Classification methods for functional data

2017 CRoNoS Spring Course on Multivariate methods with R

Enea Bongiorno

UNIVERSITÀ DEL PIEMONTE ORIENTALE

Cyprus University of Technology,
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OUTLINE

Multivariate Framework

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- a random vector

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  with positive density f

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$$\mathbb{P}(Y = g) = \pi_g > 0, \quad \sum_{g=1}^{G} \pi_g = 1.$$

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- $f(x|g)$, the density function of $(X|Y = g)$

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   $\Longrightarrow$ supervised classification (discriminant) - Bayes rule

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- Heuristic and Geometric procedures as hierarchical clustering, k-means, ... [Ward'63, Hartigan'75]
- Probabilistic approaches as model-based algorithm, density based clustering [Hartigan'75, Wishart'69]

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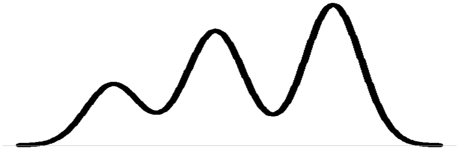
Regions with high density identify clusters [Wishart'69]:

- Fix c, consider the connected components of $\{f > c\}$



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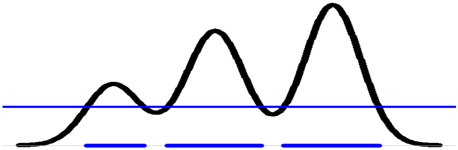

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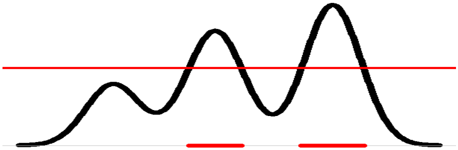

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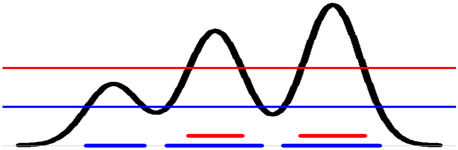

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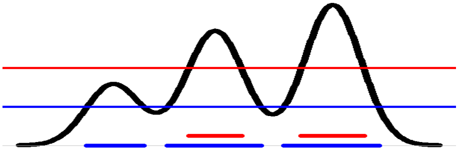

Clusters number depends on the threshold level c

In many cases, MODES depict structural differences among data

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- If $f(x|g)$ were known ($f(x|g) > 0$):

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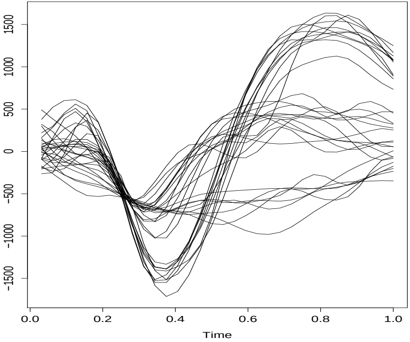
[Bosq'00, Ferraty,Vieu'06, Ramsay,Silverman'05]

Example of Functional Data 1/2

Neuronal experiment on a monkey: (Voltage of neurons) vs. Time

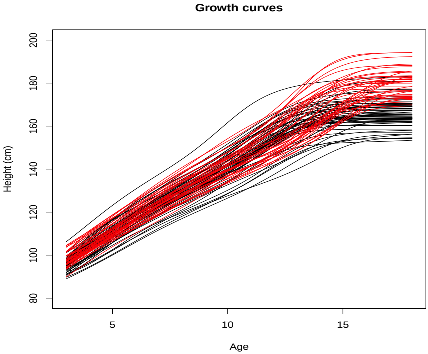


GOAL
spike sorting: distinguish different activities of neurons (clustering)

[Thanks to Andrew Schwartz motorlab in Pittsburgh]

Example of Functional Data 2/2

Berkeley growth curves: Boys (red), Girls (black)



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retrieve the gender of subjects (clustering if sex is treated as a hidden variable, discriminant otherwise)

