

# Denoising and Trimming for Improved Cluster Solutions with Applications to Customs Frauds

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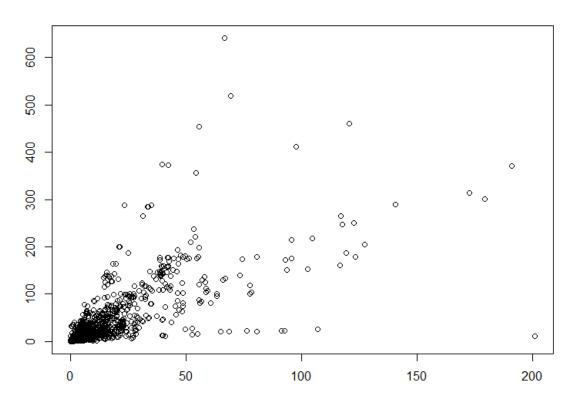


#### Plan of the talk

Trimmed & Constrained Maximum Likelihood (ML) proposals for Model Based Clustering

Robustness is based on the joint application of trimming & constraints

Clustering of Regression models
Application to Comext data

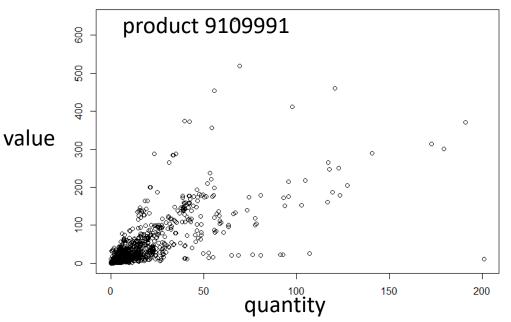


The ComExt Extra-European trade database provides statistics on merchandise trade among European Union member states, and between member states and global partners. ComExt, published by Eurostat, is based on data provided by the statistical agencies of the EU member states and trading partners. The statistics of interest for anti-fraud are mainly the traded volumes and values for a fixed product, which are aggregated monthly by Eurostat.

We are interested in applying robust clustering procedures for identifying outliers in the ComExt Extra-European trade database by thinking about its usefulness in fraud detection.

There are robust procedures available for clustering data in different settings, including ones devoted to identifying clusters around linear subspaces which appear to be well suited for

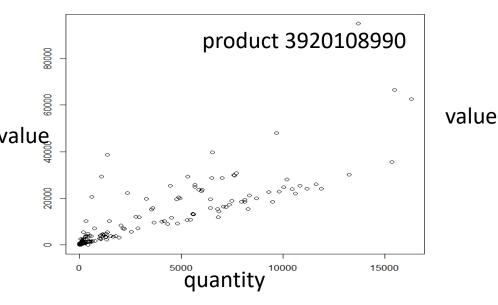
datasets in this database.

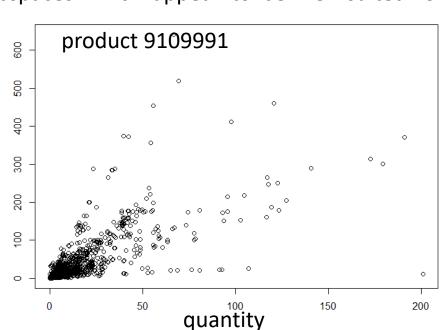


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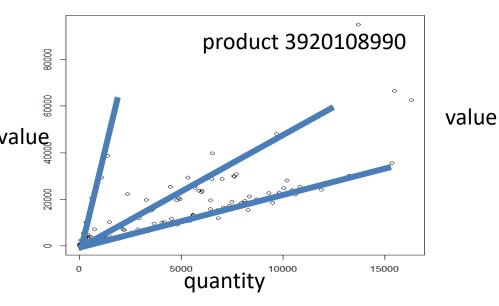


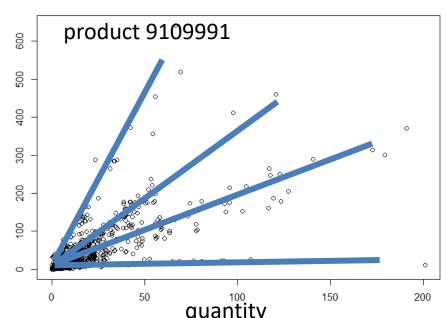
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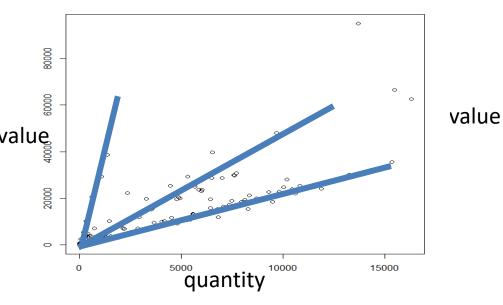


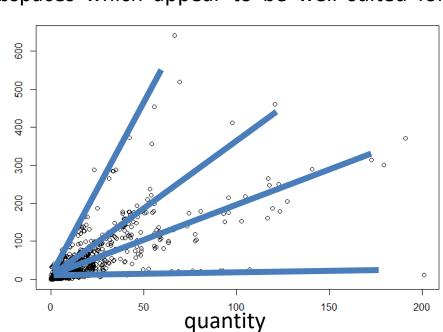
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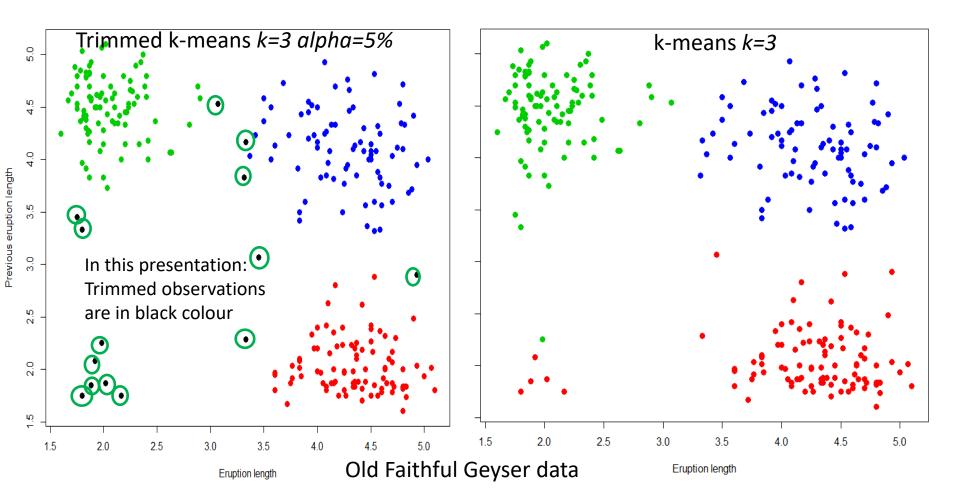
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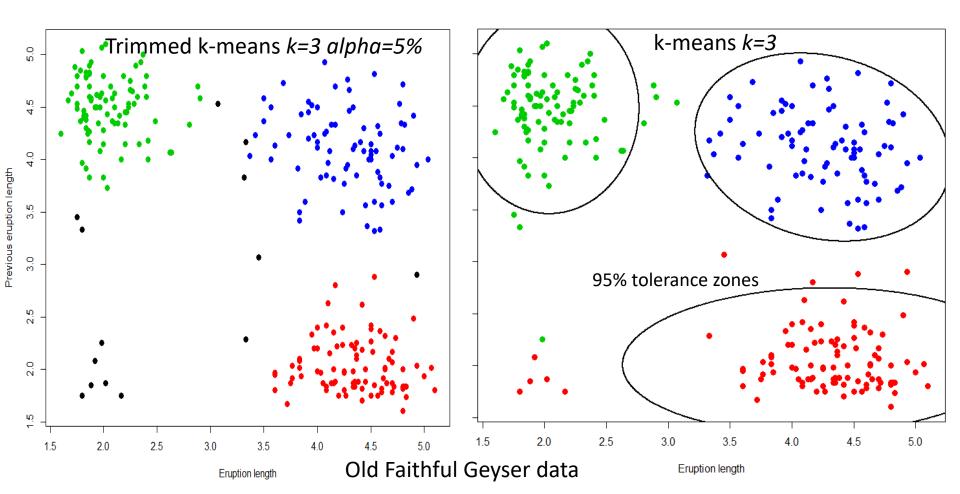


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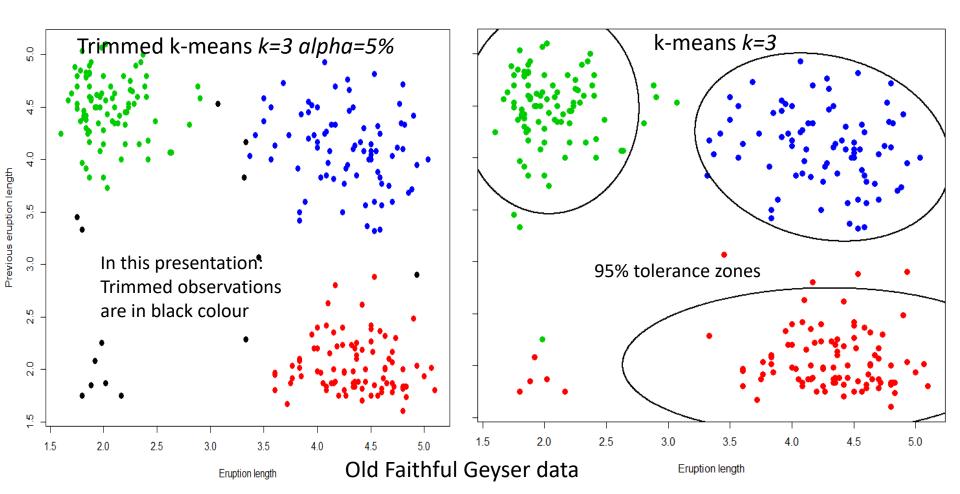
Trimmed k-means. Cuesta, Gordaliza and Matran (1997) Trimmed k-means: an attempt to robustify quantizers. The Annals of Statistics, 25(2), 553-576.



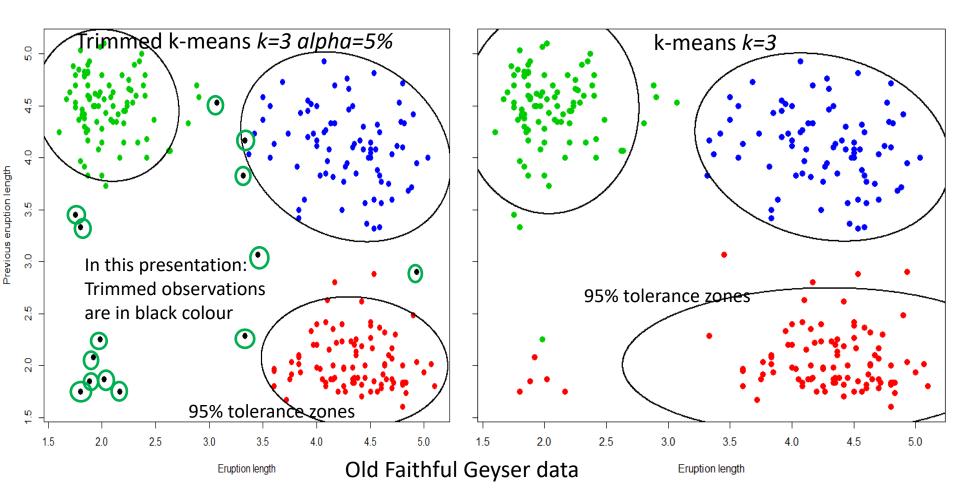
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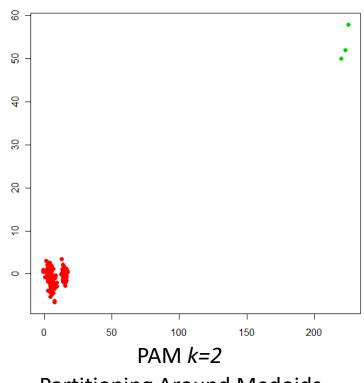


k-means is not a robust procedure.

Possible effects produced by contamination in clustering:

- To change the estimation of location and scatter corresponding to each true group
- To merge several real groups in one component of the solution

Alternatives based on M-estimators increase the resistance against the influence of outliers.



Partitioning Around Medoids

But, our recommendation is to use trimming for avoiding the influence of contamination in the cluster parameters estimation. The level of trimming,  $\alpha$ , is given in advance and has to be greater than the contamination level.

Robustness is based on impartial trimming: the sample decides which is the best way to trim.

Given a sample 
$$\{x_1...x_i...x_n\}$$

to find the best k quantizers

in the sense of 
$$\left(\mu_1...\mu_j...\mu_k\right)$$
 Trimmed k-means  $k$ =3 alpha=5% arg  $\min_{\mu,z} \min_{A/\mathbf{P}_n(A)=1-\alpha} \sum_{i=1}^n I_A(x_i) \sum_{j=1}^k z_{ij} \left\|x_i - \mu_j\right\|^2$  where

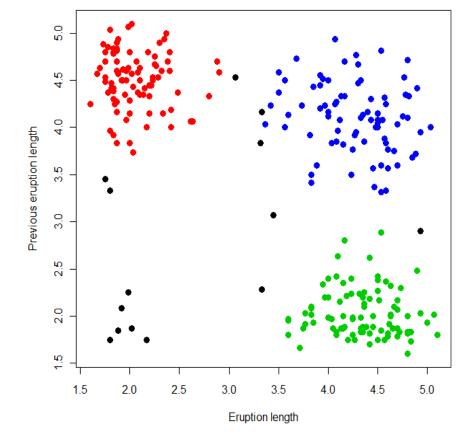
 $z_{ij}=0$  or 1 with  $\sum_{j=1}^k z_{ij}=1$  defines the assignment  $I_A(x)$  Indicator of belonging to A is a set with size 1- $\alpha$  containing the non-trimmed observations.

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 arg  $\min_{\mu,z}$ 



Trimmed k-means *k=3 alpha=5%* 

$$\sum_{i=1}^k z_{ij} \left\| x_i - \mu_j \right\|^2$$

where

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Robustness is based on impartial trimming: the sample decides which is the best way to trim.

Given a sample  $\{\chi_1 ... \chi_i ... \chi_n\}$ 

To find the best *k* quantizers

in the sense of 
$$\left(\mu_1...\mu_j...\mu_k\right)$$
 
$$\underset{\mu,z}{\arg\min} \min_{A/\mathrm{P}_n(A)=1-\alpha} \sum_{i=1}^n I_A(x_i) \sum_{j=1}^k z_{ij} \left\|x_i-\mu_j\right\|^2$$

$$\arg \sup_{\mu, z} \sup_{A/P_n(A)=1-\alpha} \sum_{i=1}^n I_A(x_i) \sum_{j=1}^k z_{ij} \log \left( \pi_j N_{\mu_j, \Sigma_j}(x_i) \right)$$

previous eruption length 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 Eruption length

$$\sum_{j=1}^{N_i} \sum_{ij} \|X_i - \mu_j\|$$
 $\sum_{ij} \log \left(\pi_j N_{\mu_i, \Sigma_i}(x_i)\right)$ 

with the constraints  $\sum_{1=\ldots=\pi_{j}=\ldots=\pi_{k}=m} = \sum_{1=\ldots=\pi_{k}=m} =$ 

Normal density

Robustness is based on impartial trimming: the sample decides which is the best way to trim.

Given a sample  $\{\chi_1 ... \chi_i ... \chi_n\}$ 

To find the best *k* quantizers

in the sense of

arg min

$$\underset{a,z}{\operatorname{rg sup}} \sup \sum_{A/P} \sum_{i=1}^{n} I_A(x_i) \sum_{i=1}^{k} z_{ij} \log \left( \pi_j N_{\mu_j, \Sigma_j}(x_i) \right)$$

with the constraints  $\sum_1 = \ldots = \sum_j = \ldots = \sum_k = \lambda I_p$   $\pi_1 = \ldots = \pi_i = \ldots = \pi_\iota$ 

previous eruption length

3.5

4.5

5.0

 $\mathbf{Y}_{A}(x_{i}) \sum_{ij}^{k} z_{ij} \left\| x_{i} - \mu_{j} \right\|^{2}$ 

Robustness is based on impartial trimming: the sample decides which is the best way to trim.

