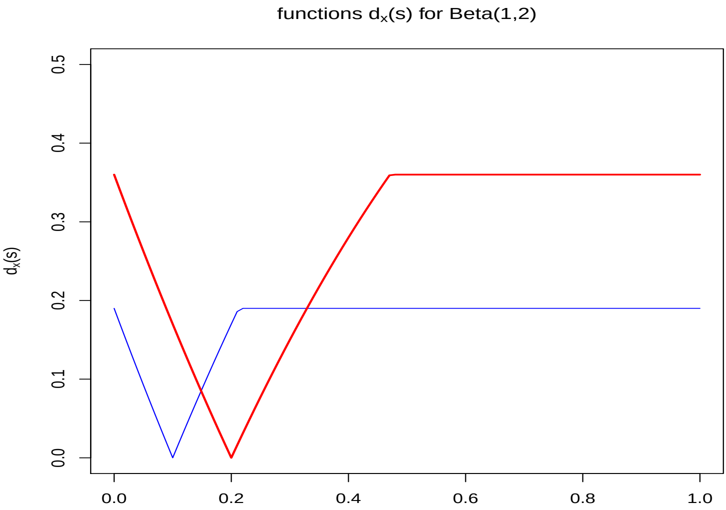

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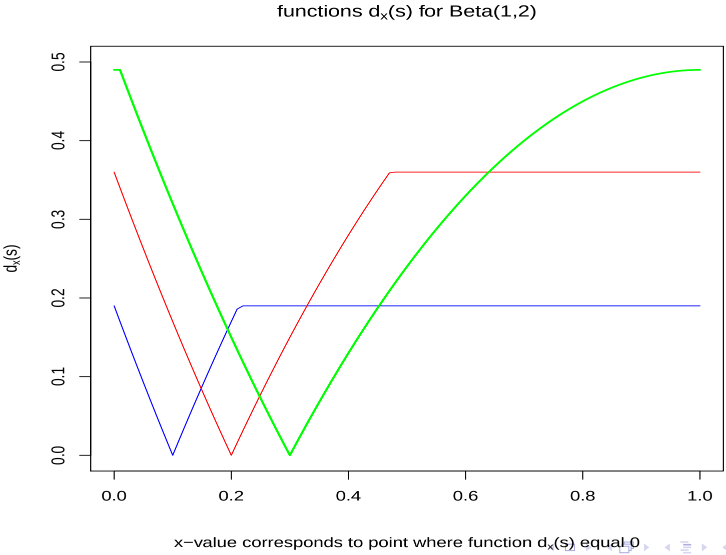

functions $d_x(s)$ for Beta(1,2)
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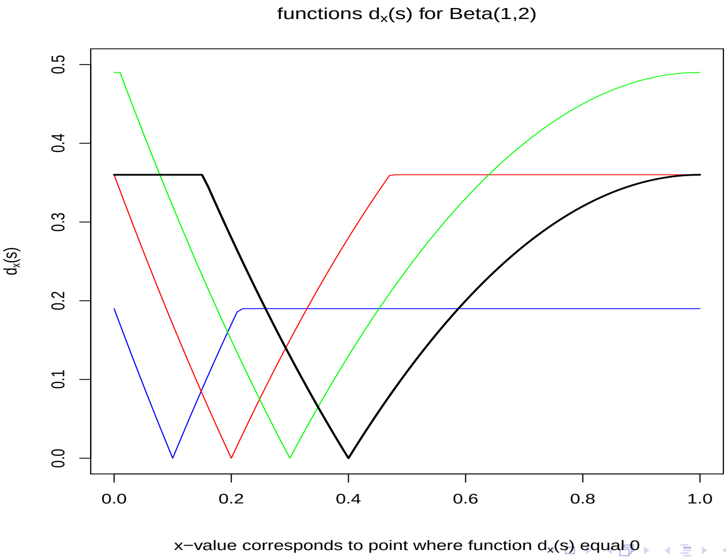
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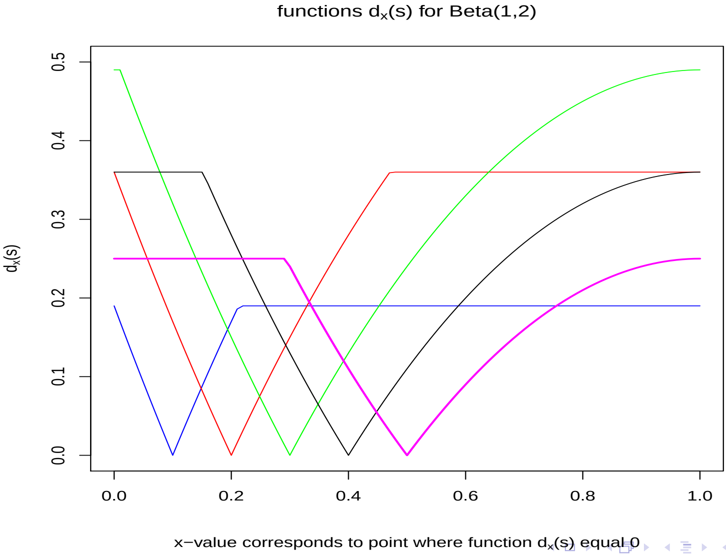
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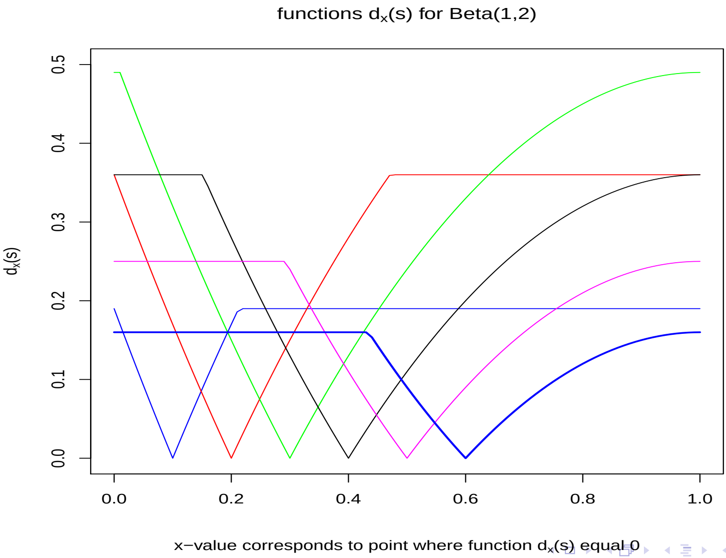