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   - Parametric mixture model for coefficients of some basis

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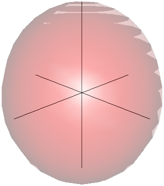

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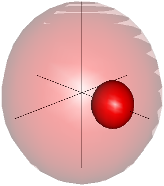

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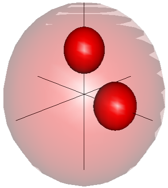

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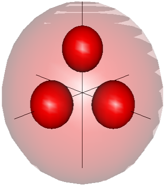

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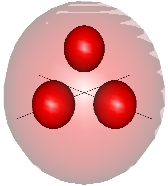
  - Then $B_i \cap B_j = \emptyset$, $i \neq j$, $B \supset \bigcup B_j$ and $\nu(B) \geq \sum_j \nu(B_j) = \infty$



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Ψ = intensity of SmBP = density "surrogate"
ϕ = Volume parameter

Some references

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- applications:

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Proposition [B.,Goia'16b]

Fix d. As $\varepsilon \to 0$, $\quad \varphi(x,\varepsilon) \sim f_d(x) V_d(\varepsilon) \mathcal{R}(x,\varepsilon,d)$

- $V_d(\varepsilon)$ = volume of the d–dimensional ball of radius ε.
- $\mathcal{R}(x,\varepsilon,d) = \mathbb{E}\left[(1-S)^{d/2}\,\mathbb{I}_{\{S\leq 1\}}\right]$
- $S = S(x,\varepsilon,d) = \frac{1}{\varepsilon^2}\sum_{j\geq d+1}(\theta_j - \langle x, \xi_j\rangle)^2$

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Some settings lead to define an intensity $\Psi(x)$ of the SmBP:

1. $\mathcal{R}(x,\varepsilon,d)$ is independent on x,
   Ex.: when $\langle x,\xi_j\rangle = 0$ for any $j \geq d_0 + 1$
   (e.g. the Gaussian processes are included: for any $d \geq d_0$,
   $\Psi(x) = \exp\left\{-\sum_{j\leq d_0} x_j^2/(2\lambda_j)\right\}$)

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3. $$\begin{cases} \mathcal{R}(x,\varepsilon,d) \to 1, \\ \varphi(x,\varepsilon) \sim f_d(x) V_d(\varepsilon), \end{cases} \qquad \varepsilon \to 0,\ d(\varepsilon) \to \infty.$$

SmBP Asymptotic: let $d(\varepsilon) \to \infty$

- Consider:
  - $\{\lambda_j, \xi_j\}_{j=1}^{\infty}$ eigenelements of $\Sigma[\cdot]$
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Proposition [B.,Goia'16b]

As $\varepsilon \to 0$, it is possible to choose $d = d(\varepsilon) \to \infty$ so that:

$$\varphi(x, \varepsilon) \sim f_d(x_1, \ldots, x_d)\, \phi(d, \varepsilon)$$

This generalizes [Delaigle,Hall'10] where PCs are **independent**

SmBP Asymptotic: let $d(\varepsilon) \to \infty$

Proof Sketch.

STEP 1. Fix $d \in \mathbb{N}$. Taylor leads to

$$\left| \frac{\varphi(x,\varepsilon)}{f_d V_d \mathcal{R}} - 1 \right| \leq \frac{C\varepsilon^2}{\lambda_d}$$

SmBP Asymptotic: let $d(\varepsilon) \to \infty$

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STEP 2. Use the $\{\lambda_j\}$ decay to choose $d = d(\varepsilon)$ so that

$$d \to \infty, \qquad 1 - C\frac{d+2}{\varepsilon^2} \sum_{j \geq d+1} \lambda_j \leq \mathcal{R} \leq 1$$

That is $\mathcal{R}(x, \varepsilon, d(\varepsilon)) \to 1$ as $\varepsilon \to 0$.