Given a sample 
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To find the best *k* quantizers

in the sense of  $(\mu_1...\mu_j...\mu_k)$  arg  $\min_{\mu,z} \min_{A/P_n(A)=1-\alpha} \sum_{i=1}^n I_A(x_i) \sum_{j=1}^k z_{ij} \left\| x_i - \mu_j \right\|^2$  Trimming & constraints  $\arg\sup_{\mu,z} \sup_{A/P_n(A)=1-\alpha} \sum_{i=1}^n I_A(x_i) \sum_{j=1}^k z_{ij} \log \left(\pi_j N_{\mu_j,\Sigma_j}(x_i)\right)$  with the constraints  $\sum_{1}^n \sum_{j=1}^n \sum_{m=1}^n \sum_{m$ 

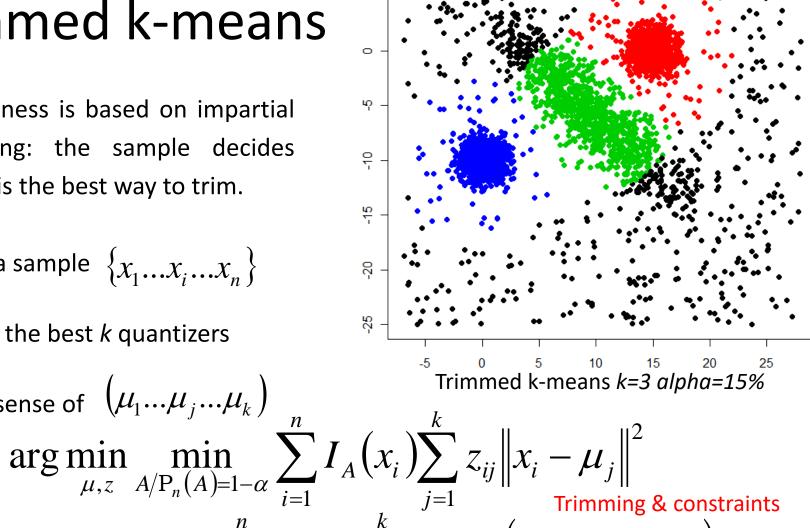
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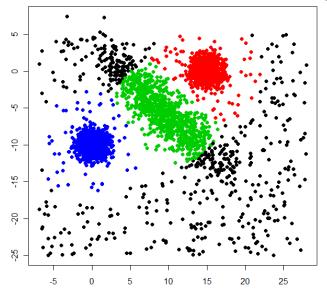
$$\underset{\mu,z}{\operatorname{arg \, min}} \min_{A/P_n(A)=1-\alpha}$$



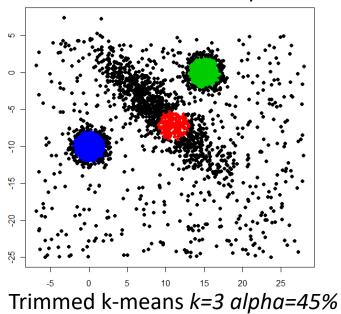
$$\arg\sup_{\mu,z} \sup_{A/P_n(A)=1-\alpha} \sum_{i=1}^{n} I_A(x_i) \sum_{j=1}^{k} z_{ij} \log(\pi_j N_{\mu_j,\Sigma_j}(x_i))$$

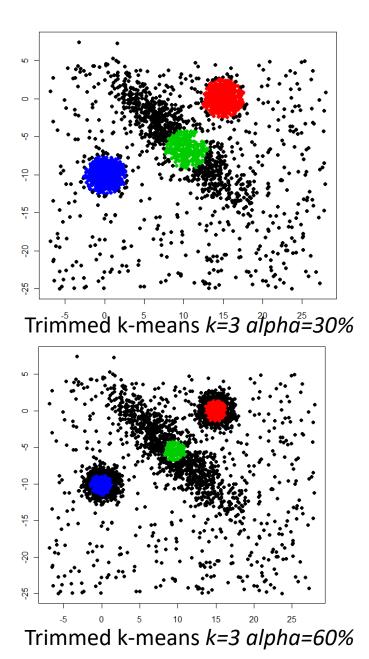
$$\lim_{\mu,z} \sup_{A/P_n(A)=1-\alpha} \sum_{i=1}^{n} I_A(x_i) \sum_{j=1}^{k} z_{ij} \log(\pi_j N_{\mu_j,\Sigma_j}(x_i))$$
with the constraints  $\Sigma_1 = \dots = \Sigma_n = \lambda I$ 

with the constraints  $\Sigma_1 = \dots = \Sigma_j = \dots = \Sigma_k = \lambda I_p$   $\pi_1 = \dots = \pi_j = \dots = \pi_k$  Very strong constraints



Trimmed k-means *k=3 alpha=15%* 





# **TCLUST** methodology

García-Escudero, Gordaliza, Matrán and M-I (Annals of Stat. 2008).

Estimator (likelihood based)

$$\arg \sup_{\theta \in R, z} \sup_{A/\#A = n(1-\alpha)} \sum_{i=1}^{n} \sum_{j=1}^{\kappa} I_{A}(x_{i}) z_{ij} \log(\pi_{j} N_{\mu_{j}, \Sigma_{j}}^{p}(x_{i}))$$

where k is the number of components

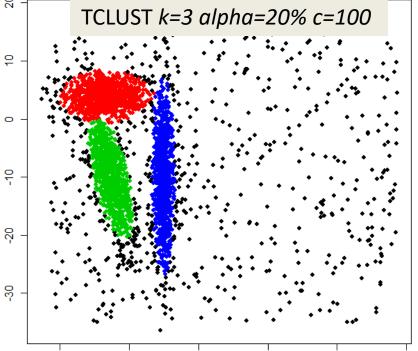
 $X_1, X_2, ..., X_n$  is a random sample

 $N_{\mu,\Sigma}^{p}(x)$  is the Normal density

$$\theta = \left(\pi_1, \mu_1, \Sigma_1, ..., \pi_j, \mu_j, \Sigma_j, ..., \pi_k, \mu_k, \Sigma_k\right)$$

- Missing information
  - $\begin{array}{ll} \bullet \text{ Membership} & Z_{ij} \\ \text{which verifies} & \sum_{j=1}^k Z_{ij} = 1 & \text{\&} & Z_{ij} = 0 \text{ or } 1 \\ \bullet \text{ Genuineness} & I_A \Big( X_i \Big) \\ \end{array}$
  - which verifies  $\sum_{i=1}^{n} I_{A}(x_{i}) = n(1-\alpha)$

 $\Sigma_1 = \dots - \Sigma_j = \dots = \Sigma_k = \lambda I_p \text{ weaker}$   $\pi_1 = \dots = \pi_j = \dots = \pi_k \text{ constraints}$ 

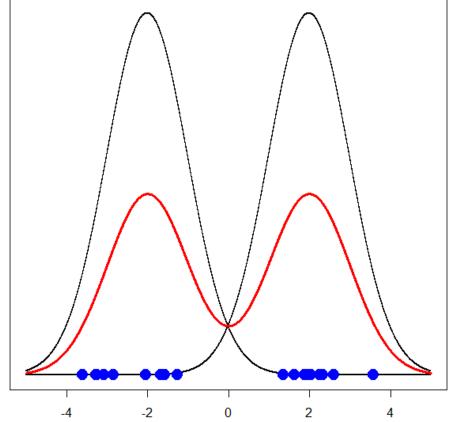


#### Mixture of normal distributions

Density of a mixture of normal distributions

$$\sum_{j=1}^{G} \pi_j \, N_{\mu_j, \Sigma_j}(x)$$

 $N_{\mu,\Sigma}(x)$  is the density of a Normal distribution with parameters  $\mu$  and  $\Sigma$  Mixture distribution parameter  $\psi = \{\theta_1, \theta_2, \dots, \theta_G\}$  where  $\theta_j = (\pi_j, \mu_j, \Sigma_j)$  j = 1...G



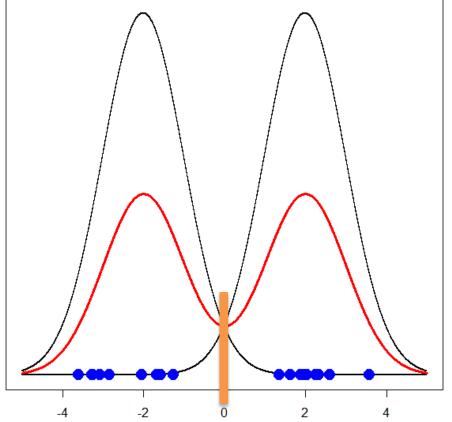
density of a mixture of normals (red) and normal components (black) points from a random sample of the mixture (blue)

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density of a mixture of normals (red) and normal components (black) points from a random sample of the mixture (blue)

Maximum likelihood estimation for finite mixture model/clustering model

$$x_1, x_1, \dots, x_n$$

Likelihood mixture model

$$\arg \sup_{\theta} \sum_{i=1}^{n} \log \left( \sum_{j=1}^{k} \pi_{j} \frac{1}{(2\pi)^{p/2} |\Sigma_{j}|^{1/2}} exp\left( -(1/2) (x_{i} - \mu_{j})' \Sigma_{j}^{-1} (x_{i} - \mu_{j}) \right) \right)$$

Likelihood clustering

$$\arg \sup_{\theta} \sum_{i=1}^{n} \sum_{j=1}^{k} \log(\pi_{j}) z_{ij} - (1/2) \log(|\Sigma_{j}|) z_{ij} - (1/2) z_{ij} (x_{i} - \mu_{j})' \Sigma_{j}^{-1} (x_{i} - \mu_{j})$$

Without constraints, the estimation problem is not well posed.

There are singularities in the likelihood

By choosing  $\mu_1 = x_1$  and  $|\Sigma_1| \to 0$ , we can get the likelihood goes to  $\infty$ . Then, how we can define Maximum Likelihood Estimator?

Maximum likelihood estimation for finite mixture model/clustering model

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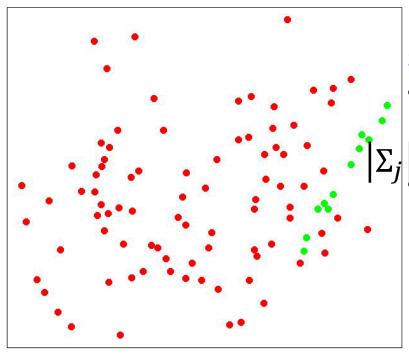
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Then, how we can define Maximum Likelihood Estimator?

maximum of local maximizers??

$$\arg \sup_{\theta} \sum_{i=1}^{n} \log \left( \sum_{j=1}^{k} \pi_{j} \frac{1}{(2\pi)^{p/2} |\Sigma_{j}|^{1/2}} exp\left( -(1/2) (x_{i} - \mu_{j})' \Sigma_{j}^{-1} (x_{i} - \mu_{j}) \right) \right)$$



#### Synthetic data set 2 (McP2000)

Mixture of two normal heteroscedastic populations without contamination

#### **Spurious clusters**

- "little practical use or real-world interpretation" (McLachlan &Peel, 2000
  McP2000)
  - "It often seems in these cases that the model is fitting a small localized random pattern in the data rather than any underlying group structure" . (McP2000)

Maximum likelihood function for a finite mixture model

How to define MLE?

$$\arg \sup_{\theta} \sum_{i=1}^{n} \log \left( \sum_{j=1}^{k} \pi_{j} \frac{1}{(2\pi)^{p/2} |\Sigma_{j}|^{1/2}} exp\left( -(1/2) (x_{i} - \mu_{j})' \Sigma_{j}^{-1} (x_{i} - \mu_{j}) \right) \right)$$

To apply constraints

$$\Sigma_i = \lambda I$$
 (k-means // trimmed k-means)

$$\Sigma_i = \Sigma$$

$$|\Sigma_j| = |\Sigma|$$

Hathaway proposal for univariate mixtures (Annals Stat. 1985): In order to get a well posed estimation-problem, to constrain the relative variability between components

$$\sigma_i \leq c\sigma_j$$
 for each  $i, j \ 1 \leq i, j \leq k$ 

#### **TCLUST. Constraints**

In order to get a well posed estimation-problem a solution is to restrict the relative variability between components (Hathaway, Annals Stat. 1985)

For the multivariate case, implemented in TCLUST:

• Eigenvalue constraints (Ingrassia and Rocci, 2007)

$$\frac{\lambda_{\Sigma_{j_1}}^{l_1}}{\lambda_{\Sigma_{j_2}}^{l_2}} \le c , \ 1 \le j_1, j_2 \le k \qquad 1 \le l_1, l_2 \le p$$

c is a boundary for the relative variability. It corresponds to restr.fact in R TCLUST.

To set the boundary for the restrictions equal to c is equivalent to bound the relative size of the tolerance ellipsoids' axis by  $\sqrt{c}$ 

These constraints are not affine equivariant

• Determinant constraints (McLachlan and Peel, 2000 - McP2000). These are affine equivariant constraints

$$\frac{\left|\Sigma_{j_1}\right|}{\left|\Sigma_{j_2}\right|} \le c , \ 1 \le j_1, j_2 \le k$$

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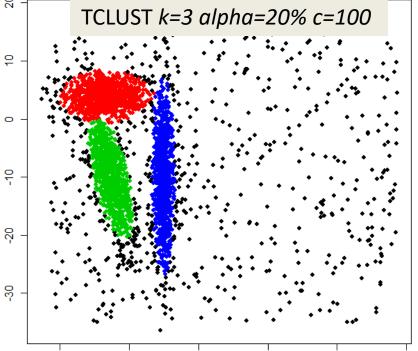
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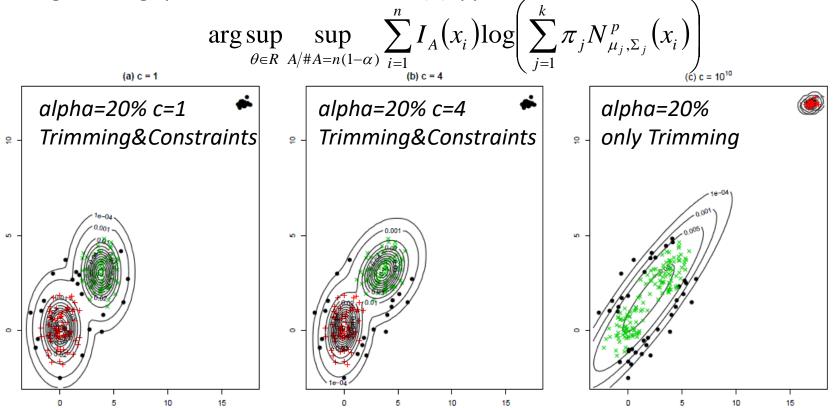
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# Trimmed & Constrained Maximum likelihood Mixture Normal models

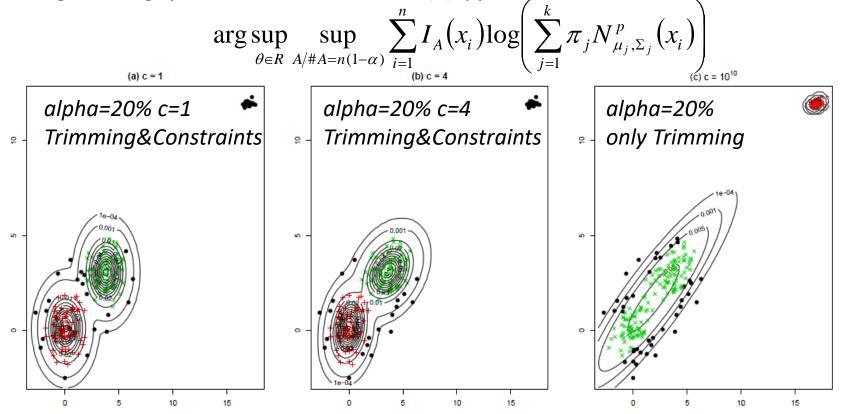
Trimming & Eigenvalue constraints applied to ML finite mixture models estimation García-Escudero, Gordaliza and M-I (2014). A constrained robust proposal for mixture modeling avoiding spurious solutions. ADAC 8 (1), pp 27-43



Fitted mixtures for the data in scenario S2 with n = 200 when G = 2 and  $\alpha = 0.2$ . Restriction value c = 1 is used in (a), c = 4 in (b) and  $c = 10^{10}$  (almost unrestricted) in (c).

# Trimmed & Constrained Maximum likelihood Mixture Normal models

Trimming & Eigenvalue constraints applied to ML finite mixture models estimation García-Escudero, Gordaliza and M-I (2014). A constrained robust proposal for mixture modeling avoiding spurious solutions. ADAC 8 (1), pp 27-43



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#### Genuine bank notes identification

**Bank notes.** Flury, B. and Riedwyl, H. (1988). 200 printed Swiss 1000-franc bank notes divided in two groups: 100 genuine and 100 counterfeit notes. It is a well known benchmark data set

Dotto, F., Farcomeni, A., García-Escudero, L. A., & M-I, A. (2018). A reweighting approach to robust clustering. Stat. and Comp., 28(2), 477-493.

Fritz, H., Garcia-Escudero, L. A., & M-I, A. (2012). tclust: An R package for a trimming approach to cluster analysis. Journal of Statistical Software, 47(12), 1-26. García-Escudero, L. A., Gordaliza, A., Matrán, C., & M-I, A. (2011). Exploring the number of groups in robust model-based clustering. Stat. & Comp., 21(4), 585-599.

Image from Flury and Riedwyl (1988).