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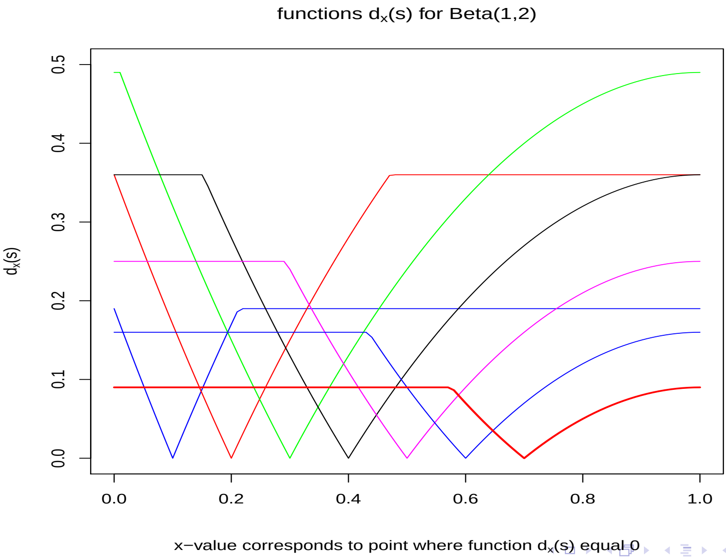
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Choose cone tip s randomly, i.e let $S \sim G$ on ℓ. Consider the cdf of $d_{x,\ell}(S)$

$$P(d_{x,\ell}(S) \leq t) = G\big(s \in \ell : d_{x,\ell}(s) \leq t\big).$$

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$\rightsquigarrow$ put all depth functions onto same 'scale'

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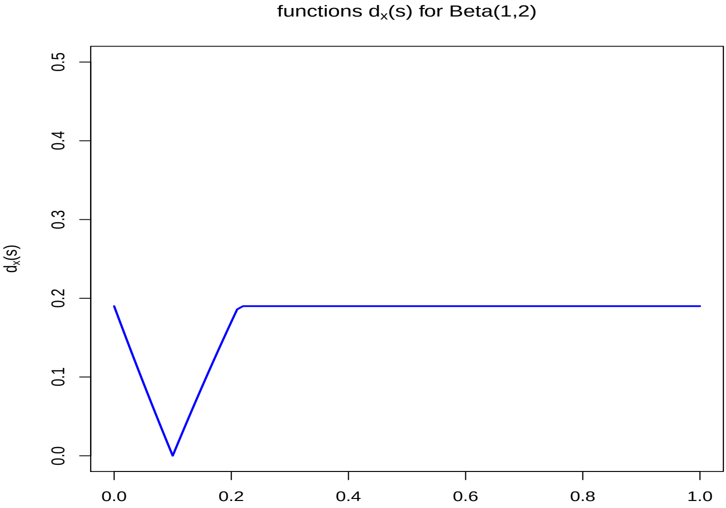

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Questions

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- *What information is contained in depth quantile functions?*
- *How to use for statistical inference?*

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- $\lim_{\delta \to 0} \frac{q_{x,\ell}(\delta)}{\alpha^d} = C \frac{f(x)}{g(x)}$, where C is known (localization)

  f, g are densities of F and G.