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STEP 3. Errors in 1-2 are controlled at the same time exploiting $\{\lambda_j\}$ decay (the faster they decay, the smaller the total error is)
$\Rightarrow$ The basis provided by KL decomposition is OPTIMAL

SmBP Asymptotic: comment 1/3

$\varphi(x,\varepsilon) \sim f_d(x)\phi(d,\varepsilon)$ as $\varepsilon \to 0$ and $d(\varepsilon) \to \infty$

In general, f_d still depends on ε through $d(\varepsilon)$
$\Longrightarrow$ it is not an intensity of the SmBP
BUT, some settings lead to an intensity $\Psi(x)$ of the SmBP:

- If $\{\theta_j\}$ are independent with density $\propto \exp\left\{-\left(|x_j|/\sqrt{\lambda_j}\right)^p\right\}$. Then

$$f_d(x) \to \Psi(x) = \exp\left\{-\frac{1}{2}\sum_{j=1}^{\infty}\left(|x_j|/\sqrt{\lambda_j}\right)^p\right\}, \text{ for any } x \in H$$

  is an intensity for the SmBP (Gaussian processes are included in this family).

SmBP Asymptotic: comment 2/3

$\varphi(x,\varepsilon) \sim f_d(x)\phi(d,\varepsilon)$ as $\varepsilon \to 0$ and $d(\varepsilon) \to \infty$

The form of the volumetric term $\phi(d,\varepsilon)$ depends on the eigenvalues decay rate. As example:

- Exponential decay (e.g. $\lambda_j = e^{-\beta j^\alpha},\ \beta > 0, \alpha \geq 1$):

$$\lambda_d^{-1} \sum_{j \geq d+1} \lambda_j < C, \quad \forall d$$

$$\phi(d,\varepsilon) = \exp\left\{\tfrac{1}{2} d \left[\log(2\pi e \varepsilon^2) - \log(d) + \delta(d,\alpha)\right]\right\}$$

- Hyper-exponential decay (e.g. $\lambda_j = e^{-\beta j^\alpha},\ \beta > 0, \alpha > 1$):

$$d\lambda_d^{-1} \sum_{j \geq d+1} \lambda_j = o\left(1\right), \text{ as } d \to \infty$$

$\phi(d,\varepsilon) = \frac{\varepsilon^d \pi^{d/2}}{\Gamma(d/2+1)}$ (Volume of a d-dim ball)

SmBP Asymptotic: comment 3/3

$\varphi(x,\varepsilon) \sim f_d(x)\phi(d,\varepsilon)$ as $\varepsilon \to 0$ and $d(\varepsilon) \to \infty$

There are situations in which $\varphi \sim f_d(x)\phi(d,\varepsilon)$ for slower (than exponential) decays. E.g. Wiener process:

$$\lambda_j \sim j^{-2}, \qquad \varphi(x,\varepsilon) \sim \exp\left\{-1/2 \int_0^1 x'(t)dt\right\} \phi(\varepsilon)$$

SmBP Mixture

- Consider the conditioned SmBP

$$\varphi(x, \varepsilon | g) = \mathbb{P}\left(\|X - x\| < \varepsilon \mid Y = g\right) \qquad g = 1, \ldots, G,$$

- Mixture

$$\varphi(x, \varepsilon) = \sum_{g=1}^{G} \pi_g \varphi(x, \varepsilon | g)$$

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$$\varphi(x, \varepsilon | g) = \mathbb{P}(\|X - x\| < \varepsilon \mid Y = g) \qquad g = 1, \ldots, G,$$

- Mixture $\quad + \quad$ Factorization

$$\varphi(x, \varepsilon) = \sum_{g=1}^{G} \pi_g \varphi(x, \varepsilon | g) \sim f_d(x_1, \ldots, x_d)\phi(d, \varepsilon), \quad \varepsilon \to 0$$

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Surrogate density f_d:

- carries spatial information on the mixture
- endorses "density oriented" clustering approach on f_d

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$$\sim \sum_{g=1}^{G} \pi_g f_{d_g}(x_1, \ldots, x_{d_g} | g)\phi(d_g, \varepsilon)$$

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$$\sim \sum_{g=1}^{G} \pi_g f_{d_g}(x_1,\dots,x_{d_g}|g)\phi(d_g,\varepsilon)$$

Under suitable assumptions on Σ, as $\varepsilon \to 0$:

$$f_d(x_1,\dots,x_d) \sim \sum_{g=1}^{G} \pi_g f_d(x_1,\dots,x_d|g), \quad \varepsilon \to 0$$

$\Longrightarrow$ discriminant analysis using $\pi_g f_d(x|g)$.