(a) Three clearaffication (lat vs. 4th)

(b) Initial clearating (c) Final clearating

(c) Final clearating

(c) Final clearating

(c) Final clearating

(d) Three clearaffication (lat vs. 4th)

(e) Initial clearating

(f) Final clearating

(g) Initial clearating

(g) Ini

Fig. 8 Fourth against the sixth variable of the Swiss Bank Notes data set. (a) G stands for genuine bills, F for forged ones and 15 bills listed in Flury and Riedwyl (1988) as anomalous ones are surrounded by "o" symbols. (b) The initial TCLUST solution with  $\alpha_0=0.33$  (c) Final solution when applying the proposed iterative approach. Trimmed observations not coinciding with those in Flury and Riedwyl's list are surrounded by " $\Box$ " symbols in (b) and

#### Genuine bank notes identification

Bank notes. Flury, B. and Riedwyl, H. (1988). 200 printed Swiss 1000-franc bank notes divided in two groups: 100 genuine and 100 counterfeit notes. It is a well

known benchmark data set Image from Flury and Riedwyl (1988). Length of the diagonal 12 0.05 0.10 0.15 0.20

Distance of the inner frame to lower border

### **TCLUST. Trimming & Constraints**

#### Early impartial trimming references

- Rousseeuw, P. J., JASA (1984) & Mathematical Statistics and Applications, B, (1985)
- Neykov, N. M. and P. N. Neytchev (1990). Short communications of COMPSTAT
- Gordaliza, A. (1991). Journal of Approximation Theory
- Cuesta-Albertos, J. A., Gordaliza, A., & Matrán, C. (1997). The Annals of Statistics
- Hadi, AS Luceño (1997). Computational Statistics & Data Analysis
- Vandev, D. L., & Neykov, N. M. (1998). A Journal of Theoretical and Applied Statistics
- García-Escudero, Gordaliza, Matrán and M-I. (2008) Annals of Statistics

#### Early references related with constraints application proposals

- Hathaway (1985). Annals of Statistics
- Gallegos and Ritter (2005). Annals of Statistics
- Ingrassia and Rocci (2007). Computational Statistics & Data Analysis
- García-Escudero, Gordaliza, Matrán and M-I. (2008) Annals of Statistics

# TCLUST Statistical properties

#### Statistical methodology

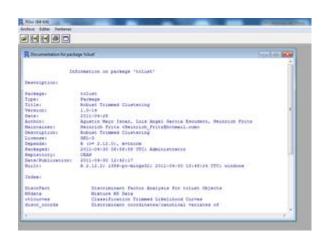
- Well posed statistical problem. We are interested in the maximum in the restricted parameter space.
- Existence and Consistency (García-Escudero, Gordaliza, Matrán and M-I, Annals of Stat. 2008).
- Breakdown point≈alpha (in the sense of Hennig (2004))

# TCLUST Algorithm

Fast algorithm for TCLUST (Fritz, García-Escudero and M-I. CSDA, 2013)

- Random starts
- Iterations
  - E step, to assign each point to the closest component, in the sense given by a greatest value in the discriminant functions  $\pi_j N_{\mu_j,\Sigma_j}(x_i)$  and to obtain the **optimal** *A* **set** is given by the 1- $\alpha$  proportion of closest points to the model in the sense of  $\pi_{j^{opt}} N_{\mu_{iopt},\Sigma_{jopt}}(x_i)$
  - M step, to obtain the best value for the parameters in **the constrained space**. The current release of the algorithm reduces this search to a set of kp + 2 possible solutions obtained in a explicit way. In relation with the classical ML estimator, the change appears in the estimation of  $\Sigma_j$ , which corresponds to the projection of matrices  $S_i$  in the constrained space.

#### TCLUST R & MATLAB





TCLUST in CRAN. TCLUST package. Maintainer: Valentin Todorov

Fritz, García-Escudero and M-I (2012) Tclust: An R Package for a Trimming Approach to Cluster Analysis. J.Stat. Soft. 47(12), 1-26.

TCLUST in Matlab. FSDA library.

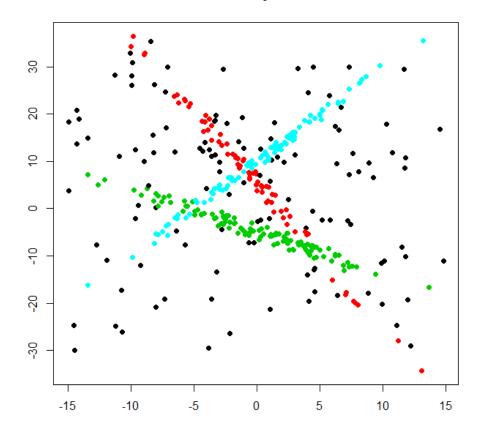
Riani, Perrotta & Torti, F. 2012. FSDA: A MATLAB toolbox for robust analysis and interactive data exploration. *Chemometrics and Intelligent Laboratory Systems*, 116, 17–32 Ro.Sta.Bi.Da.C - CENTRO DI STATISTICA ROBUSTA PER GRANDI BANCHE DATI (ROBUST STATISTICS FOR BIG DATA CENTRE) of University of Parma. Marco Riani and Andrea Cerioli. JRC Ispra. Domenico Perrotta and Francesca Torti.

# Clustering/mixture regression models

## Trimming & Constraints Clustering of regression models

Trimming & Constraints in order to get robust clustering of regression models. García-Escudero, Gordaliza, M-I & San Martín (CSDA, 2010).

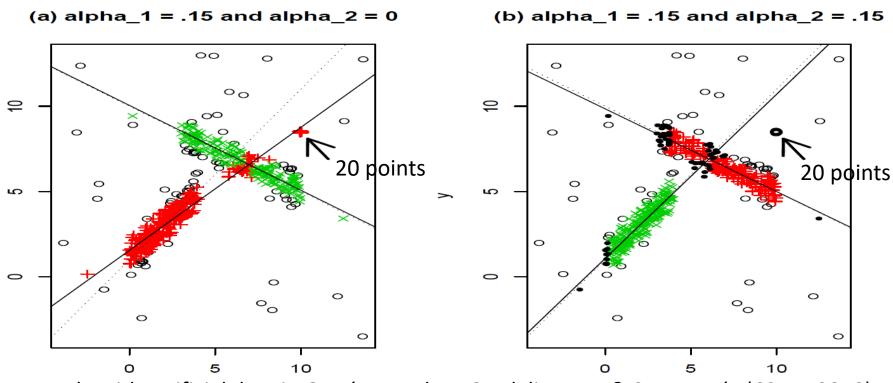
$$\arg \sup_{\theta \in R} \sup_{z} \sup_{A/\#A = n(1-\alpha)} \sum_{i=1}^{n} \sum_{j=1}^{k} I_{A}(x_{i}, y_{i}) z_{ij} \log \left(\pi_{j} N_{0, \sigma_{j}}^{1} \left(y_{i} - \beta_{0} - \beta_{j} x_{i}\right)\right)$$



$$\frac{\sigma_{j_1}^2}{\sigma_{j_2}^2} \le c , \ 1 \le j_1, j_2 \le k$$

## Trimming & Constraints Clustering of regression models

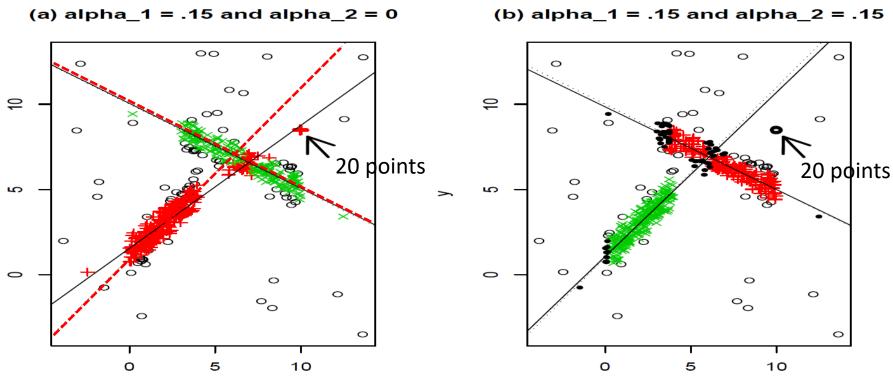
Trimming & Constraints in order to get robust clustering of regression models. García-Escudero, Gordaliza, M-I & San Martín (CSDA, 2010). A second trimming can be included in the E step of EM algorithm in order to eliminate outliers in explanatory variables.



Example with artificial data in García-Escudero Gordaliza, M-I & San Martín (CSDA, 2010).

## Trimming & Constraints Clustering of regression models

Trimming & Constraints in order to get robust clustering of regression models. García-Escudero, Gordaliza, M-I & San Martín (CSDA, 2010). A second trimming can be included in the E step of EM algorithm in order to eliminate outliers in explanatory variables.



Example with artificial data in García-Escudero Gordaliza, M-I & San Martín (CSDA, 2010).

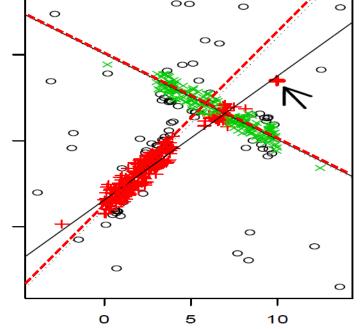
#### Cluster weighted model

Cluster Weighted Model (CWM) is a mixture approach to modeling the joint probability of data coming from a heterogeneous population. Introduced in Gershenfeld (1997) under Gaussian and linear assumptions.

CWM decomposes the joint probability in each component of the mixture as the product of the marginal and the conditional distributions.

$$\sum_{j=1}^{k} \pi_{j} N_{0,\sigma_{j}}^{1} \left( y - \beta_{0} - \beta_{j} x \right) N_{\mu,\Sigma_{j}}^{p} \left( x \right)$$

Ingrassia et al. (2012) shows that Gaussian ©
CWM includes, as special cases,
Multivariate Finite Mixture Models & ©
Classical Finite Mixture Regression Models



## Trimming & Constraints Cluster weighted model

Trimmed Cluster Weighted Restricted Modeling (TCWRM). García-Escudero, Gordaliza, Greselin, Ingrassia & M-I (Stat&Comp, 2017)

$$\arg \sup_{\theta \in R} \sup_{A/\#A = n(1-\alpha)} \sum_{i=1}^{n} I_{A}(x_{i}, y_{i}) \log \left( \sum_{j=1}^{k} \pi_{j} N_{0,\sigma_{j}}^{1} (y_{i} - \beta_{0} - \beta_{j} x_{i}) N_{\mu,\Sigma_{j}}^{p} (x_{i}) \right)$$

We apply jointly trimming and two kind of constraints

Eigenvalue constraints for controlling the relative variability of regression errors

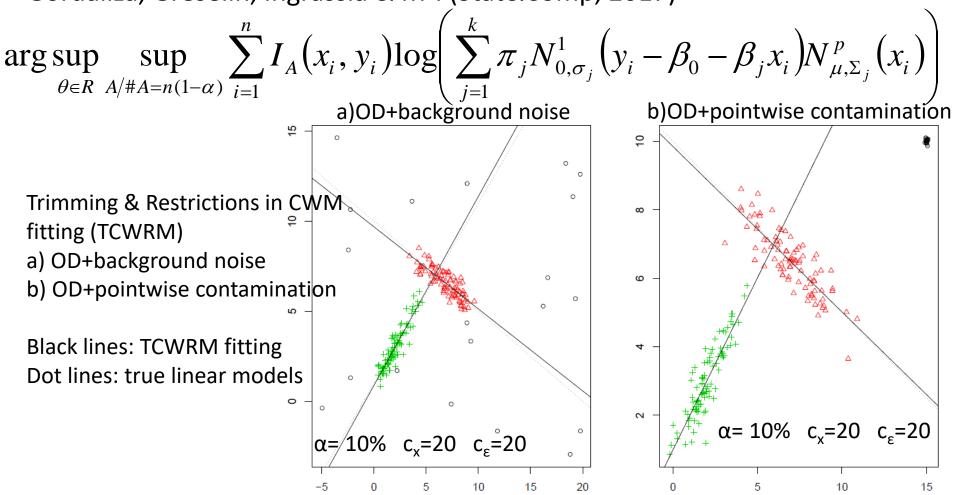
$$\frac{\sigma_{j_1}^2}{\sigma_{j_2}^2} \le c_x, \ 1 \le j_1, j_2 \le k$$

 Eigenvalue constraints for controlling the relative variability of explanatory variables ,

$$\frac{\lambda_{\Sigma_{j_1}}^{l_1}}{\lambda_{\Sigma_{j_2}}^{l_2}} \leq c_{\varepsilon} , \ 1 \leq j_1, j_2 \leq k \qquad 1 \leq l_1, l_2 \leq p$$

## Trimming & Constraints Cluster weighted model

Trimmed Cluster Weighted Restricted Modeling (TCWRM). García-Escudero, Gordaliza, Greselin, Ingrassia & M-I (Stat&Comp, 2017)



From García-Escudero, Gordaliza, Greselin, Ingrassia & M-I (2014)

### TCLUST REG // TCLUST CWM

Torti, F., Perrotta, D., Riani, M., & Cerioli, A. (2019). Assessing trimming methodologies for clustering linear regression data. *Advances in Data Analysis and Classification*, 13(1), 227-257.

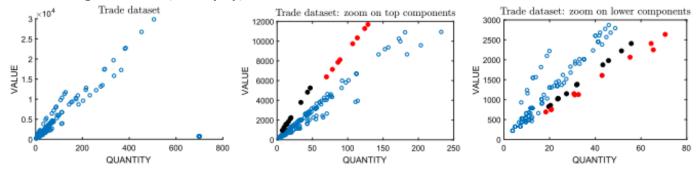


Fig. 12 Scatterplots of case study 5. Trade dataset formed by customs declarations made by an EU importer. The axes report the declared values (y-axis) and quantities (x-axis). The left panel plots the data in the original scale. The central and right panels zoom in the data to highlight the presence of components that are difficult to notice in the original scale

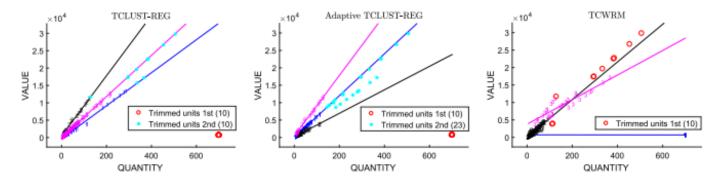


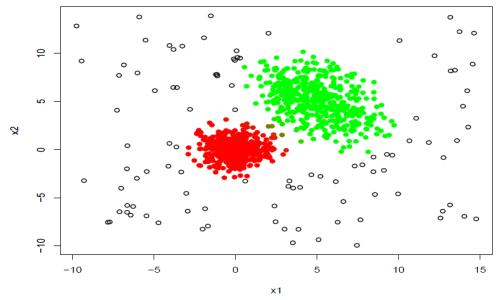
Fig. 13 Case study 5. Dataset of Figure 12 analyzed with three components (G = 3) with, from left to right, TCLUST-REG, Adaptive TCLUST-REG and TCWRM

## **Fuzzy TCLUST**

#### **Trimming & Constraints Fuzzy clustering**

Fritz, García-Escudero and M-I (2013), Robust Constrained Fuzzy Clustering. Information Sciences, 245, 38-52

$$\arg \sup_{\mu,u} \sup_{A/P_n(A)=1-\alpha} \sum_{i=1}^n I_A(x_i) \sum_{j=1}^k u_{ij}^m \log \left(\pi_j N_{(\mu_j, \Sigma_j)}(x_i)\right) \frac{\lambda_{\Sigma_{j_1}}^{l_1}}{\lambda_{\Sigma_{j_2}}^{l_2}} \le c, \ 1 \le j_1, j_2 \le k \qquad 1 \le l_1, l_2 \le p$$



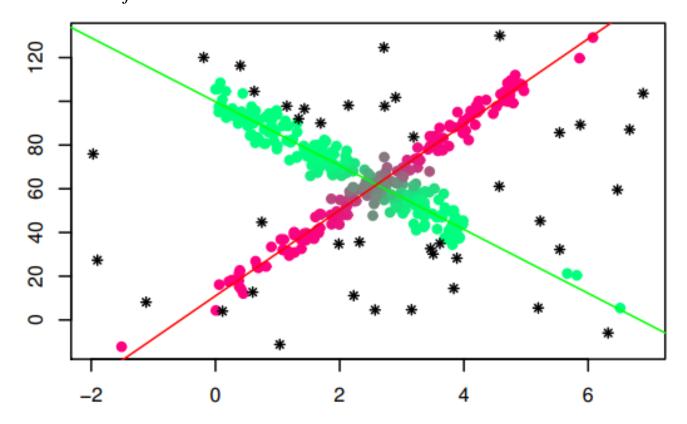
 $\alpha=0.1$  for a 10% contamination level  $\Rightarrow$  Trimmed points: " $\circ$ "

