UNIVERSITÀ DEGLI STUDI DI PALERMO

dSEAS dipartimento scienze economiche aziendali e statistiche

CRoNoS

Workshop on Multivariate Data Analysis and Software

A new method for curves clustering in general dependence models

Gianluca SOTTILE and Giada ADELFIO

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Literature review

The problem of curves clustering is very complex and has been recently addressed in several fields:

- *structural averaging* in the context of computing an average (Kneip and Gasser, 1992);
- *curves registrastion* in statistics (Silverman, 1995; Ramsay and Li, 1998);
- *time warping* in engineering (Wang and Gasser, 1997)

Literature review

In statistics:

- Silverman, (1995) proposed a general approach, in which a target curve must satisfy a predefined criterion;
- Ramsay and Li, (1998) used a Procrustes fitting procedure (Gower, 1975) to provide maximal alignment to the target function;
- James, (2007) introduced a method for finding similarities between functions by equating the moments among all curves;
- Garcia-Escudero and Gordaliza, (2005) proposed a new approach based on the trimmed *k*-means Robust Curve Clustering;
- Adelfio et al., (2012) introduced a procedure to identify clusters of multivariate waveforms;
- Adelfio et al., (2016) focused on finding clusters of multidimensional curves with spatio-temporal structure.

WHAT ABOUT CURVES CLUSTERING IN GENERAL DEPENDENCE MODELS?

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QR Koenker and Bassett Jr, (1978) and Koenker, (2005)

Let be y a response variable, and $\boldsymbol{x}$ a q-dimensional vector of covariates. We assume that $Q(p \mid \boldsymbol{x}) = \boldsymbol{x}^T\beta(p)$ is the p-th quantile of y, given $\boldsymbol{x}$. The vector of quantile regression coefficients, $\beta(p)$, can be estimated by

$$\hat{\beta}(p) = \arg\min_{\boldsymbol{\beta}\in\mathcal{R}^q} \sum_{i=1}^{n} \omega_{p,i}(y_i - \boldsymbol{x}_i^T\beta)$$

where $\omega_{p,i} = \mathcal{I}(y_i \leq \boldsymbol{x}_i^T\beta)$ and $\mathcal{I}(\cdot)$ is the indicator function.

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Issues

- quantiles are estimated one at the time
- the estimated coefficients are generally non-smooth functions of p

QR Koenker and Bassett Jr, (1978) and Koenker, (2005)

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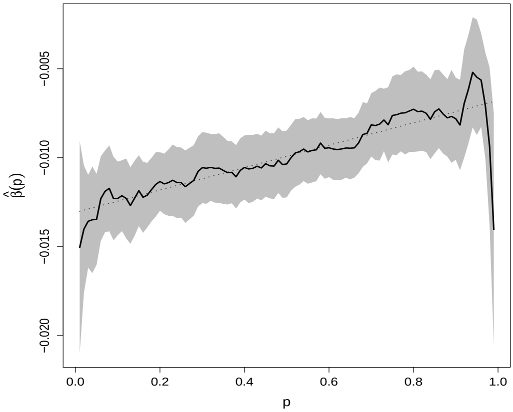

Estimated quantile regression coefficient and 95% pointwise confidence intervals (shaded area). The dotted line suggests a possible linear trend.

Contents

QRCM Frumento and Bottai, (2016)

A parametric approach to model the quantile function estimating the coefficients as functions of the order of the quantile $p \in (0, 1)$

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$$Q(p \mid \boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{x}^T \beta(p \mid \boldsymbol{\theta}),$$

- $\boldsymbol{x}$ is the model matrix ($N \times q$)
- $\beta(p \mid \boldsymbol{\theta}) = \boldsymbol{\theta}\boldsymbol{b}(p)$
- $\boldsymbol{b}(p) = [1, b_1(p), \ldots, b_k(p)]^T$ is a set of $(k+1)$ known functions
- $\boldsymbol{\theta}$ is the unknown parameter matrix

QRCM Frumento and Bottai, (2016)

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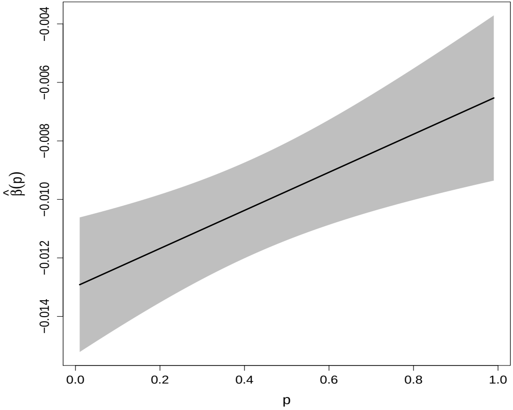