OUTLINE

1. Density oriented classification methods: a review
2. Functional Setting
3. Estimating the surrogate Density
   - Theoretical Aspects
   - Empirical Performances
4. SmBP Clustering
5. SmBP Discriminant Analysis

Estimating the surrogate Density

Multivariate kernel density estimator:

$$\widehat{f}_{d,n}\left(\widehat{\Pi}_d x\right) = \frac{1}{n}\sum_{i=1}^{n} K_H\left(\left\|\widehat{\Pi}_d\left(X_i - x\right)\right\|\right), \qquad \widehat{\Pi}_d x \in \mathbb{R}^d,$$

where:

- $K_H(\mathbf{u}) = \det(H)^{-1/2} K\left(H^{-1/2}\mathbf{u}\right)$,
- K kernel function,
- H symmetric semi-definite positive $d \times d$ matrix,
- $\widehat{\Pi}_d$ projection operator over the subspace spanned by the first d eigenfunctions of $\widehat{\Sigma}_n$

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Π_d is estimated:
¿is the rate of convergence the same as when Π_d is known?

Estimating the surrogate Density

Consider $H_n = h_n^2 I$ and suppose:

(B.1) $f_d(x) > 0$ and p times differentiable;

(B.2) $h_n \to 0 \quad \text{and} \quad nh_n^d / \log n \to \infty \quad \text{as} \quad n \to \infty$;

(B.3) K is a density, Lipschitz and bounded with cpct. support;

(B.4) $\exists s, \kappa > 0 : \quad \mathbb{E}\left[\|X - x\|^m\right] \leq m! s \kappa^{m-2}/2$.

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[B.,Goia'16b]

Assume (B.1)–(B.4) with $p > (3d+2)/2$ and consider the optimal bandwidth

$$c_1 n^{-\frac{1}{2p+d}} \le h_n \le c_2 n^{-\frac{1}{2p+d}} \qquad c_1, c_2 > 0.$$

Then, as $n \to \infty$ and uniformly in $\mathbb{R}^d$

$$\mathbb{E}\left[f_d(x) - \widehat{f}_n(x)\right]^2 = O\left(n^{-2p/(2p+d)}\right).$$

Finite dimensional process

$$\begin{cases} X(t) = a\sqrt{2/\pi}\sin(t) \ \text{(the random process)} \\ \left. a \sim \begin{cases} \text{pdf } f_a \\ \mathbb{E}[a] = 0, \ Var(a) = 1, \end{cases} \right\} \text{(the only random part)} \\ t \in [0, \pi] \\ \\ \end{cases}$$

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In this setting, it holds:

$$\varphi(x, \varepsilon) \sim f_1(x_1)\,\varepsilon\pi^{1/2}/\Gamma(1/2+1) = 2f_a(b)\,\varepsilon.$$

- $(X_1, \ldots, X_n)$ sample drawn from X
- we compare f_a with the 1–dim estimator $\widehat{f_1}$

Finite dimensional process

- Relative MSE: $\sum_b \left[\widehat{f_1}\left(\widehat{x}_1^b\right) - f_a\left(b\right)\right]^2 / \sum_b f_a^2\left(b\right)$