### **Fuzzy TCLUST Reg**

Dotto, Farcomeni, García-Escudero, M-I (2017) A fuzzy approach to robust regression clustering. ADAC

$$\arg \sup_{\theta \in R} \sup_{z} \sup_{A/\#A = n(1-\alpha)} \sum_{i=1}^{n} \sum_{j=1}^{k} I_{A}(x_{i}, y_{i}) u_{ij}^{m} \log \left(\pi_{j} N_{0, \sigma_{j}}^{1} \left(y_{i} - \beta_{0} - \beta_{j} x_{i}\right)\right)$$

$$\frac{\sigma_{j_1}^2}{\sigma_{j_2}^2} \le c , \ 1 \le j_1, j_2 \le k$$



### Robust fuzzy cluster weighted modeling

Trimming & Constraints to Fuzzy cluster weighted Model

$$\arg \sup_{\theta \in R, u} \sup_{A/\#A = n(1-\alpha)} \sum_{i=1}^{n} I_{A}(x_{i}, y_{i}) \left( \sum_{j=1}^{k} u_{ij}^{m} \log \left( \pi_{j} N_{0, \sigma_{j}}^{1} \left( y_{i} - \beta_{0} - \beta_{j} x_{i} \right) N_{\mu, \Sigma_{j}}^{p} \left( x_{i} \right) \right) \right)$$

We apply jointly trimming and two kind of constraints

• Eigenvalue constraints for controlling the relative variability of regression errors  $\sigma_{j_1}^2$ 

 $\frac{\sigma_{j_1}^2}{\sigma_{j_2}^2} \le c_x , \ 1 \le j_1, j_2 \le k$ 

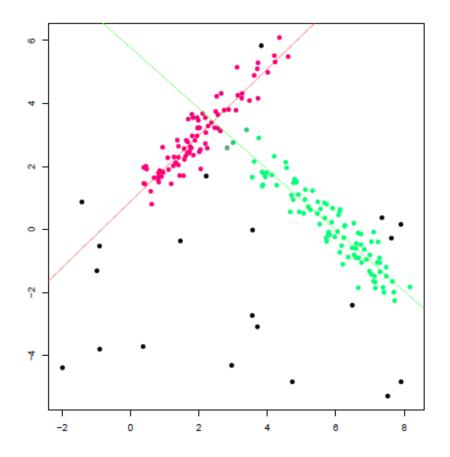
• Eigenvalue constraints for controlling the relative variability of explanatory variables  $2^{l_1}$ 

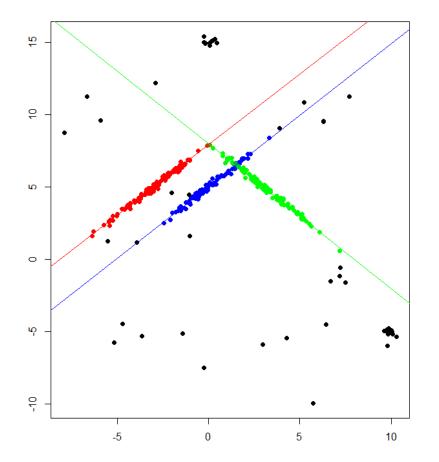
$$\frac{\lambda_{\Sigma_{j_1}}^{l_1}}{\lambda_{\Sigma_{j_2}}^{l_2}} \leq c_{\varepsilon} , \quad 1 \leq j_1, j_2 \leq k \qquad 1 \leq l_1, l_2 \leq p$$

### Robust fuzzy cluster weighted modeling

Trimming & Constraints to Fuzzy cluster weighted Model

$$\arg \sup_{\theta \in R, u} \sup_{A/\#A = n(1-\alpha)} \sum_{i=1}^{n} I_{A}(x_{i}, y_{i}) \left( \sum_{j=1}^{k} u_{ij}^{m} \log \left( \pi_{j} N_{0, \sigma_{j}}^{1} \left( y_{i} - \beta_{0} - \beta_{j} x_{i} \right) N_{\mu, \Sigma_{j}}^{p} \left( x_{i} \right) \right) \right)$$



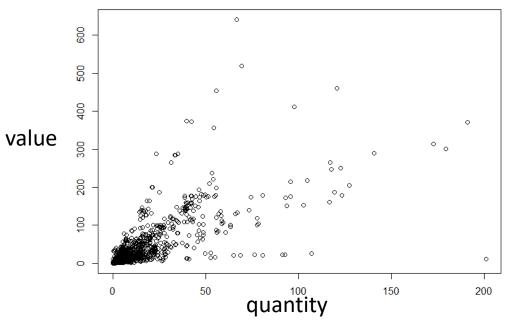


The ComExt Extra-European trade database provides statistics on merchandise trade among European Union member states, and between member states and global partners. ComExt, published by Eurostat, is based on data provided by the statistical agencies of the EU member states and trading partners. The statistics of interest for anti-fraud are mainly the traded volumes and values for a fixed product, which are aggregated monthly by Eurostat.

We are interested in applying robust clustering procedures for identifying outliers in the ComExt Extra-European trade database by thinking about its usefulness in fraud detection.

There are robust procedures available for clustering data in different settings, including ones devoted to identifying clusters around linear subspaces which appear to be well suited for

datasets in this database.



Cerioli, A. & Perrotta, D. (2014) Robust clustering around regression lines with high density regions. Adv Data Anal Classif 8, 5-26

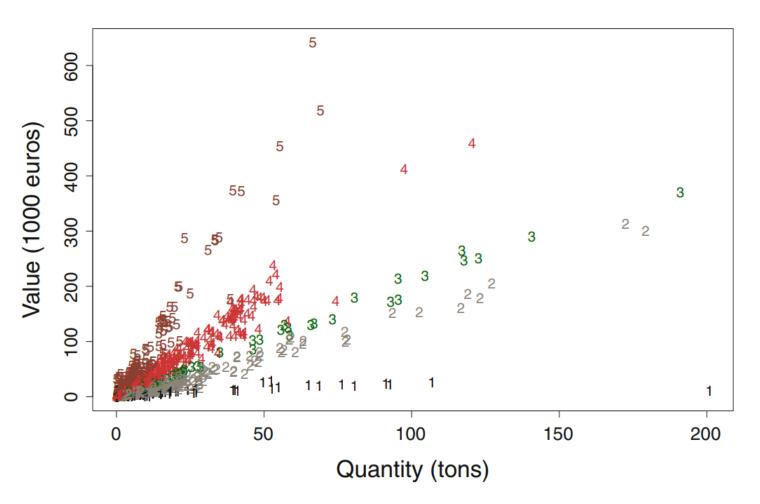
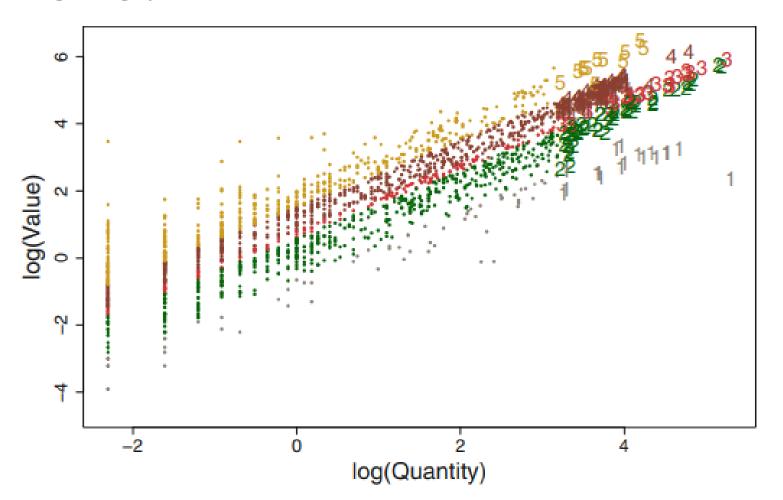


Fig. 1 Spices data set: scatter plot of value (y) and quantity (x), together with cluster membership assigned

Cerioli, A. & Perrotta, D. (2014) Robust clustering around regression lines with high density regions. Adv Data Anal Classif 8, 5-26

#### log-log plot



Cerioli, A. & Perrotta, D. (2014) Robust clustering around regression lines with high density regions. Adv Data Anal Classif 8, 5-26

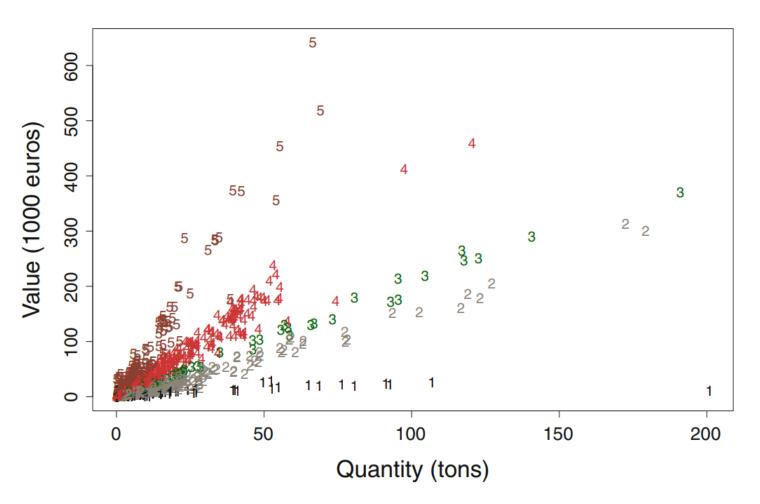


Fig. 1 Spices data set: scatter plot of value (y) and quantity (x), together with cluster membership assigned

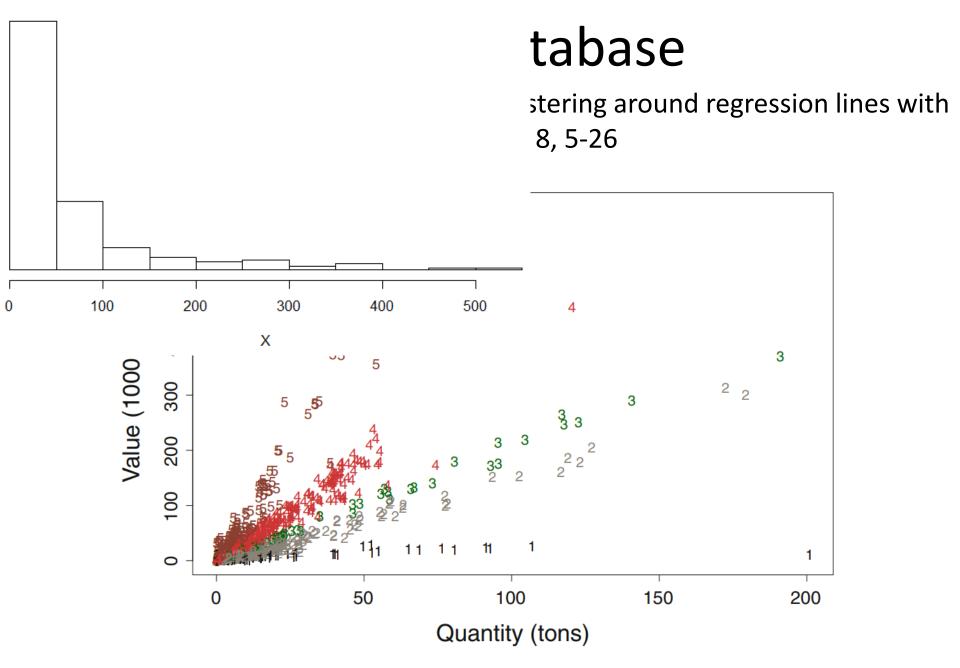


Fig. 1 Spices data set: scatter plot of value (y) and quantity (x), together with cluster membership assigned

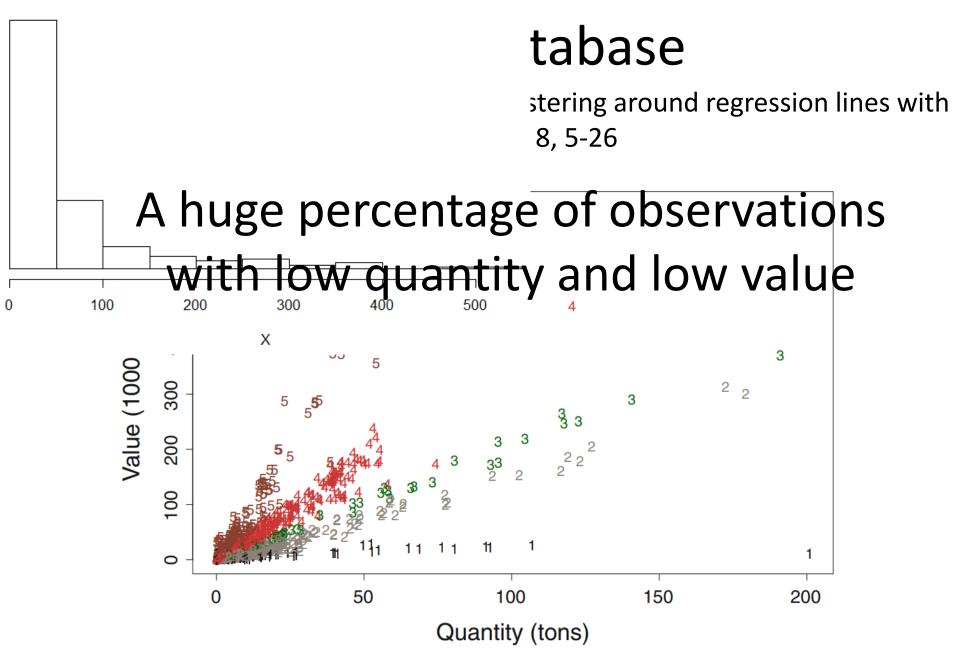


Fig. 1 Spices data set: scatter plot of value (y) and quantity (x), together with cluster membership assigned

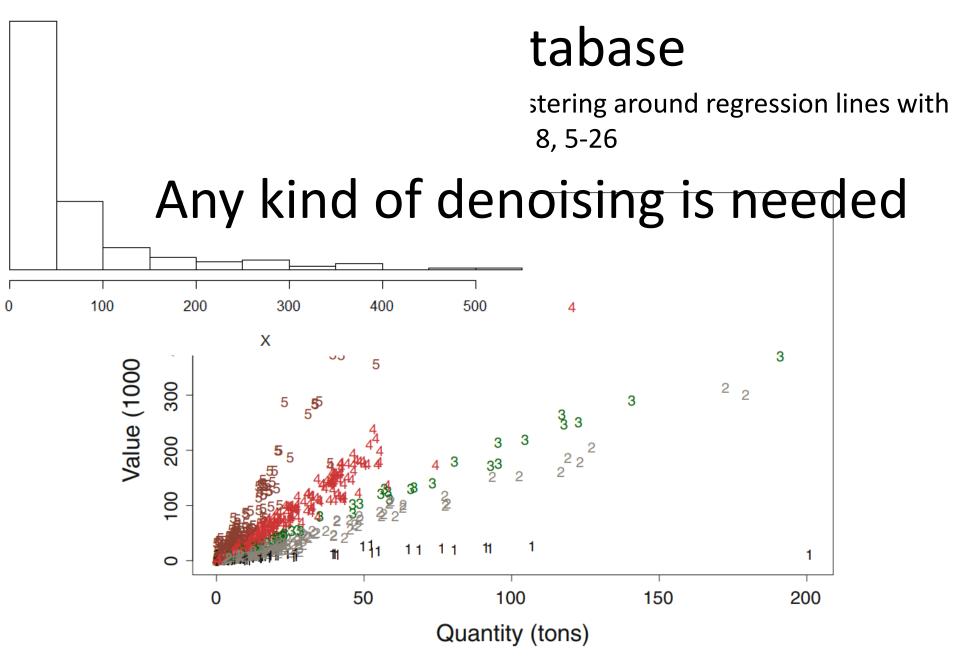


Fig. 1 Spices data set: scatter plot of value (y) and quantity (x), together with cluster membership assigned

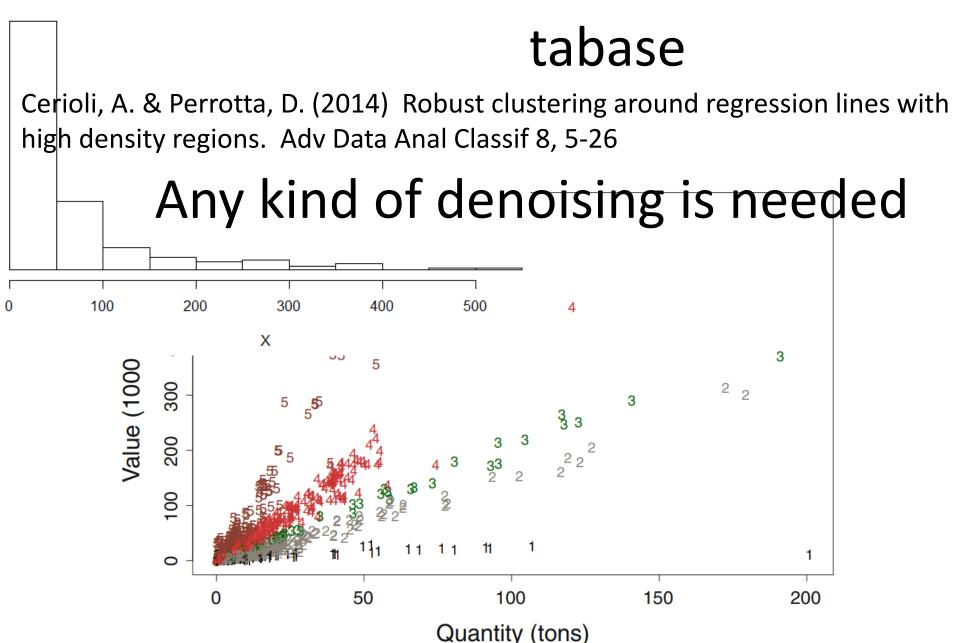


Fig. 1 Spices data set: scatter plot of value (y) and quantity (x), together with cluster membership assigned