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CEC method Sottile and Adelfio

Aims

Our goal is to use the QRCM framework to answer two different questions:

- **Univariate case.** Given one response variable we estimate $\beta_1(p \mid \boldsymbol{\theta}), \ldots, \beta_q(p \mid \boldsymbol{\theta}) \Rightarrow$ the **aim** is to assess if these q curves, can be clustered based on similarities of effects

CEC method Sottile and Adelfio

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- **Multivariate case.** Given m response variables we estimate $\beta_{11}(p \mid \boldsymbol{\theta}), \ldots, \beta_{mq}(p \mid \boldsymbol{\theta}) \Rightarrow$ the **aim** is to assess if there are similar responses given covariates

Our proposal

A new dissimilarity measure, that accounts both for the **shape** and for the **distance**:

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- the *shape* evaluated using its second derivative. Moreover, two different curves are similar in shape if, at any given point, the signs of the second derivatives are concordant;

$$d^{ii'}_{\text{shape}}(\boldsymbol{p}) = \mathcal{I}(\text{sign}(\beta''_i(\boldsymbol{p} \mid \boldsymbol{\theta})) \times \text{sign}(\beta''_{i'}(\boldsymbol{p} \mid \boldsymbol{\theta})) = \mathbf{1})$$

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- the *distance* between two curves evaluated as their differences with respect to other curves. Two curves are said close if their distance at any given point is lower than a fixed value;

$$d^{ii'}_{\text{distance}}(\boldsymbol{p}) = \mathcal{I}(|\beta_i(\boldsymbol{p} \mid \boldsymbol{\theta}) - \beta_{i'}(\boldsymbol{p} \mid \boldsymbol{\theta})| \leq f(\alpha, \text{dist}(\boldsymbol{p})))$$

The cut-off function

The $f(\cdot,\cdot)$ function depends on a probability value α, and on dist(p) that is, for each percentile, the distribution of all possible distances among curves. Therefore, the cut-off function selects the α-th percentile of dist(p)

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The role of α

α is the probability value, and it has a central role for finding hoogeneous clusters. Its choice depends on the goal of the analysis and has to be fixed by the researcher.

The new dissimilarity measure

$$d(i,i') = 1 - \int_0^1 \left[d^{ii'}_{\text{shape}}(p) \cdot d^{ii'}_{\text{distance}}(p) \right] dp$$

The product of the two measures is computed, to account for their concordance at each point.

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Optimization

We implemented the above measure in the `clustEff` R package.

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Computation

Pseudo code of the algorithm implemented in the `clustEff` package

Step	Algorithm
1	fix the α-level and calculate dist($\boldsymbol{p}$) for each $p \in (0, 1)$
2	the cut-off function $f(\cdot, \cdot)$ selects the percentiles of the distribution of dist($\boldsymbol{p}$) used in $d^{ii'}_{\text{distance}}(\boldsymbol{p})$
3	compute $d^{ii'}_{\text{shape}}(\boldsymbol{p})$, $d^{ii'}_{\text{distance}}(\boldsymbol{p})$, and hence $d(i, i')$
4	apply a hierarchical clustering algorithm to the dissimilarity matrix in order to obtain the dendrogram
5	select the optimal number of clusters l^*, unless it is known in advance
6	calculate goodness-of-fit measures

Choice of the number of clusters

Effects curves

$$\pi^l = l \sum_{j=1}^{l} q_j^{-1} \sum_{i=1}^{q_j} \left\{ \int_0^1 \mathcal{I}\left(\overline{\text{LB}}_j(p) \leq \beta_j^i(p \mid \boldsymbol{\theta}) \leq \overline{\text{UB}}_j(p) \right) dp \right\},$$

The value l^* is identified by that partition for which $\pi^l - \pi^{l+1}$ is minimized

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General curves

$$\text{dist}_{\text{rel}}^l = l \sup_{j \in \{1,\dots,l\}} \left\{ q_j^{-1} \sum_{i=1}^{q_j} \int_0^1 |\overline{\beta}_j(p) - \beta_j^i(p \mid \boldsymbol{\theta})| \, dp \right\}.$$

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Simulation scenario 1

Clusters of effects

We considered a multivariate scenario in which the general quantile function was defined by

$$Q(p \mid x, \boldsymbol{\theta}) = \beta_0(p \mid \boldsymbol{\theta}) + \beta_1(p \mid \boldsymbol{\theta})x$$

where $x \sim \mathcal{U}(0, 5)$.