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	$a \sim N(0,1)$, $b \in [-4,4]$		$a \sim t(5)/\sqrt{5/3}$, $b \in [-4,4]$		$a \sim \left(\chi^2(8) - 8\right)/4$, $b \in [-2,6]$	
n	Mean	Std.	Mean	Std.	Mean	Std.
50	3.235	(2.681)	5.921	(2.557)	4.081	(2.842)
100	1.860	(1.444)	4.775	(1.503)	2.401	(1.619)
200	1.091	(0.824)	4.138	(0.878)	1.422	(0.887)
500	0.546	(0.355)	3.737	(0.477)	0.753	(0.443)
1000	0.330	(0.220)	3.606	(0.327)	0.453	(0.233)

- RMSE ($\times 10^2$) decreases as the sample size increases:
  - better estimates of projections $\widehat{\theta}$ and $\widehat{x}^b$
  - better performances of the kernel estimator
- Shape of distributions matters: long tails and asymmetries worse estimates

Finite dimensional process

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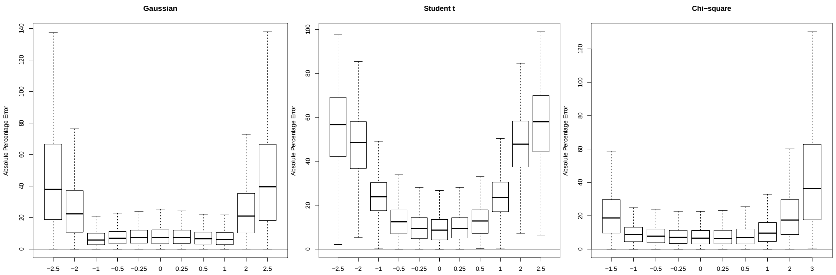

Estimate worsens at the edges due to limitations of kernel density estimator in evaluate the tails.

Infinite dimensional process

- X Stand. Brownian Motion on $[0, 1]$ ($\lambda_j \sim cost \cdot j^{-2}$).
- $x(t) = b\frac{2\sqrt{2}}{\pi}\sin\left(\frac{\pi t}{2}\right), \qquad t \in [0, 1], b \in \mathbb{R}$

$$\varphi(x, \varepsilon) \sim \exp\left\{-b^2/2\right\}\varphi(0, \varepsilon), \qquad \text{as } \varepsilon \to 0,$$

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- $x(t) = b\frac{2\sqrt{2}}{\pi}\sin\left(\frac{\pi t}{2}\right), \qquad t \in [0,1], b \in \mathbb{R}$

$$\varphi(x,\varepsilon) \sim \exp\left\{-b^2/2\right\}\varphi(0,\varepsilon), \qquad \text{as } \varepsilon \to 0,$$

- 1000 MC replication of BM sample $(X_1, \ldots, X_n)$
- the used dimension d varies in $1, \ldots, 5$
- $b \in [-4, 4]$

Infinite dimensional process

n	$d = 1$	$d = 2$	$d = 3$	$d = 4$	$d = 5$
50	3.36 (2.51)	7.20 (3.73)	13.53 (7.34)	22.03 (12.05)	31.90 (15.87)
100	1.95 (1.20)	4.82 (2.59)	9.47 (5.54)	15.86 (8.71)	23.99 (12.27)
200	1.16 (0.72)	3.14 (1.60)	6.64 (3.77)	11.51 (6.30)	17.89 (9.48)
500	0.57 (0.33)	1.78 (0.93)	4.17 (2.36)	7.77 (4.23)	12.96 (6.88)
1000	0.35 (0.19)	1.15 (0.63)	2.82 (1.64)	5.86 (3.13)	10.09 (5.43)

- Fix d, RMSE reduces (both in mean and var.) increasing n
- Fix n, RMSE increases (both in mean and var.) with d (curse of dim.)
- d vs. n: it is possible to use large d at the cost of use large samples (read diagonally the table).