## **Thinning**

For avoiding the influence of concentrated contamination when estimating mixture of regressions (Cerioli and Perrotta, 2014)

weighting based on density (inverse to the density) & sampling based on this weighting

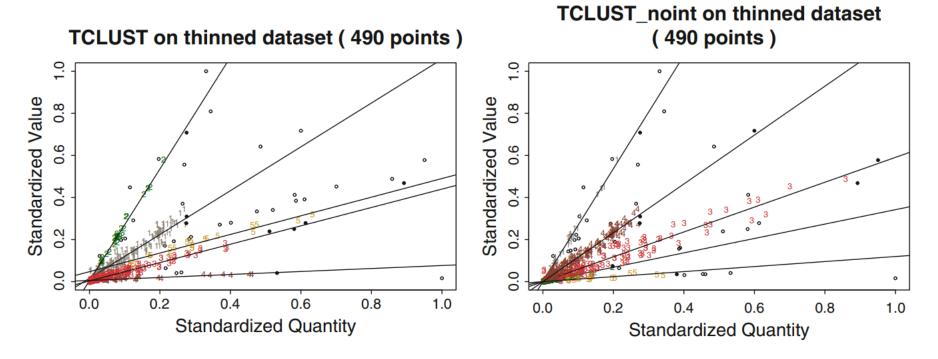


Fig. 7 Thinned Spices data set: robust fit using TCLUST-REG with G = 5 and trimming level 0.06. Left panel with intercept terms; right panel without intercept terms

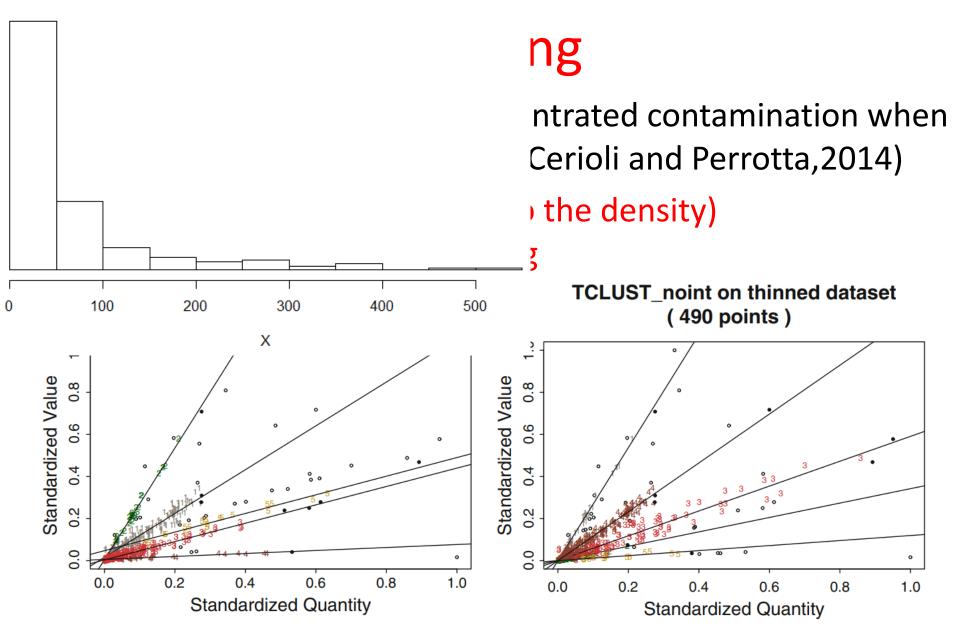
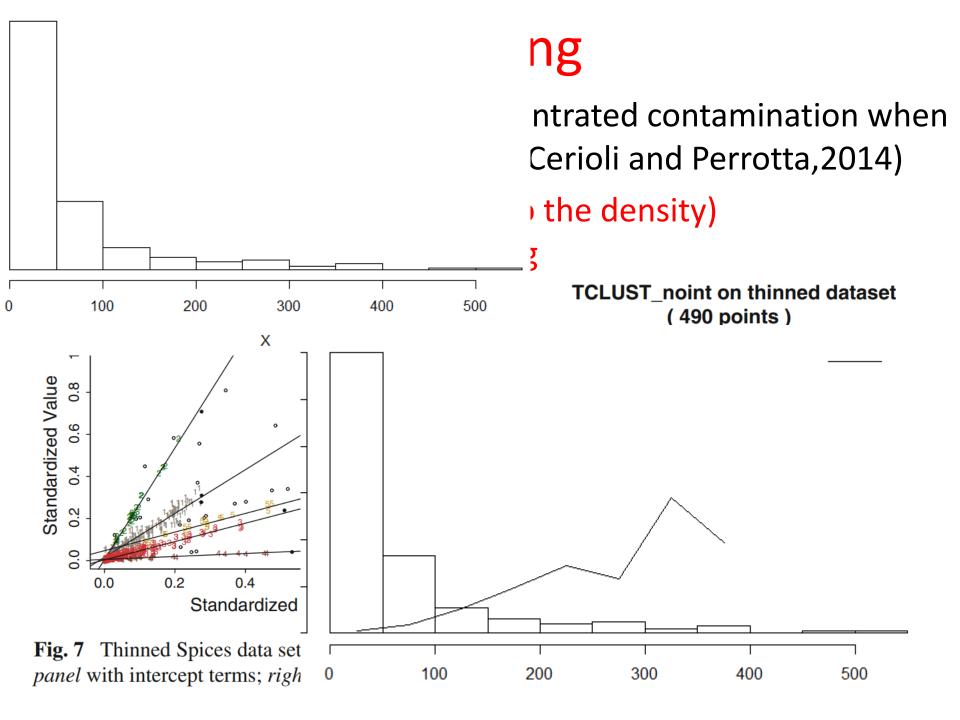
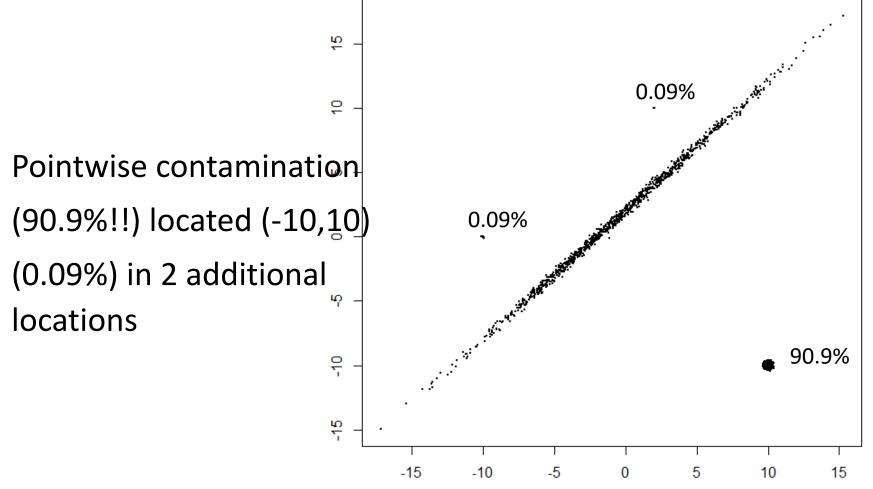


Fig. 7 Thinned Spices data set: robust fit using TCLUST-REG with G = 5 and trimming level 0.06. Left panel with intercept terms; right panel without intercept terms



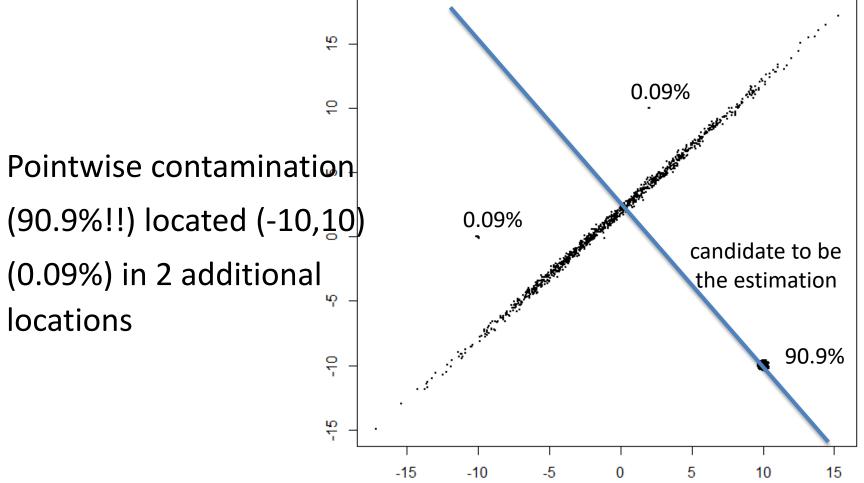
Pointwise contamination is not necessarily close to the regression line

A huge challenge, even, for Robust Statistics



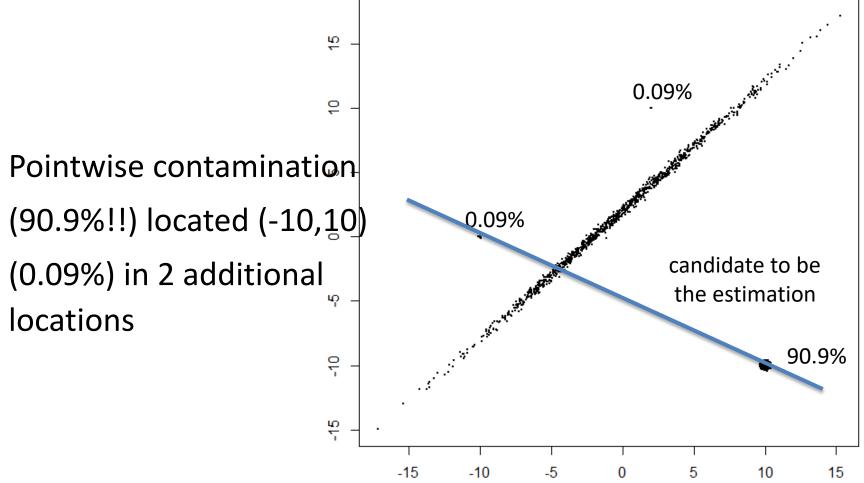
Pointwise contamination is not necessarily close to the regression line

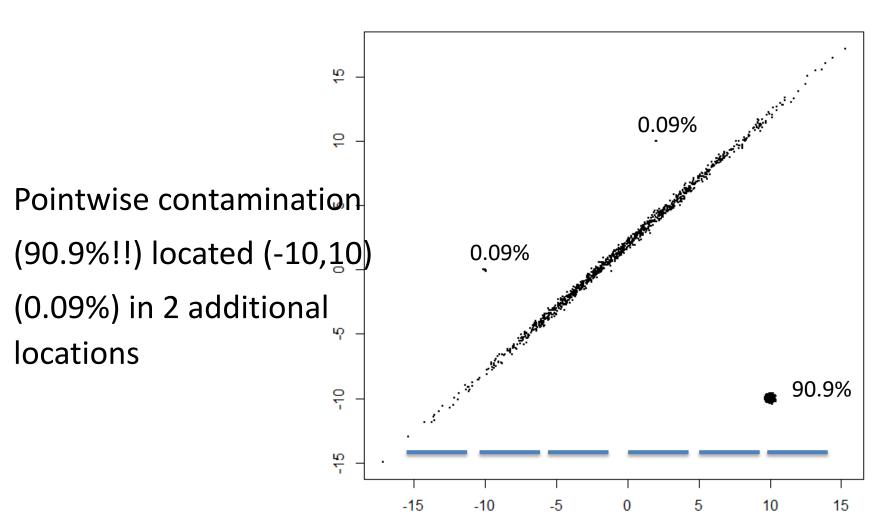
A huge challenge, even, for Robust Statistics

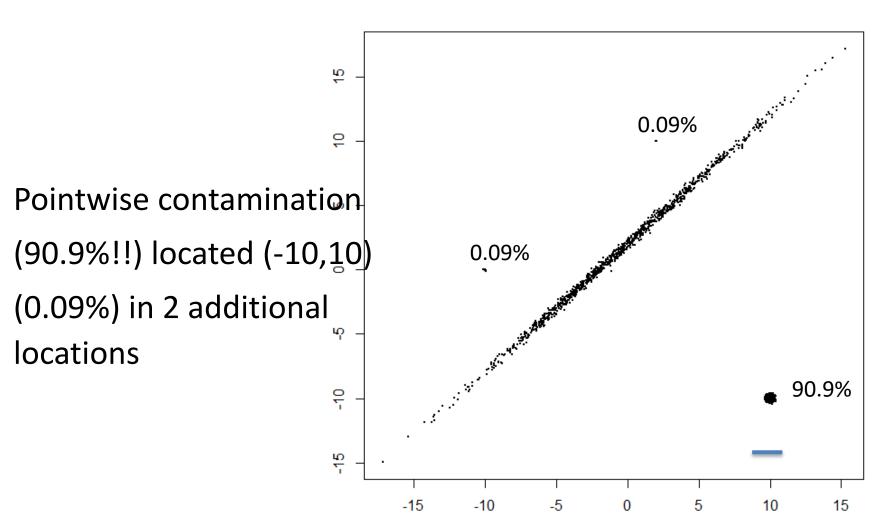


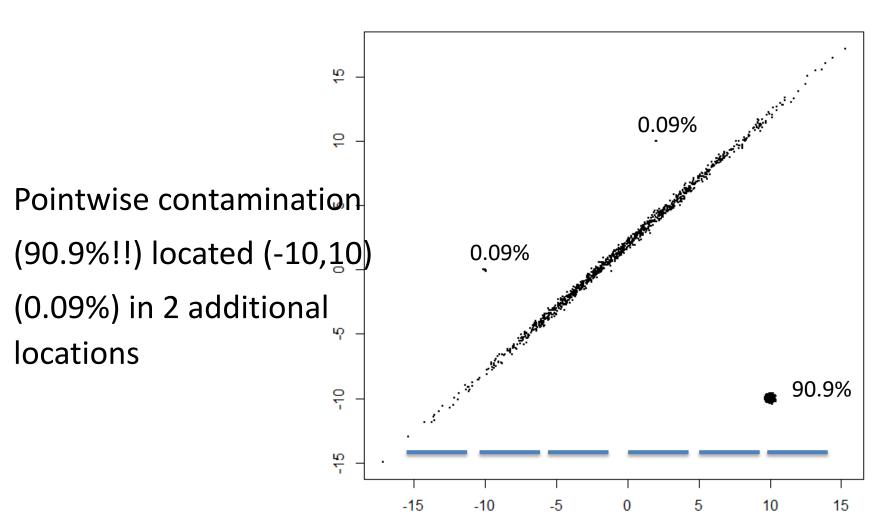
Pointwise contamination is not necessarily close to the regression line