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where $x \sim \mathcal{U}(0, 5)$.

We defined three quantile functions and generated 30 response variables, 10 for each of them, using polynomial trends, i.e.,

1. $Q_1(p \mid x, \boldsymbol{\theta}_1) = (1 + \phi(p)) + (.5 + .5p + p^2 + 2p^3)x$
2. $Q_2(p \mid x, \boldsymbol{\theta}_2) = (1 + \phi(p)) + (-3 + .5p + p^2 + .5p^3)x$
3. $Q_3(p \mid x, \boldsymbol{\theta}_3) = (1 + \phi(p)) + (.3 - .5p - p^2 + 2p^3)x$

Simulation scenario 1

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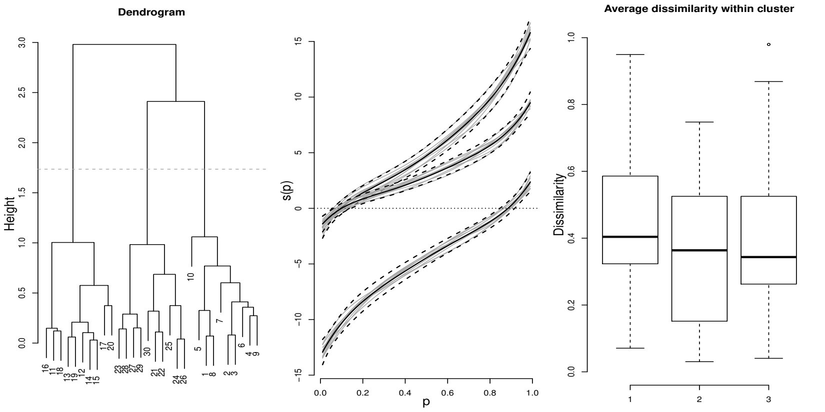

Output of the proposed algorithm for one replicate. The left panel shows the dendrogram; the middle panel shows the 30 curves clustered in 3 groups; the right panel shows the boxplot of the average dissimilarity within each cluster.

Simulation scenario 2

Waveform clustering

We simulated 30 harmonic functions evaluated at a grid of size 1000

1. $f(t) = \sin(3\pi t)$ ($\times 10$)
2. $g(t) = \cos(3\pi t)$ ($\times 13$)
3. $h(t) = \sin(3\pi t)\cos(\pi t)$ ($\times 5$)
4. $l(t) = 0$ ($\times 2$)

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A random error $\epsilon_t \sim \mathcal{N}(0, \sigma_t)$ was added to each curve to define a segmented relation with multiple change-points, such as

$$\sigma_t = 4\max(t - 0.2, 0) - 8\max(t - 0.5, 0) + 4\max(t - 0.8, 0)$$

Simulation scenario 2

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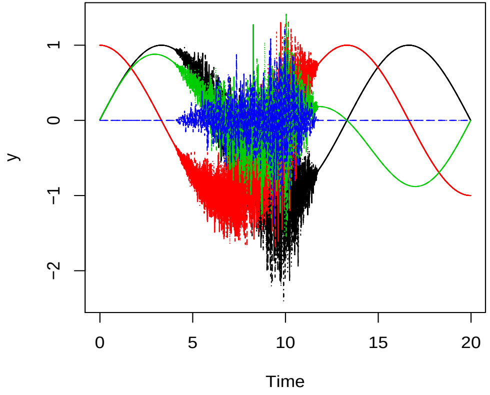

One simulated dataset

Simulation scenario 2

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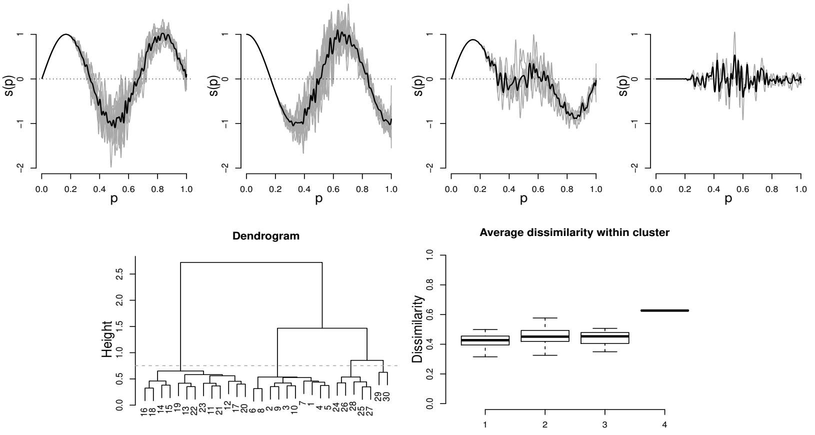

Output of the proposed algorithm for one replicate. Upper panels show the 4 clusters; bottom-left panel shows the dendrogram; bottom-right panel shows the boxplot of the average dissimilarity within each cluster.