"multiscale"

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Computation: Embarrassingly parallelizable (if needed).

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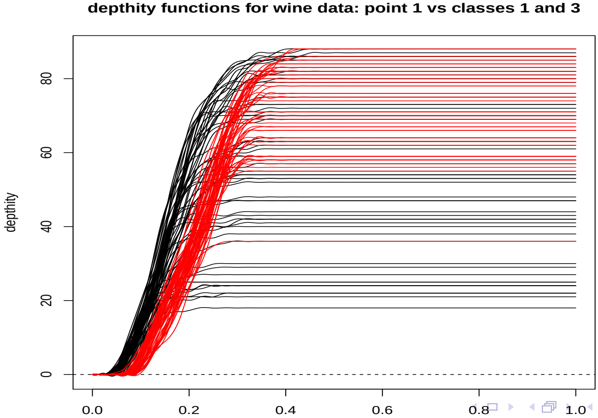

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$K \geq 1$ classes

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- For each fixed X_i, average $\widehat{q}_{ij}(\delta)$ over all X_j in class k

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Averaged feature functions

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- For each point, we obtain K functions $(\widehat{q}_i^{(1)}(\delta), \ldots, \widehat{q}_i^{(K)}(\delta))$

Example: Iris data

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Iris data (Fisher, 1936); $d = 4$; $K = 3$, $n = 150$

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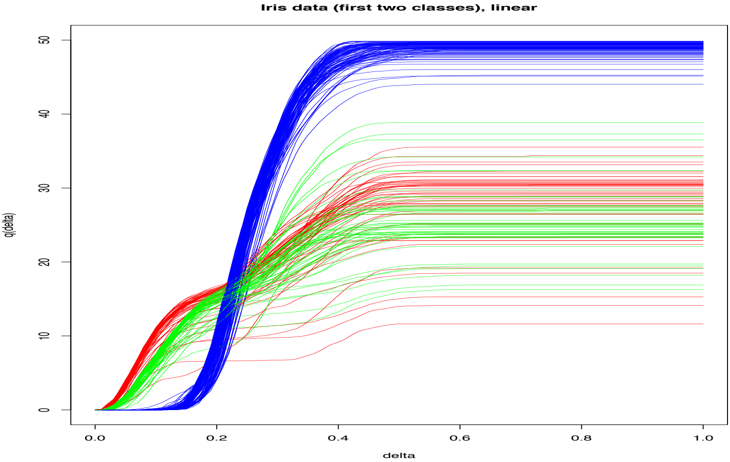
only used classes 1 and 2



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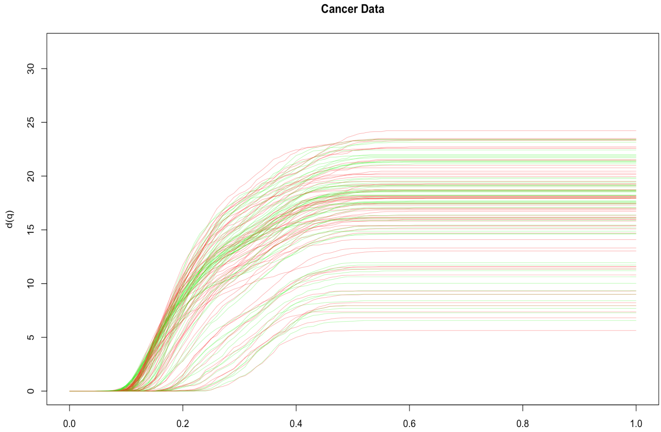

More information on depth quantile functions

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Enhance understanding of our approach by relating it to

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Enhance understanding of our approach by relating it to

- *multidimensional scaling*

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More information on depth quantile functions

Enhance understanding of our approach by relating it to

- *multidimensional scaling*
- *Choquet capacities*
- *shorth plot (one-dimensional case)*

Depth quantiles and multidimensional scaling

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Observe: Given a line $\ell \subset \mathbb{R}^d$, depth quantile functions only depend on number of points in cones (with axis of symmetry being ℓ).