A huge challenge, even, for Robust Statistics

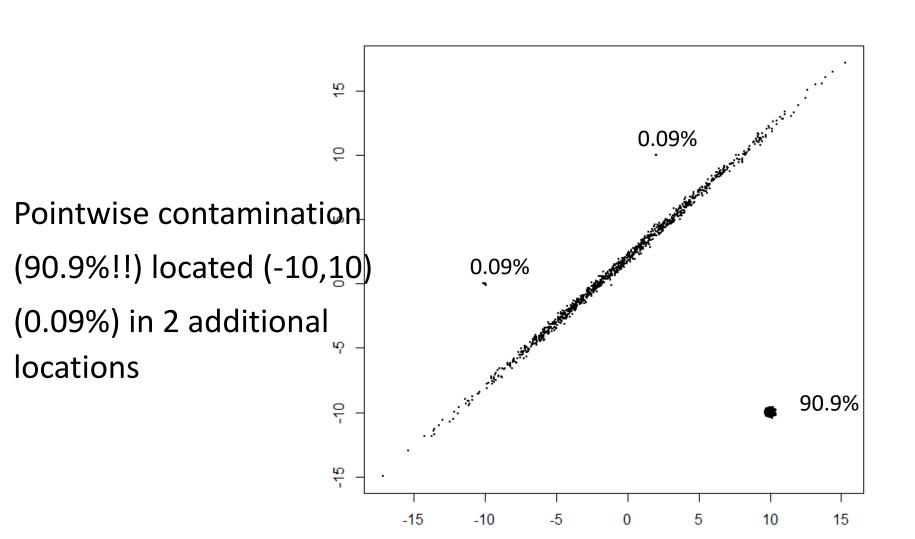


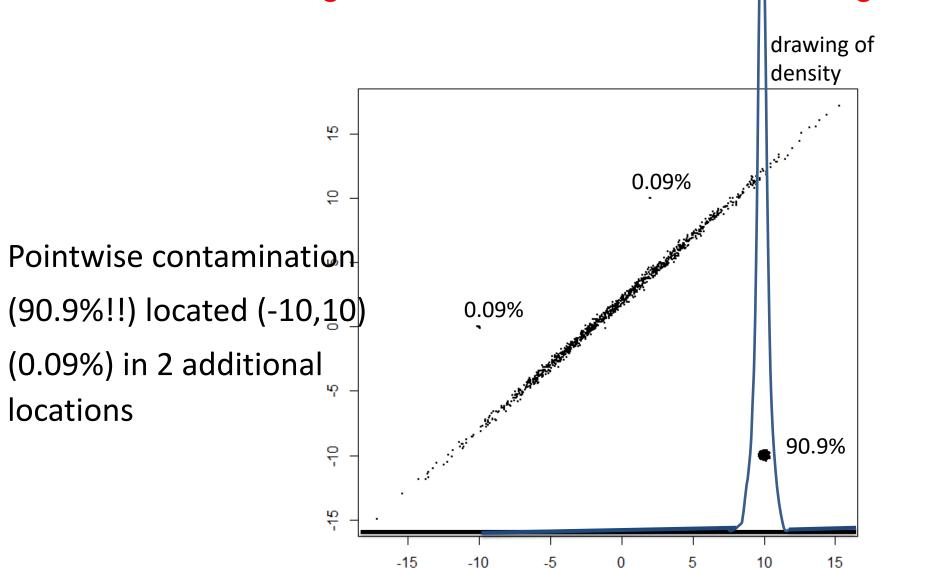




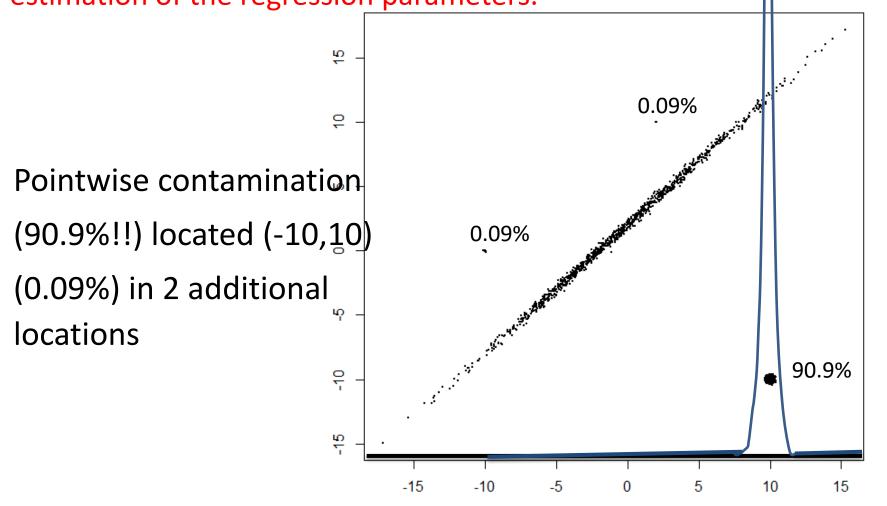


Thinning (Cerioli & Perrotta, 2014). De-construction of it

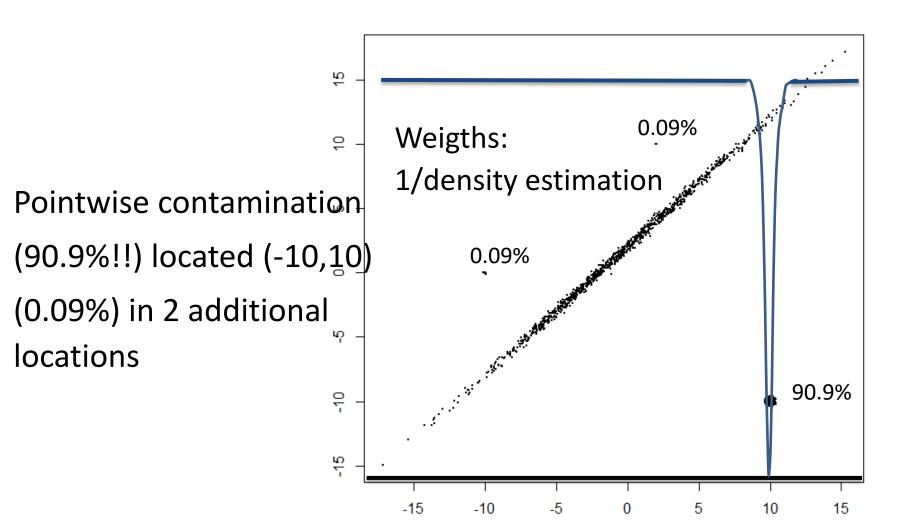




We are interested in a regression solution based on the whole range of x Any weighting based on the explanatory variable gives consistent estimation of the regression parameters.



Any weighting based on the explanatory variable gives consistent estimation of the regression parameters.



Any weighting based on the explanatory variable gives consistent estimation of the regression parameters.

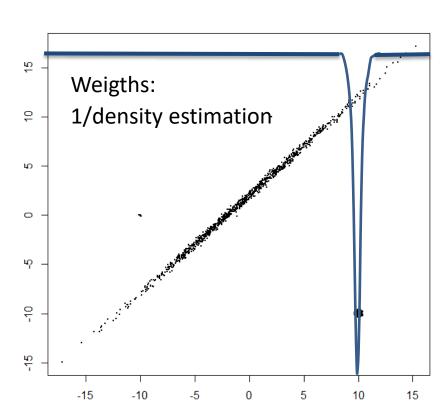
To apply weighting based on density allows us to reduce the influence of concentrated contamination.

Trimming based on this weighting (not a fix proportion of observations,

a fix proportion of weight)

Pointwise contamination (90.9%!!) located (-10,10) (0.09%) in 2 additional locations

trimming level 20%



Any weighting based on the explanatory variable gives consistent estimation of the regression parameters.

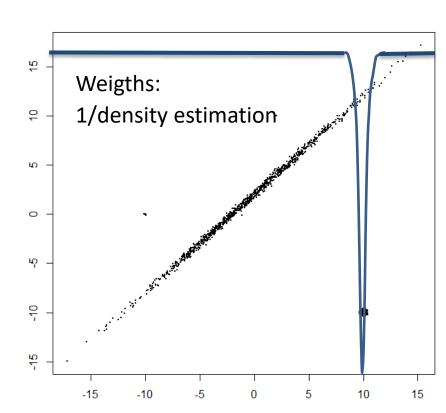
To apply weighting based on density allows us to reduce the influence of concentrated contamination.

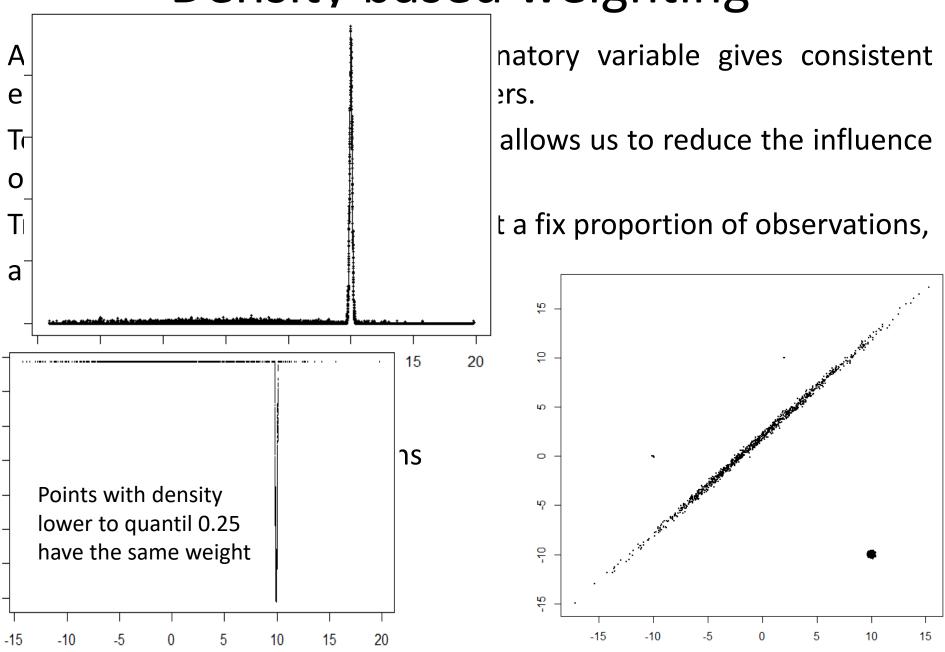
Trimming based on this weighting (not a fix proportion of observations,

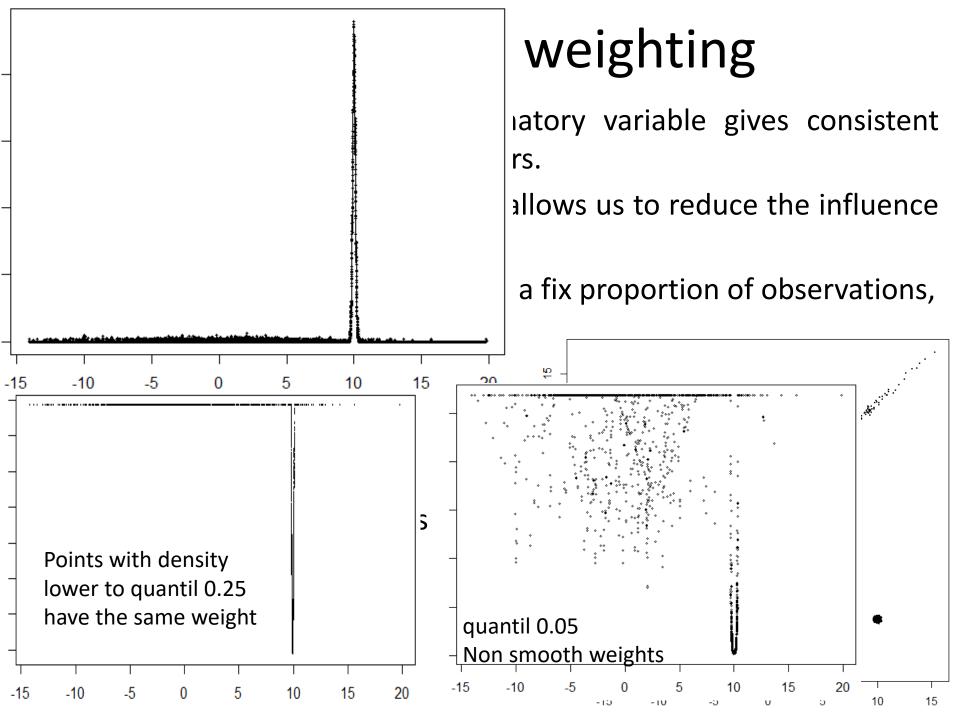
a fix proportion of weight)

Pointwise contamination (90.9%!!) located (-10,10) (0.09%) in 2 additional locations

trimming level 20%







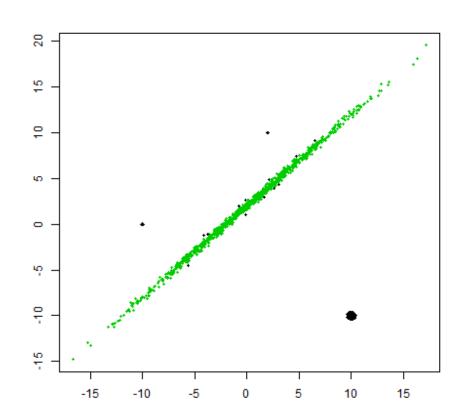
Any weighting based on the explanatory variable gives consistent estimation of the regression parameters.

To apply weighting based on density allows us to reduce the influence of concentrated contamination.

Trimming based on this weighting (not a fix proportion of observations,

a fix proportion of weight)

Pointwise contamination (90.9%!!) located (-10,10) (0.09%) in 2 additional locations



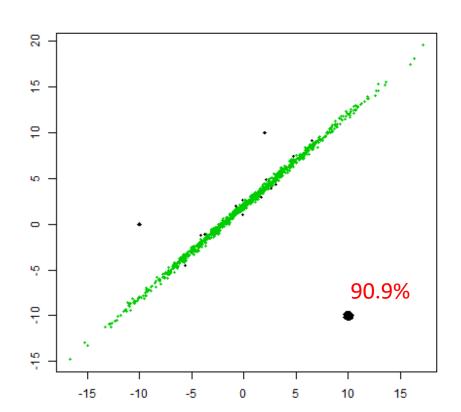
Any weighting based on the explanatory variable gives consistent estimation of the regression parameters.

To apply weighting based on density allows us to reduce the influence of concentrated contamination.

Trimming based on this weighting (not a fix proportion of observations,

a fix proportion of weight)

Pointwise contamination (90.9%!!) located (-10,10) (0.09%) in 2 additional locations



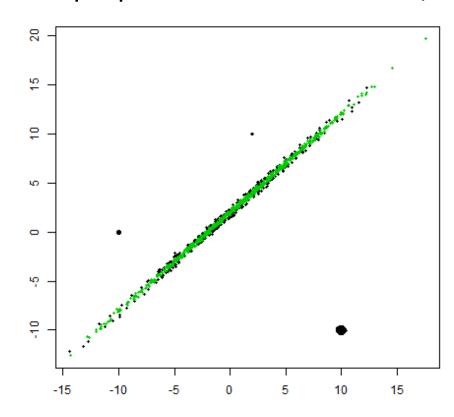
Any weighting based on the explanatory variable gives consistent estimation of the regression parameters.

To apply weighting based on density allows us to reduce the influence of concentrated contamination.

Trimming based on this weighting (not a fix proportion of observations,

a fix proportion of weight)

Pointwise contamination (90.9%!!) located (-10,10) (0.09%) in 2 additional locations



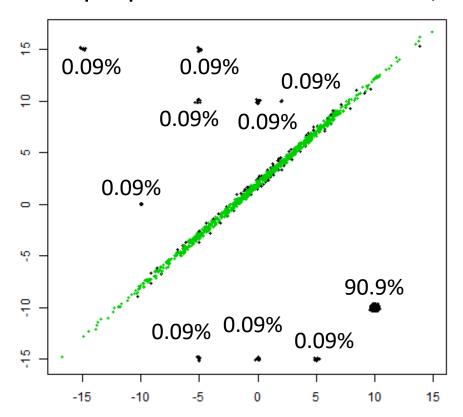
Any weighting based on the explanatory variable gives consistent estimation of the regression parameters.

To apply weighting based on density allows us to reduce the influence of concentrated contamination.

Trimming based on this weighting (not a fix proportion of observations,

a fix proportion of weight)

Pointwise contamination (90.9%!!) located (-10,10) (0.09%) in 10 additional locations



#### Density based weighting (Clustering)

Any weighting based on the explanatory variable gives consistent estimation of the clustering of regression parameters.

To apply weighting based on density allows us to reduce the influence of concentrated contamination.

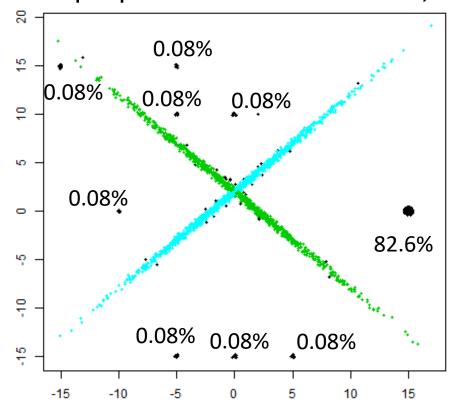
Trimming based on this weighting (not a fix proportion of observations,

a fix proportion of weight)

Pointwise contamination

(82.6%!!) located (-10,10)

(0.08%) in 10 additional locations



#### Density based weighting (Clustering)

Any weighting based on the explanatory variable gives consistent estimation of the clustering of regression parameters.

To apply weighting based on density allows us to reduce the influence of concentrated contamination.

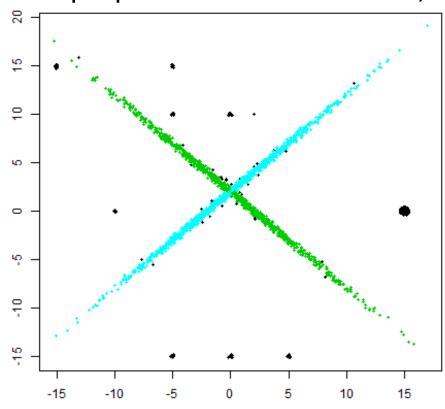
Trimming based on this weighting (not a fix proportion of observations,

a fix proportion of weight)

Pointwise contamination

(82.6%!!) located (-10,10)

(0.08%) in 10 additional locations



Any weighting based on the explanatory variable gives consistent estimation of the clustering of regression parameters.

To apply weighting based on density allows us to reduce the influence of concentrated contamination.