OUTLINE

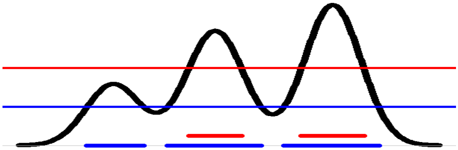
Multivariate Clustering

$$f(x) = \sum_{g=1}^{G} \pi_g f(x|g), \qquad x \in \mathbb{R}^d$$

IDEA

Regions with high density identify clusters [Wishart'69]:

- Fix c, consider the connected components of $\{f > c\}$



Clusters number depends on the threshold level c

In many cases, MODES depict structural differences among data

SmBP Mixture

- Consider the conditioned SmBP

$$\varphi(x,\varepsilon|g) = \mathbb{P}\left(\|X - x\| < \varepsilon \mid Y = g\right) \qquad g = 1, \ldots, G,$$

- Mixture + Factorization

$$\varphi(x,\varepsilon) = \sum_{g=1}^{G} \pi_g \varphi(x,\varepsilon|g) \sim f_d(x_1, \ldots, x_d)\phi(d,\varepsilon), \quad \varepsilon \to 0$$

Surrogate density f_d:

- carries spatial information on the mixture
- endorses "density oriented" clustering approach on f_d

SmBP Clustering

Consider the sample $\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ drawn from (X, Y)

- X_i are observed
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METHOD

Regions with "locally high surrogate density (f_d)" identify groups

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4. Label the unclassified X_i with the $\widehat{K}$ prototypes groups by means of a k-NN procedure.

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  Hartigan $\iff$ global threshold
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- Dependent Approach: PCs are just uncorrelated
  ([Jacques,Preda'13, Jacques,Preda'14]: PCs independent)
- Tuning d (or ε) and/or tuning the bandwidth matrix lead to different phenomenon scales

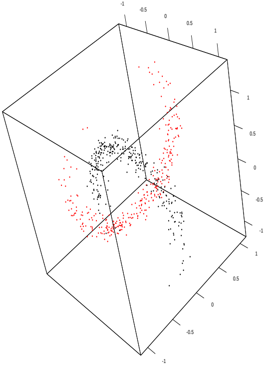
Example: Synthetic Data

$$X_i^{(g)}(t) = \sum_{l=0}^{L} \sqrt{\lambda_l}\tau_{i,l}^{(g)}\varphi_l(t),$$

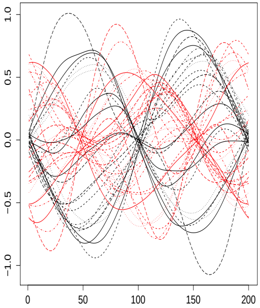
$t \in [0,1],\ i = 1,\ldots,N,\ g = 1,\ldots,G.$

- $\{\varphi_l(t)\}_l$ Fourier Basis
- $\lambda_l = 0.7 \times 3^{-l}$ $(l = 1,\ldots,L = 150)$, so that the first 3 PCs explain always more than 99%
- $G = 2$ groups and $N = 300$ curves for each group
- uncorrelated but dependent coefficients $(\tau_{i,l}^{(g)})_{l=1}^{L}$ so that the first 3 PCs looks like two bound up "bananas".

Example: Synthetic Data



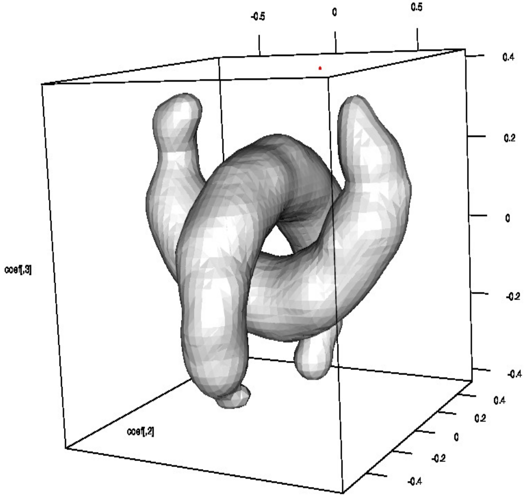
$\tau_{i,l}^{(g)}, \quad l = 1, 2, 3, \quad g = 1, 2$



sample of curves

Example: Synthetic Data

Maximum iso–surfaces (prototypes)