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- distance to line (Z_2^x)

Used two-dimensional data: (Z_{1i}^x, Z_{2i}^x), $i = 1, \ldots, n$

$\rightsquigarrow$ two-dimensional depth-quantile functions with $x = 0$; exactly the same as depth quantile functions based on original high-dimensional data

$\rightsquigarrow$ spirit of multidimensional scaling

Depth quantiles and multidimensional scaling

Given data, our construction gives

$\rightsquigarrow \binom{n}{2}$ different lines

$\rightsquigarrow \binom{n}{2}$ different (Z_1, Z_2)-plots

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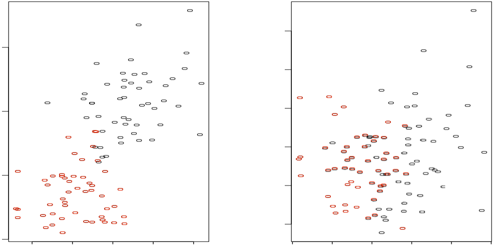


Figure 3: First two classes of iris data

different class　　　　same class

Depth quantiles and multidimensional scaling

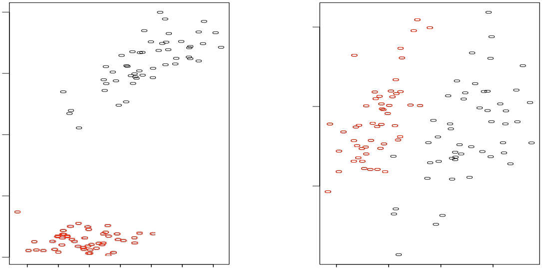
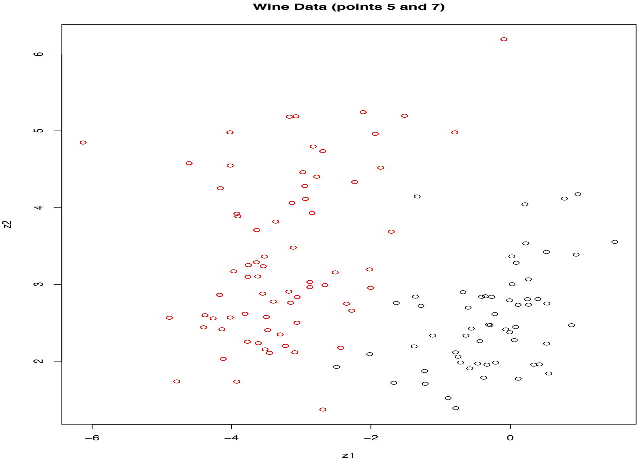


Figure 2: Second and third classes of iris data

different class　　　　　same class

Depth quantiles and multidimensional scaling



Depth quantiles in infinite dimensions

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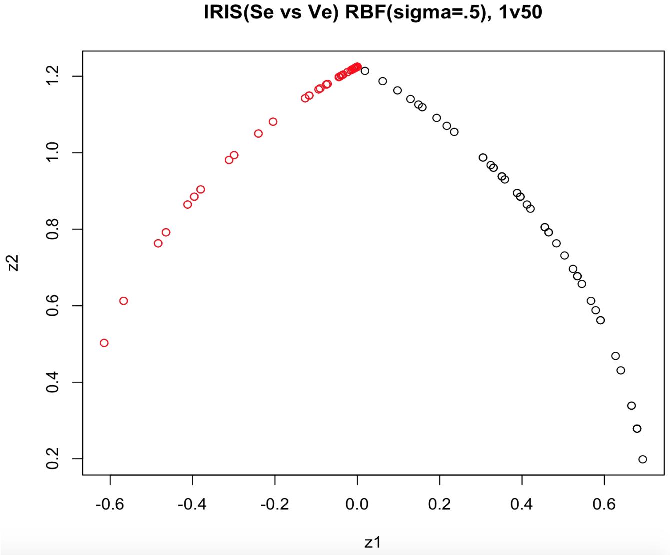
In particular:

Visualization of RKHS geometries

Examples: Iris data



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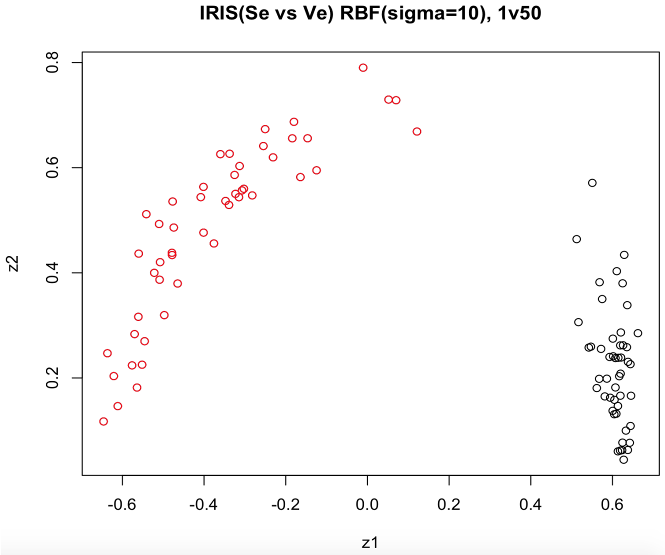