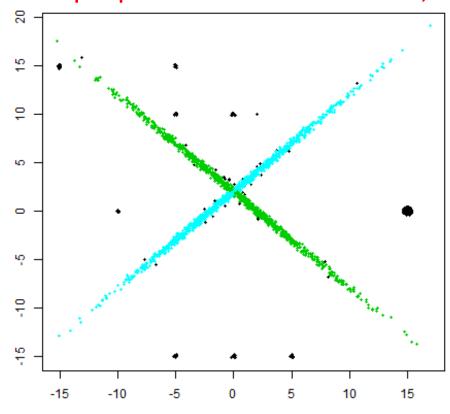
Trimming based on this weighting (not a fix proportion of observations,

a fix proportion of weight)

Pointwise contamination

(82.6%!!) located (-10,10)

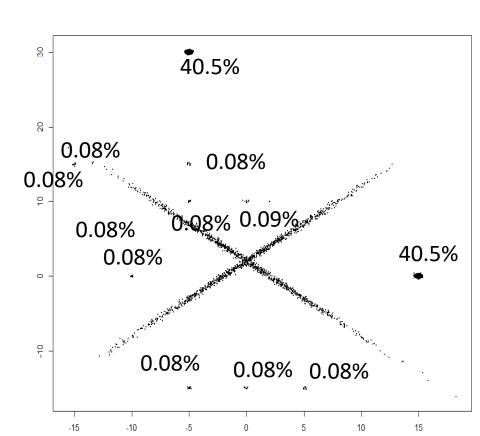
(0.08%) in 10 additional locations



Pointwise contamination

(40.5%!!) located (0,15)

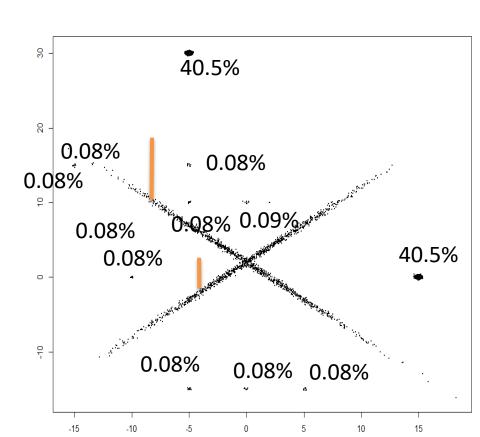
(40.5%!!) located (-5,30)



Pointwise contamination

(40.5%!!) located (0,15)

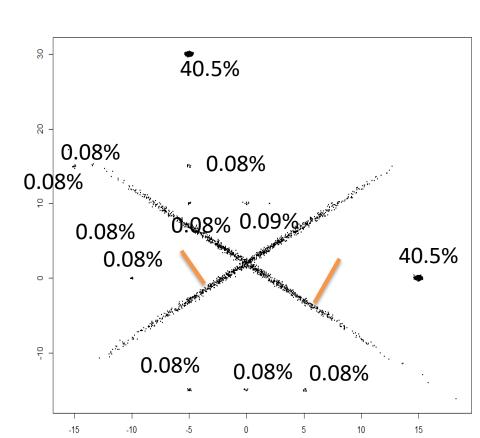
(40.5%!!) located (-5,30)



Pointwise contamination

(40.5%!!) located (0,15)

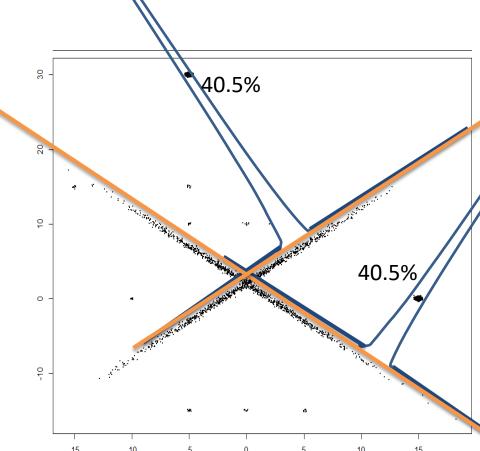
(40.5%!!) located (-5,30)



Pointwise contamination

(40.5%!!) located (0,15)

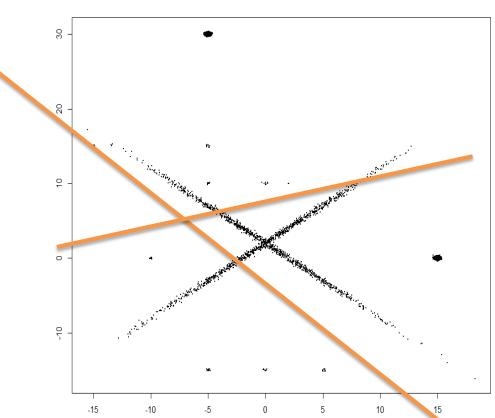
(40.5%!!) located (-5,30)



Pointwise contamination

(40.5%!!) located (0,15)

(40.5%!!) located (-5,30)



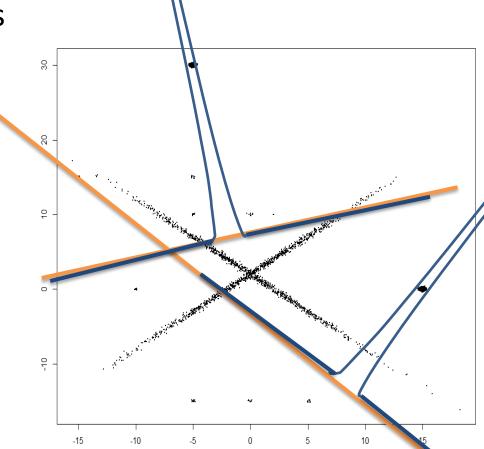
Pointwise contamination

(40.5%!!) located (0,15)

(40.5%!!) located (-5,30)

(0.08%) in 10 additional locations

It is necessary to include the density estimation in each step of the algorithm



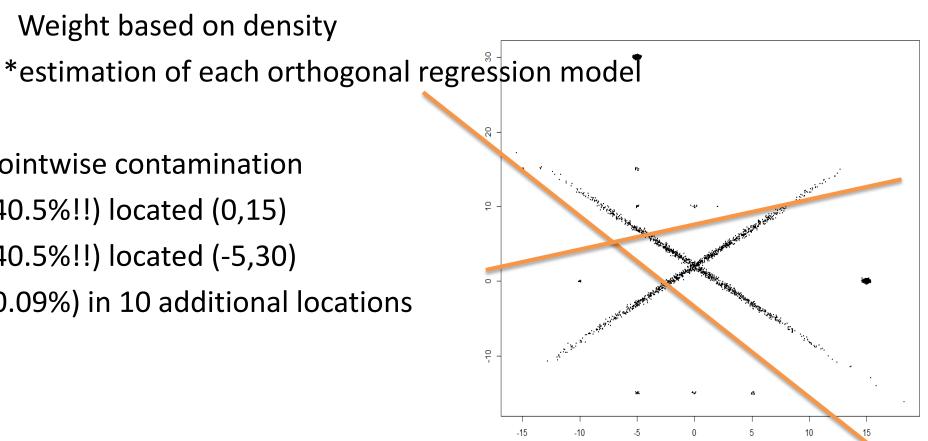
Start with k random linear models **Iterations** 

\*Assign each observation to the closest model

Estimate density in each model separately

Weight based on density

Pointwise contamination (40.5%!!) located (0,15) (40.5%!!) located (-5,30)

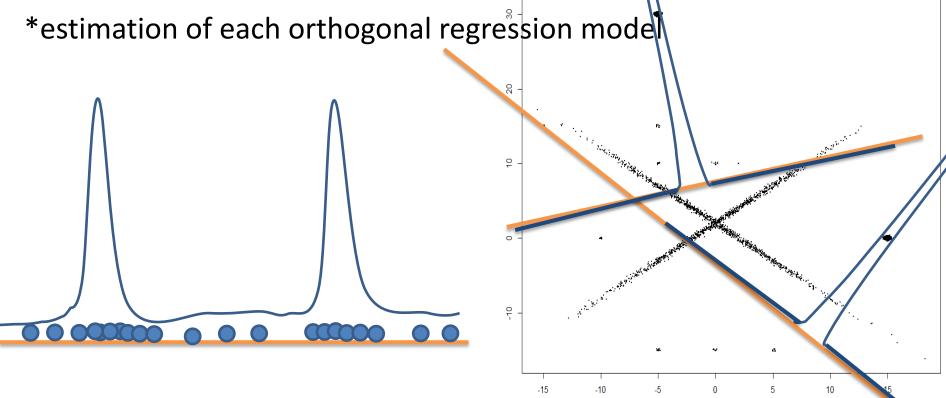


Start with *k* random linear models Iterations

\*Assign each observation to the closest model

Estimate density in each model (jointly with a the observations)

Weight based on density



Start with *k* random linear models Iterations

\*Assign each observation to the closest model

Estimate density in each model

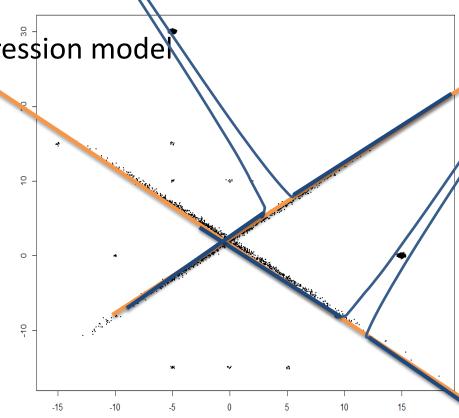
Weight based on density

\*estimation of each orthogonal regression model

Pointwise contamination

(40.5%!!) located (0,15)

(40.5%!!) located (-5,30)

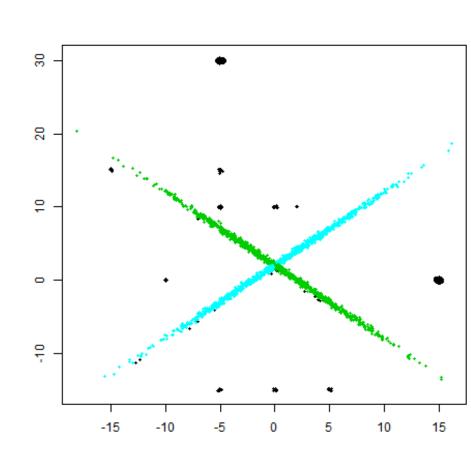


Pointwise contamination

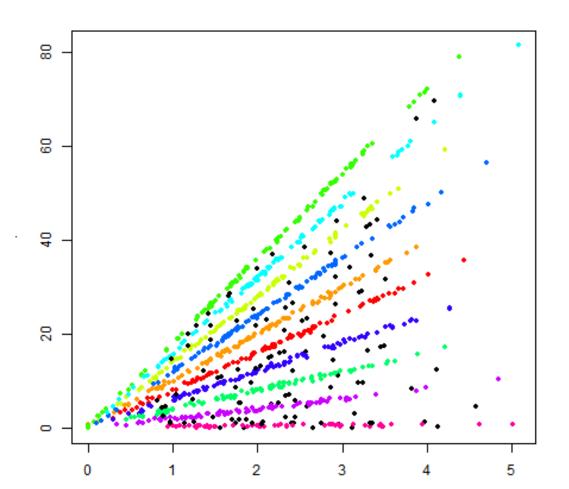
(40.5%!!) located (0,15)

(40.5%!!) located (-5,30)

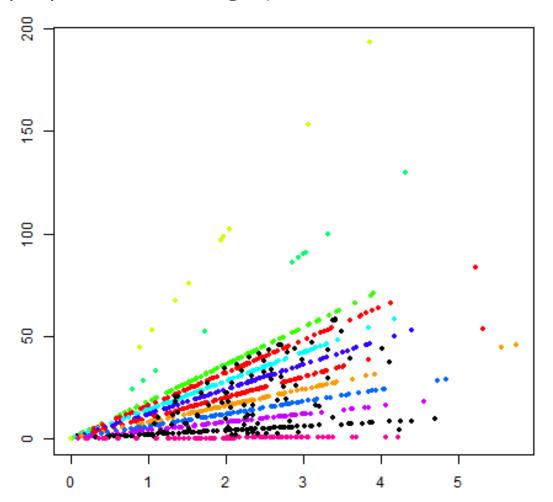
(0.08%) in 10 additional locations



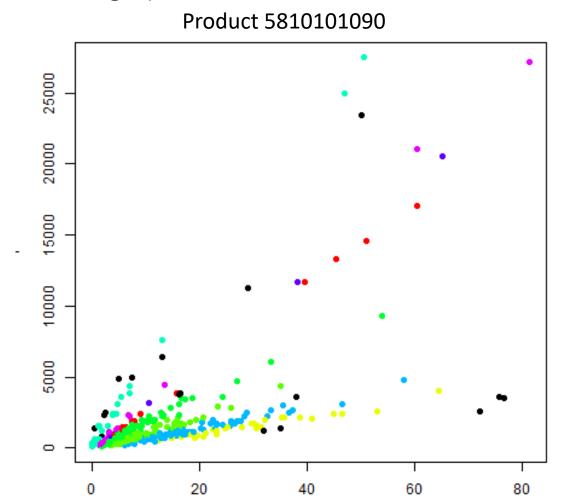
Weighting based on explanatory variables density and estimated beta Trimming based on this weighting (not a fix proportion of observations, a fix proporttion of weight)



Weighting based on explanatory variables density and estimated beta Trimming based on this weighting (not a fix proportion of observations, a fix proporttion of weight)



Weighting based on density and estimated beta Trimming based on this weighting (not a fix proportion of observations, a fix proporttion of weight)



# Benford's Law Conference

10-12 July 2019 - Stresa, Italy

# Thank you!!!

Denoising and Trimming for Improved Cluster Solutions with Applications to Customs Frauds

Andrea Cerioli<sup>1</sup>, Luis Ángel García-Escudero<sup>2</sup>, Alfonso Gordaliza<sup>2</sup>, Carlos Matrán<sup>2</sup>, Agustín Mayo-Iscar<sup>2</sup>, Domenico Perrotta<sup>3</sup>, Marco Riani<sup>1</sup> and Francesca Torti<sup>3</sup>

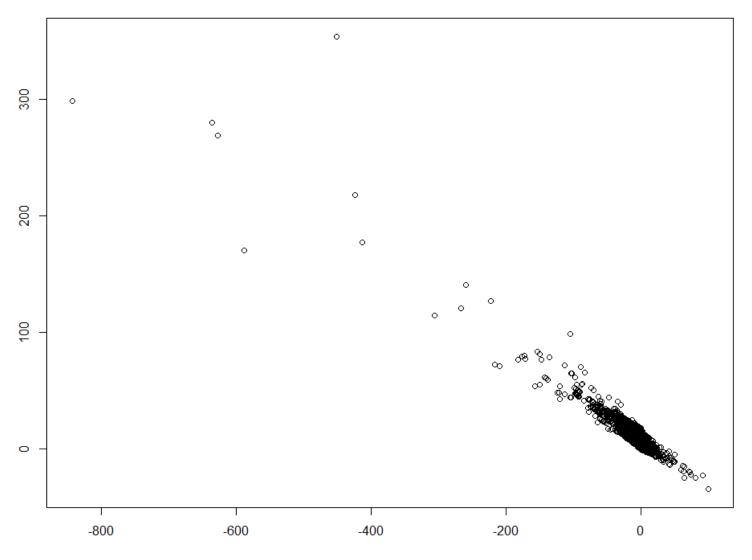
- 1. Department of Economics & Ro.S.A. University of Parma
- 2. Department of Statistics and O.R. & IMUVA. University of Valladolid