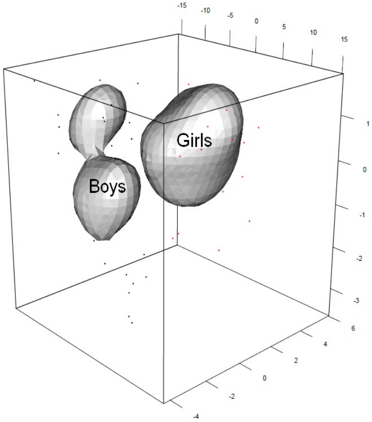
Example: Synthetic Data

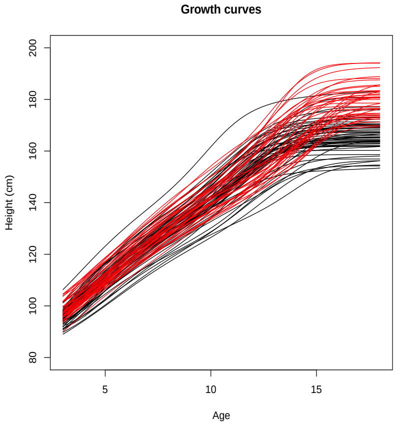
$d = 3$ (FEV criterion)
400 Monte Carlo replications

Algorithm	Miscl. Error		$\widehat{G}$		
	Mean	St. Dev.	$q_{0.5}$	$q_{0.75}$	$q_{0.9}$
SmBP	**0.088**	**0.174**	**2**	**2**	**2**
Functional K-means ($G = 2$)	0.377	0.068	–	–	–
Gaussian Mixture ($G = 2$)	0.153	0.106	–	–	–
GM BIC selection	0.666	0.034	9	10	11

Example: Growth Curves

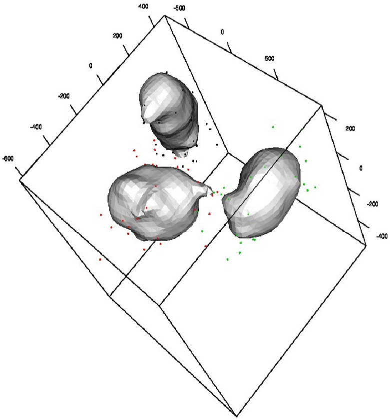
$d = 3$ (FEV) - 97.9% correct classification with respect sex

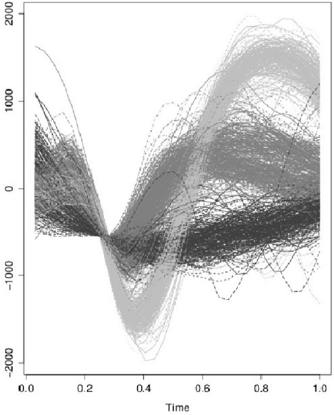




Example: Neuronal data

Iso–surfaces and Clusters





OUTLINE

Multivariate Discriminant Analysis

$$f(x) = \sum_{g=1}^{G} \pi_g f(x|g), \qquad x \in \mathbb{R}^d$$

GOAL

To label a new incoming observation x

- **Bayes Classification Rule**: assign x to the class $\gamma(x) \in \{1, \ldots, G\}$ with the highest posterior probability

$$\gamma(x) = \underset{g=1,\ldots,G}{\arg\max}\ \mathbb{P}(Y = g|X = x)$$

- If $f(x|g)$ were known ($f(x|g) > 0$):

$$\gamma(x) = \underset{g=1,\ldots,G}{\arg\max}\ \pi_g f(x|g).$$

Generalized Bayes Classification Rule

- X and Y are observed
- Consider the mixture of SmBP

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Generalized Classification Rule: assign a new functional observation x to g-th group for which, as ε tends to 0,

$$\frac{\mathbb{P}(Y=g|\ \|X-x\|<\varepsilon)}{\mathbb{P}(Y=g'|\ \|X-x\|<\varepsilon)} > 1, \qquad \text{for any } g \in \{1,\ldots,G\},\ g' \neq g.$$