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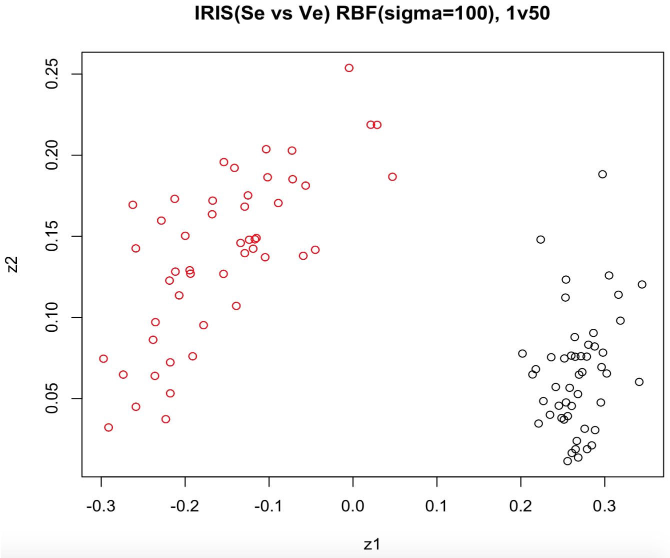

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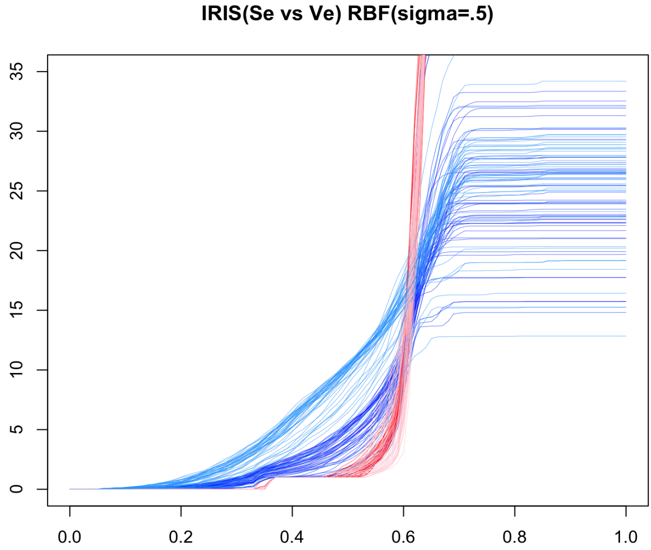

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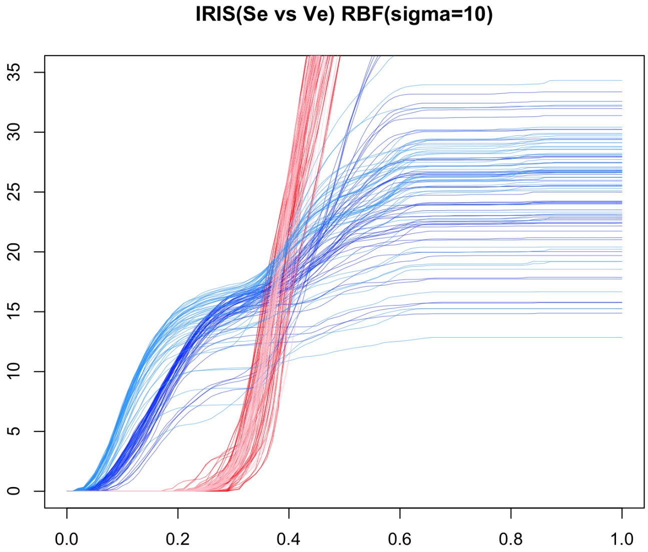

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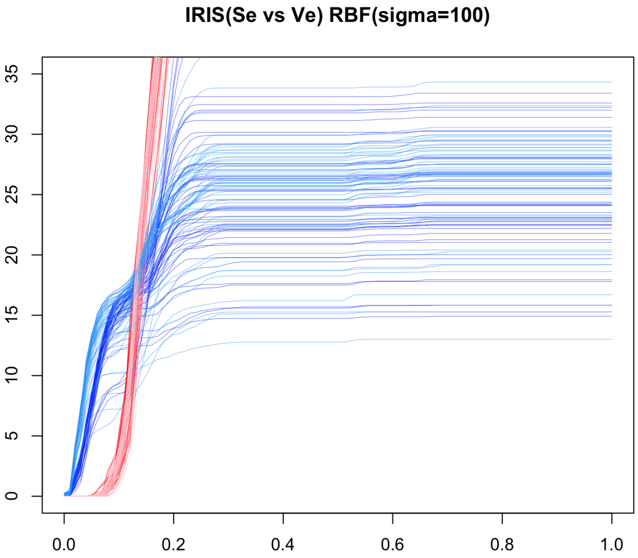