Simulations

Methods

- `funFem`: a functional mixture model (Bouveyron and Brunet-Saumard, 2014)
- `FPCA`: a k-means algorithm based on the principal component rotation of data (Adelfio et al., 2011)

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Mesasures

- $\text{Area}(l^*) = l^{*-1} \sum_{j=1}^{l^*} \left\{ q_j^{-1} \sum_{i=1}^{q_j} \int_0^1 \left(\mid \overline{\beta}_j(p) - \beta_j^i(p \mid \boldsymbol{\theta}) \mid \right) dp \right.$
- $\rho_{\text{dist}}(l^*) = l^{*-1} \sum_{j=1}^{l^*} \left\{ 1 - \left[2 \Big(q_j(q_j - 1) \Big)^{-1} \sum_{i=1}^{q_j - 1} \sum_{z>i}^{q_j} \rho_{iz} \right]^2 \right\}$
- the average number of clusters l^*

Simulations

Average area, average distance based on correlation (ρ_{dist}) and average of the optimal number of discovered clusters (I^*) using the three different algorithms (clustEff, funFEM and FPCA) and as benchmark measure the true partition of curves in the 100 runs. SD in brackets.

		True	clustEff	funFEM	FPCA
Sim 1	I^*	3.00(0.00)	3.51(1.63)	5.06(0.98)	3.35(0.63)
	Area	0.216(0.091)	0.205(0.091)	0.178(0.079)	0.206(0.090)
	ρ_{dist}	0.010(0.015)	0.010(0.015)	0.008(0.008)	0.010(0.015)
Sim 2	I^*	4.00(0.00)	4.23(0.95)	3.44(1.05)	3.83(0.38)
	Area	0.133(0.102)	0.130(0.099)	0.177(0.146)	0.142(0.116)
	ρ_{dist}	0.441(0.177)	0.426(0.175)	0.436(0.203)	0.437(0.171)

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Inspiratory capacity data

A study carried out in 1988-1991 in Northern Italy

- $N = 2,045$ subjects (51% Male and 49% Female)
- $q = 9$ (age, height, body mass index (BMI), sex, current smoking status, occupational exposure, cough, wheezing and asthma)

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The model basis

- Intercept: $\boldsymbol{b}(p) = [1, \log(p), \log(1-p)]^T$
- Covariates: a shifted Legendre polynomials up to a 5$^{\text{th}}$ degree (Abramowitz and Stegun, 1964)

Inspiratory capacity data

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Table 1: Average area, average correlation (ρ_{dist}) and average of the optimal number of discovered clusters (l^*) are compared across the three algorithm (clustEff, funFEM and FPCA).

	clustEff	funFEM	FPCA
l^*	5	3	3
Area	0.004	0.039	0.039
ρ_{dist}	0.197	0.710	0.710

Inspiratory capacity data

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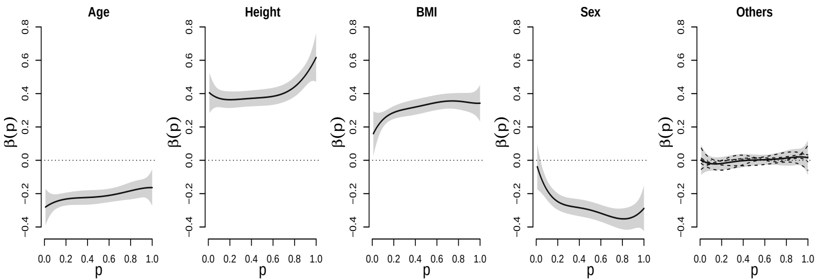

The five clusters obtained applying the clustEff algorithm on the estimated quantile regression coefficients of inspiratory capacity dataset. Black solid lines are the mean curves; the dashed lines are the effects curves; the shaded areas are identified by the mean lower and upper bands within each cluster. The dotted line indicates the zero.

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To sum-up

- We proposed a new dissimilarity measure based on similarities in shape and distance among general curves, both effects curves (in QRCM) or waveform curves;

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- We developed the `clustEff` R packages implementing the proposed algorithm;
- Results of two different simulation scenarios showed good performance of our proposal with respect of two competitors funFEM and FPCA;
- Results on the Inspiratory Capacity data showed a variable selection perspective.

Thanks for the attention!!!

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