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[B.,Goia'16a]

The Generalized Classification Rule is equivalent to

$$\gamma(x,d) = \arg\max_{g=1,\ldots,G} \pi_g f_d(x|g) \qquad \text{as } d \to \infty$$

Proof Sketch

- Bayes: $\mathbb{P}(Y = g \mid \|X - x\| < \varepsilon) = \dfrac{\pi_g \varphi(x, \varepsilon|g)}{\varphi(x, \varepsilon)}$

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- Simplification leads to Thesis.

Estimate the Classifier 1/2

Consider

- $\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ sample from (X, Y)
- $d_g = d$ for each $g = 1, \ldots, G$
- $\widehat{\Pi}_{g,d}$ = proj.oper. over the subspace spanned by the first d eigenfunctions of $\widehat{\Sigma}_g$

A <u>kernel estimator</u> for $\gamma(x, d)$ is:

$$\widehat{\gamma}_n(x, d) = \underset{g=1,\ldots,G}{\arg\max} \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}_{\{Y_i = g\}} K_{H_g}\left(\left\|\widehat{\Pi}_{g,d}(X_i - x)\right\|\right)$$

Estimate the Classifier 2/2

- Consider the Bayes probability of error

$$L^\star = \min_\gamma \mathbb{P}\left(\gamma\left(X\right) \neq Y\right)$$

and the conditional probability of error

$$L_n = \mathbb{P}\left(\widehat{\gamma}_n\left(X, d\right) \neq Y \mid \left\{\left(X_1, Y_1\right), \ldots, \left(X_n, Y_n\right)\right\}\right)$$

- Assume that there exists a positive integer d^* such that $\gamma(x, d) = \gamma(x, d^*)$ for any $d \geq d^*$.

[B.,Goia'16a]

Take $H_g = h_g I$.

$$L_n \longrightarrow L^\star \qquad \text{in probability} \qquad n \to \infty$$

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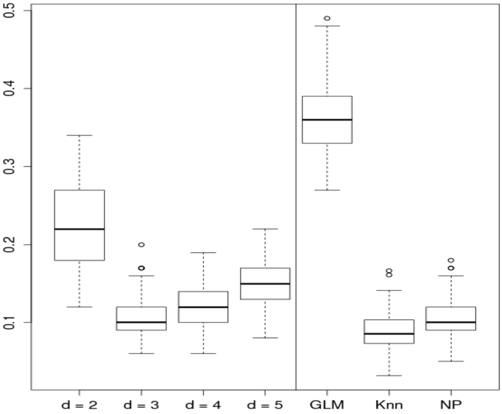
- Curse-of-dimensionality affects performances of the methodology

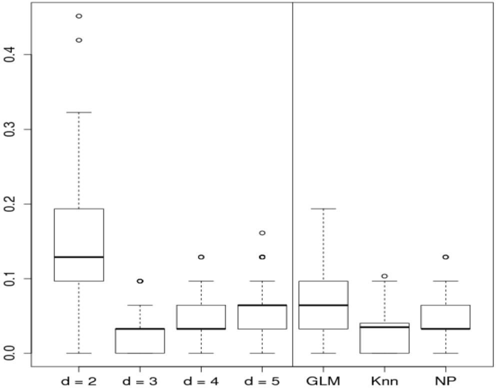
Example: Synthetic data

- Two Bananas data-set with $\pi_g = 0.5$
- Sample of size $n = 300$ split in two parts:
  training-sets ($n_{in} = 200$) $+$ test-set ($n_{out} = 100$)
- Out-of-sample misclassification error over 100 MC replications



Example: Growth curves

Out-of-sample misclassification errors over 100 MC replications (training-set is 2/3 of the sample)



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- Performances are studied on simulated and real dataset

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Thanks for your Attention