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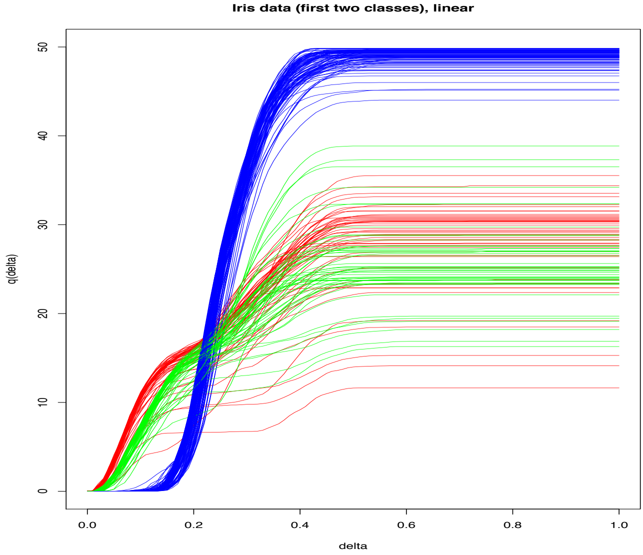

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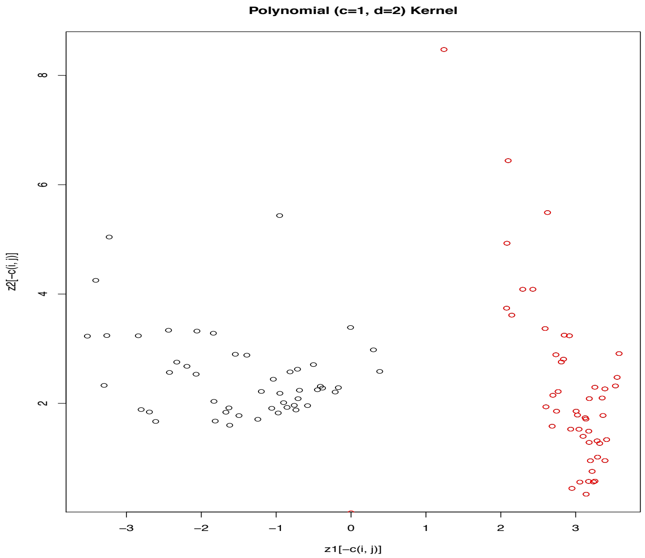

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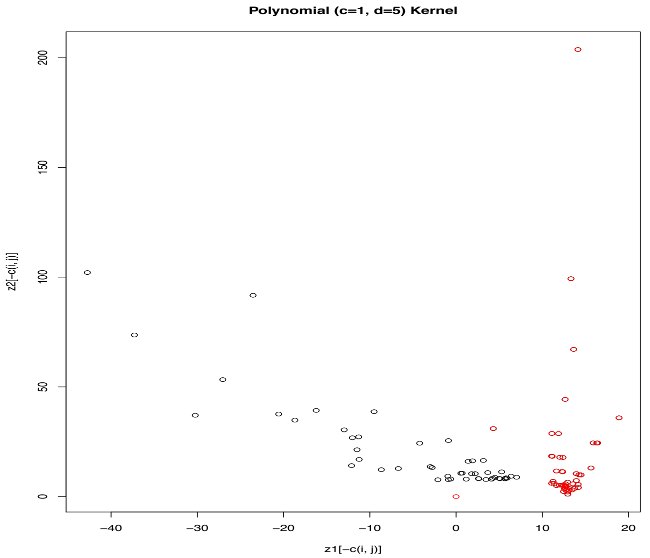

Statistical inference based on averaged feature functions

Classification analysis using FDA

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Avoid defining 'features' of depth quantile functions $\rightsquigarrow$ FDA

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For simplicity: binary classification problem, say classes 1 and 2.

- for X^* to be classified find $\widehat{q}_i^{(1)}(\delta)$ and $\widehat{q}_i^{(2)}(\delta)$

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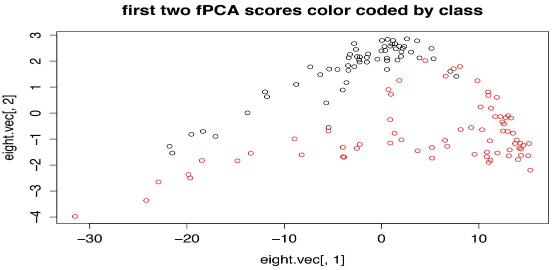
- find classification rule (SVM; kernel SVM: etc.)
- classify X^*

Illustration using wine data: Comparison to standard PCA



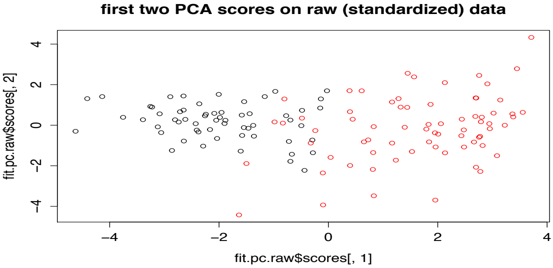


Illustration on wine data

Using leave one out procedure we obtain

misclassifications for wine data

classes	new method	1-NN
1,2	6	4
1,3	0	0
2,3	3	5

Illustration on PIMA data set

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$n = 768$; $d = 8$ covariate measurements on female Pima Indians

classification in diabetes positive/negative

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Our method is competitive with all the others tested in Dutta et al. (2015) ($\approx 25\%$ misclassification rate).

(LDA 23.37%, linear SVM 22.03%, radial SVM 24.19 %,kNN 25.73%, KDE 26.57 %, CART 27.20%, local depth based methods 25.18%)

Illustration on cancer data

gene expression data; $d = 2000, n = 62$, 2 classes (normal tissue 22, tumor tissue 40) Alon et al. 1999, PNAS

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Illustration on cancer data

leave-one-out classification gives:

- opening angle $= 60$ degrees: misclassification rate 22%
- opening angle $= 85$ degrees: misclassification rate 27.4%

(LDA 35.48%, linear SVM 16.38%, radial SVM 35.48 %, kNN 22.58%, KDE 64.52 %, CART 28.77%, local depth based methods $\approx 20\%$)

Averaged feature functions and Choquet capacities

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For this, we need some more notation:

Versions with random ℓ and x

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Note: $A_{ij}(s), B_{ij}(s)$, $d_{ij}(s), q_{ij}(\delta)$ and $q_i^{(k)}(\delta)$ are random quantities!

Averaged feature functions and Choquet capacities

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The quantity $q_i^{(k)}(\delta)$ can be expressed as:

$$q_i^{(k)}(\delta) = E_{X_j} P(Z \in \Gamma_{ij}(\delta) | X_i), \quad Z \sim F, \text{ independent of } X_i, X_j$$

where $\Gamma_{ij}(\delta)$ is a closed random set, whose distribution depends on the distributions of X_i and X_j.

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$$\Psi_i^{(k)}(z) = P(z \in \Gamma_{ij}(\delta) | X_i), \quad X_j \in \text{group } k$$

be the hitting function of the random set $\Gamma_{ij}(\delta)$, given X_i.

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Our method compares expected capacity functions of the random closed sets $\Gamma_{ij}(\delta)$ (given X_i) for different distributions of the sets, determined by the distributions of X_i and X_j. This is done for each δ.

Some asymptotics

Some asymptotics

Assumptions.

(A1) F and G posses continuous, bounded densities f and g, respectively.

(A2) For every $\epsilon > 0$ and every d there exists a set $\mathcal{R}_d(\epsilon) \subset \mathbb{R}^d$ of diameter $R_d(\epsilon)$, such that

- (i) $0 \in \mathcal{R}_d(\epsilon)$
- (ii) $R_d(\epsilon) = O(d^{1/2})$, as $d \to \infty$;
- (iii) $F(\mathcal{R}_d(\epsilon)) > 1 - \epsilon$ for every d;
- (iv) there exists a constant $c > 0$, not depending on d, such that $\sup_{x \in \mathcal{R}_d(\epsilon)} f(x) \leq c$.

(A3) $\sin \alpha = 1 - O(\frac{1}{d})$

Some asymptotics

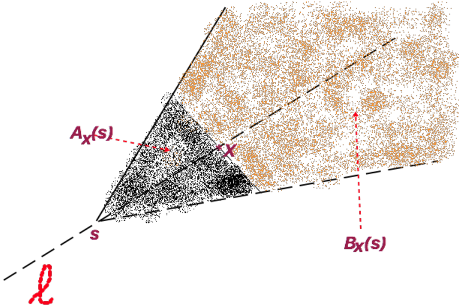
Proposition

Suppose that assumption (A1) holds, and that $X_1, \ldots, X_n, \ldots$ are iid from F. Then, for every given line $\ell \subset \mathbb{R}^d$, and every $\epsilon > 0$, there exist constants M and n_0, not varying with d, such that

$$P\left[\sup_{x,s\in\ell}\left|\sqrt{n}(\widehat{d}_{x,\ell}(s) - d_{x,\ell}(s))\right| > M\right] \leq \epsilon, \quad \textit{for } n \geq n_0.$$

Notation

Recall:



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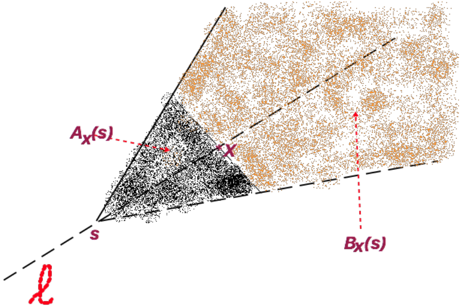

- Notation: $\mathcal{T}_{x,\ell}(s) = \underset{C \in \{A_x(s), B_x(s)\}}{\arg\min} \{F(C)\}.$

Some asymptotics

Theorem

Suppose that assumptions (A1) - (A3) hold. Let $S_{x,\ell}(c) = \{s \in \ell : |F(A_x(s)) - F(B_x(s))| \geq \frac{c}{\sqrt{n}}\}$*. With* $\mathcal{T}_{x,\ell}(s)$ *as above, let* $\mathbb{B}_x(s) = \min_{C \in \mathcal{T}_{x,\ell}(s)} B_F(C)$*. Then, for every* $\epsilon > 0$,

$$\lim_{c\to\infty} \limsup_{n\to\infty} P\Big[\sup_{x,s\in S_{x,\ell}(c)} \left|\sqrt{n}(\widehat{d}_{x,\ell}(s) - d_{x,\ell}(s)) - \mathbb{B}_x(s)\right| > \epsilon\Big] = 0.$$

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REMARK.

- This convergence is uniform in the dimension d.

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$$q_{ij}(\delta) = \inf\left\{t : \; G(s : d_{ij}(s) \leq t) \geq \delta\right\}.$$
$$\widehat{q}_{ij}(\delta) = \inf\left\{t : \; G(s : \widehat{d}_{ij}(s) \leq t) \geq \delta\right\}.$$

Recall

- ℓ determined by pair (X_i, X_j)
- x becomes midpoint $M_{ij} := \frac{X_i + X_j}{2}$

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Note: $A_{ij}(s), B_{ij}(s),\ d_{ij}(s), q_{ij}(\delta)$ and $q_i^{(k)}(\delta)$ are random quantities!

Some asymptotics

Theorem

Suppose that assumption (A1) holds. With

$$D_{ij}(c) = \{\delta \in [0,1] : s_{ij}^r(\delta), s_{ij}^l(\delta) \in S_{x,\ell}(c)\},$$

we have

$$\sup_{1 \le i < j \le n} \sup_{\delta \in D_{ij}(c)} |\widehat{q}_{ij}(\delta) - q_{ij}(\delta)| = O_P\left(\sqrt{\frac{\min\{d, \log n\}}{n}}\right).$$

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Remarks:

- Upper bound of $\left(\frac{\log n}{n}\right)^{1/2}$, independent of dimension d!

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Remarks:

- Upper bound of $\left(\frac{\log n}{n}\right)^{1/2}$, independent of dimension d!
- If data lie in affine subspace of dimension $d^* \le d$, then d can be replaced by d^*.

Some asymptotics

Conjecture

Suppose that (A1) - (A3) hold, and assume that

$$P(X_k \notin D_{ij}(c) | X_k \text{ in class } k; X_i) = o_P(1/\sqrt{n}).$$

As $n_k \to \infty$ *(*n_k *number of obs. in class* k*), then*

$$\sup_{1 \le i \le n} \sup_{\delta \in [0,1]} \left| \widehat{q}_i^{(k)}(\delta) - q_i^{(k)}(\delta) \right| = O_P\left(\sqrt{\frac{\min\{d, \log n\}}{n}} \right).$$

Some asymptotics

Conjecture

Suppose that (A1) - (A3) hold, and assume that

$$P(X_k \notin D_{ij}(c) | X_k \text{ in class } k; X_i) = o_P(1/\sqrt{n}).$$

As $n_k \to \infty$ (n_k number of obs. in class k), then

$$\sup_{1 \leq i \leq n} \sup_{\delta \in [0,1]} \left| \widehat{q}_i^{(k)}(\delta) - q_i^{(k)}(\delta) \right| = O_P\left(\sqrt{\frac{\min\{d, \log n\}}{n}} \right).$$

Same remarks as above apply.

Open questions

- more on case of $d \to \infty$
- consider different Choquet functionals?
- investigate choice of tuning parameters
  - α (opening angle of cone)
  - G (distribution of cone tips)
- What if data lie on manifolds?
- For FDA classification: estimation of modes of variation (Petersen and Müller, 2016)
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Illustration