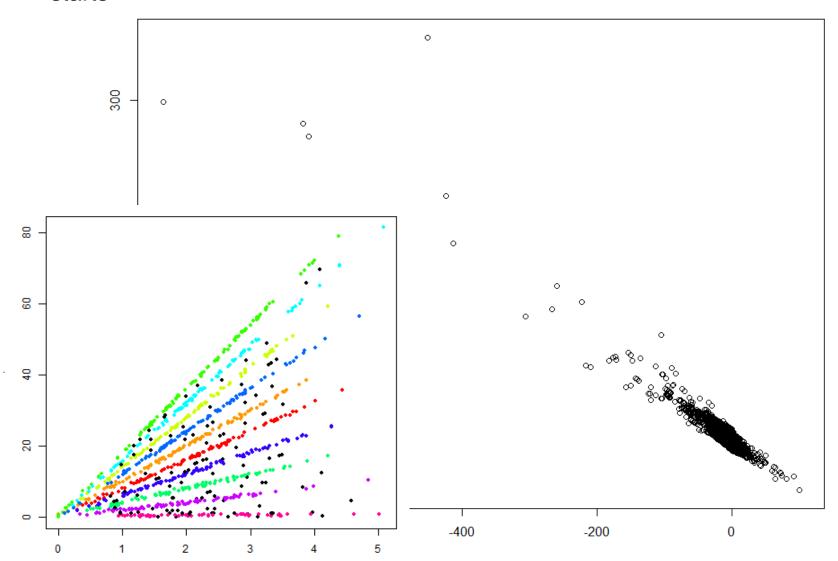


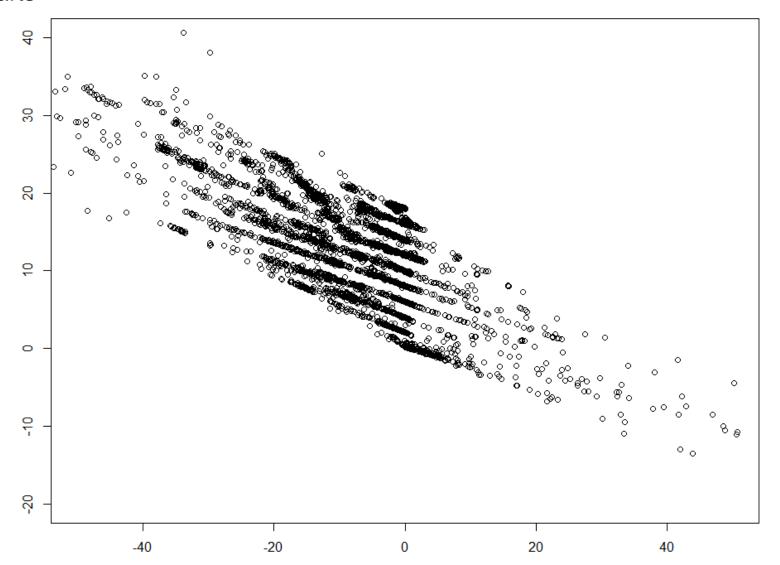


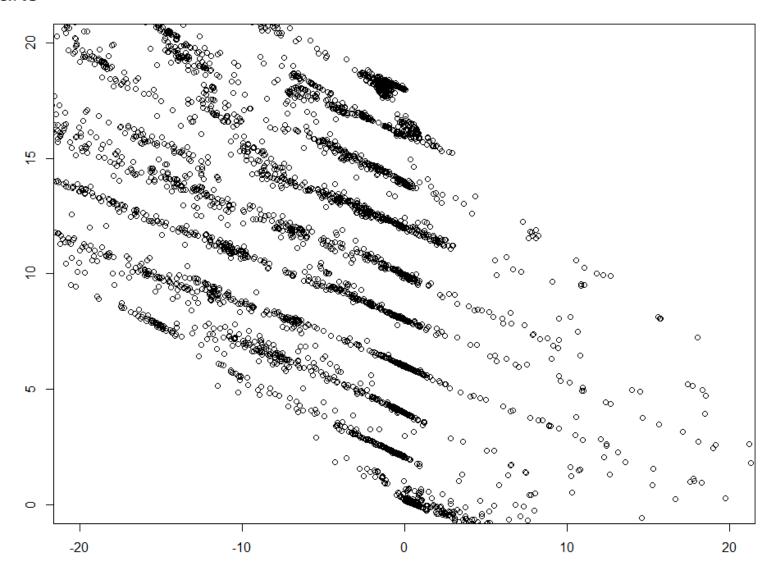












# Weights' effect

 $\arg\inf_{\mu} \inf_{z} \inf_{A/P_n(A)=1-\alpha} \sum_{i=1}^{n} \sum_{j=1}^{k} z_{ij} I_A(x_i) \|x_i - \mu_j\|^2$ Trimmed k-means  $\sup_{\mu,z} \sup_{A/P_n(A)=1-\alpha} \sum_{i=1}^n I_A(x_i) \sum_{i=1}^{k} z_{ij} \log(\pi_j N_{\mu_j,\Sigma_j}(x_i))$ arg sup Trimmed k-means k=3 alpha=20% c=1 TCLUST *k=3 alpha=20% c=1*  $\pi_1 = ... = \pi_i = ... = \pi_k$  $\pi_1 = ... = \pi_r = ... = \pi_k$ 

#### Input parameters

k: number of clusters

 $\alpha$ : level of trimming

c: strength of the constraints

These input parameters have to be provided, in advance, by the user.

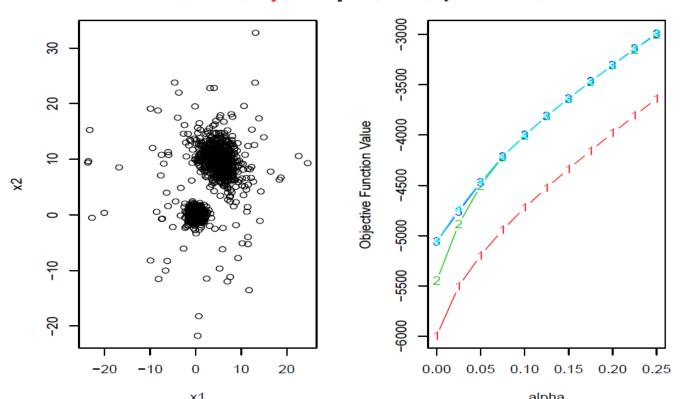
# Input parameters – k & alpha

García-Escudero, Gordaliza, Matrán & M-I (2011). Exploring the number of groups in robust model-based clustering. *Stat & Comp*, *21*(4), 585-599.

#### • Classification Trimmed Likelihood Curves with ctlcurves:

This tool is given by curves which represents the objective function value for a pairs of (k,alpha). These curves can assist users in the selection of values for k and alpha.

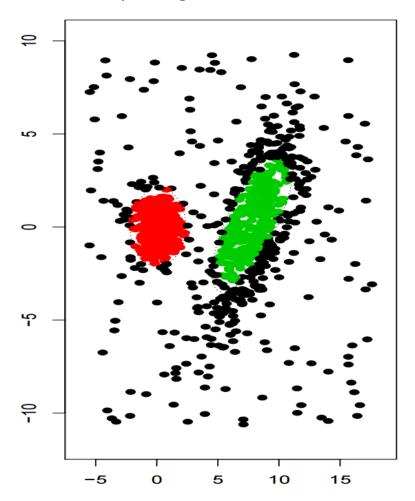
> ctlcurves (x,k=1:4,alpha=seq (0,0.25,by = 0.05), restr.fact=100)



#### Input parameters - alpha

#### ReWeighted TCLUST

Dotto, Farcomeni, García-Escudero & M-I (2018). A Reweighting Approach to Robust Clustering. *Statistics and Computing*.

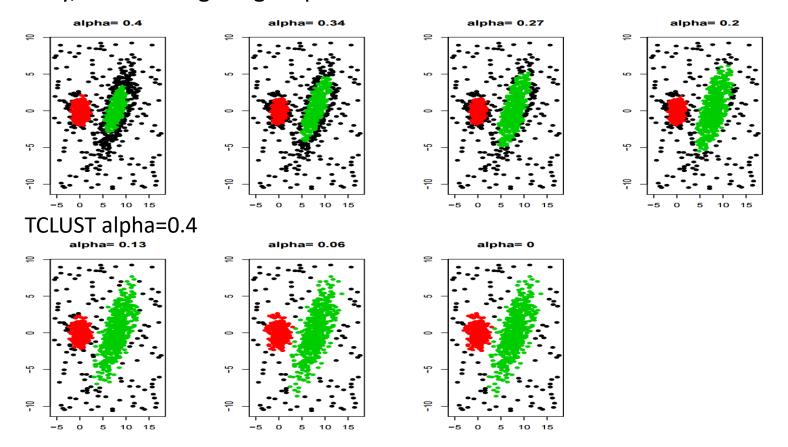


#### Input parameters - alpha

#### ReWeighted TCLUST

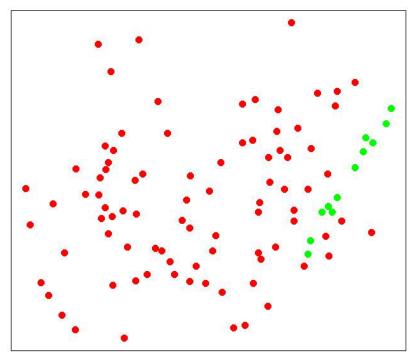
Dotto, Farcomeni, García-Escudero & M-I (2018). A Reweighting Approach to Robust Clustering. *Statistics and Computing* 

Starting from a TCLUST solution (high level of trimming), to improve it, sequentially, with reweighting steps



#### Input parameters - constraints

Eigenvalue constraints applied to ML finite mixture models estimation García-Escudero, Gordaliza, Matrán and M-I (2015) Avoiding Spurious Local Maximizers in Mixture Modeling. Stat & Comp, 25 (3) pp 619-633



Synthetic data set 2 (McP2000)

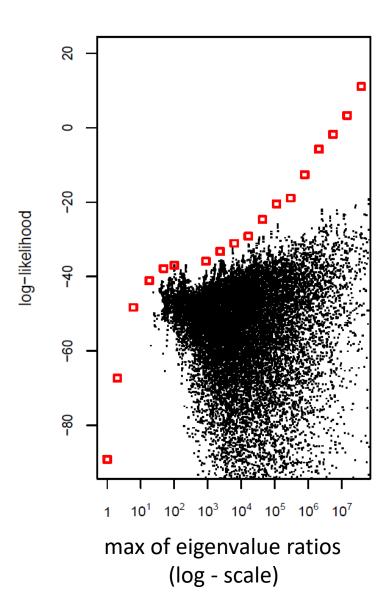
Mixture of two normal heteroscedastic populations without contamination

#### Spurious clusters

- "little practical use or real-world interpretation" (McLachlan &Peel, 2000 McP2000)
- "It often seems in these cases that the model is fitting a small localized random pattern in the data rather than any underlying group structure". (McP2000)

Constraints for avoiding spurious clusters in the solution

#### Input parameters - constraints



Eigenvalue constraints applied to ML finite mixture models estimation

García-Escudero, Gordaliza, Matrán and M-I (2015) Avoiding Spurious Local Maximizers in Mixture Modeling. Stat & Comp, 25 (3) pp 619-633

Prevalence of spurious local maximizers in ML mixture models estimation

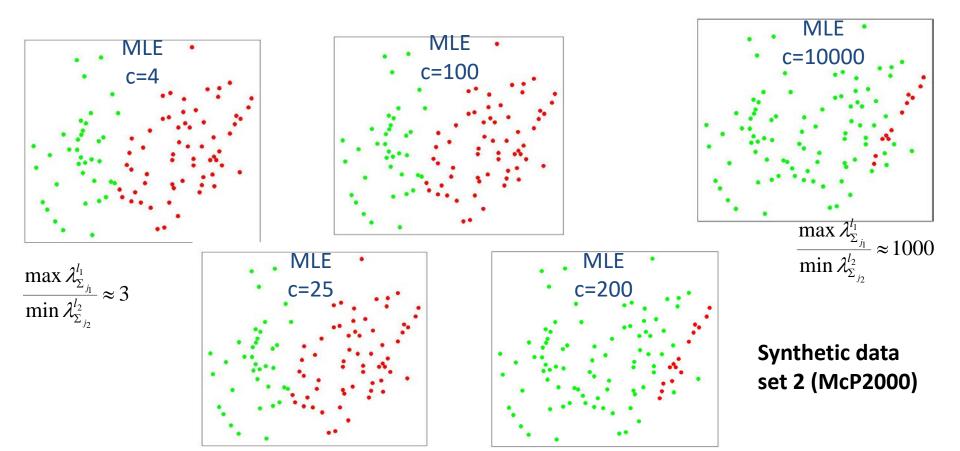
When applying the EM algorithm after thousands of random starts, thousands of different solutions appear.

How to choose the estimation?

The plot shows Log-likelihoods and maximum of eigenvalues-ratios for thousands of local ML maximizers corresponding to ML estimation of two populations for the virginica species subset of the Iris data.

#### Input parameters - constraints

Eigenvalue contraints applied to ML finite mixture models estimation García-Escudero, Gordaliza, Matrán and M-I (2015) Avoiding Spurious Local Maximizers in Mixture Modeling. Stat & Comp, 25 (3) pp 619-633



#### Input parameters – k &constraints

#### BIC based choice of contraints level

Cerioli, A., García-Escudero, L.A., M-I, A., & Riani, M. (2018) Finding the Number of Normal Groups in Model-Based Clustering via Constrained Likelihoods. Journal of Computational and Graphical Statistics, 27(2), 404-416.

Trimmed BIC approach based on monitoring

 $(k, c) \rightarrow -2 L(k, \alpha, c) + v(k, \alpha, c)$  when  $\alpha$  is fixed

where  $v(k, \alpha, c)$  penalizes a higher (than needed) "model complexities"

Analogous to other BIC approaches but n is replaced by  $[n(1 - \alpha)]$ 

 $v(k, \alpha, c)$  is an increasing function on c (higher  $c \Rightarrow less-constrained Sj matrices <math>\Rightarrow$  higher model complexity...)

### **TCLUST Parsimonious modelling**

We are interested in applying trimming & constraints in the estimation of 14 Parsimonious models from Celeux and Govaert (1995). Punzo & McNicholas (2013) gave robust estimators for these models.

We are collaborating with Marco Riani and Andrea Cerioli (University of Parma) in applying trimming & contraints for estimating these models.

Table 1: Nomenclature, covariance structure, and number of free parameters in  $\Sigma_g$  for each member of the PMCGD family.

Family	Model	Volume	Shape	Orientation	$oldsymbol{\Sigma}_g$	# Free parameters in $\Sigma_g$
Spherical	EII	Equal	Spherical	_	$\lambda I$	1
	VII	Variable	Spherical	-	$\lambda_g oldsymbol{I}$	G
Diagonal	EEI	Equal	Equal	Axis-Align	$\lambda \Gamma$	p
	VEI	Variable	Equal	Axis-Align	$\lambda_g \mathbf{\Gamma}$	G + p - 1
	EVI	Equal	Variable	Axis-Align	$\lambda \Gamma_g$	$1 + G\left(p - 1\right)$
	VVI	Variable	Variable	Axis-Align	$\lambda_g \mathbf{\Gamma}_g$	Gp
General	EEE	Equal	Equal	Equal	$\lambda \Gamma \Delta \Gamma'$	$p\left(p+1\right)/2$
	VEE	Variable	Equal	Equal	$\lambda_g \mathbf{\Gamma} \mathbf{\Delta} \mathbf{\Gamma}'$	G + p - 1 + p(p - 1)/2
	EVE	Equal	Variable	Equal	$\lambda \Gamma_g \Delta \Gamma_g'$	1 + G(p-1) + p(p-1)/2
	EEV	Equal	Equal	Variable	$\lambda \mathbf{\Gamma} \mathbf{\Delta}_g \mathbf{\Gamma}'$	p + Gp(p-1)/2
	VVE	Variable	Variable	Equal	$\lambda_g \mathbf{\Gamma}_g \mathbf{\Delta} \mathbf{\Gamma}_g'$	Gp + p(p-1)/2
	VEV	Variable	Equal	Variable	$\lambda_g \mathbf{\Gamma} \mathbf{\Delta}_g \mathbf{\Gamma}'$	G + p - 1 + Gp(p - 1)/2
	EVV	Equal	Variable	Variable	$\lambda \Gamma_q \Delta_q \Gamma_q'$	1 + G(p-1) + Gp(p-1)/2
	VVV	Variable	Variable	Variable	$\lambda_g \Gamma_g \Delta_g \Gamma_g'$	$Gp\left(p+1\right)/2$

From Punzo & McNicholas (2013)

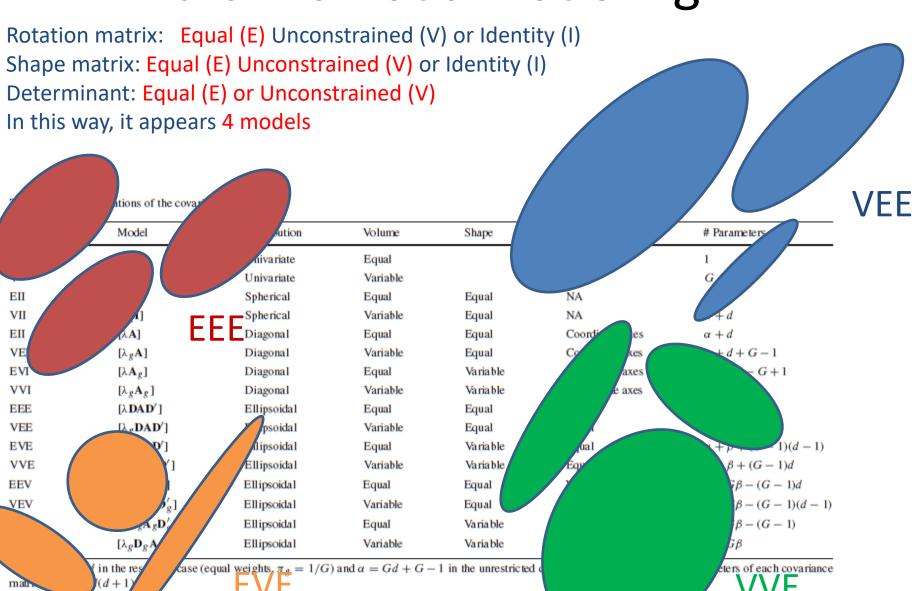
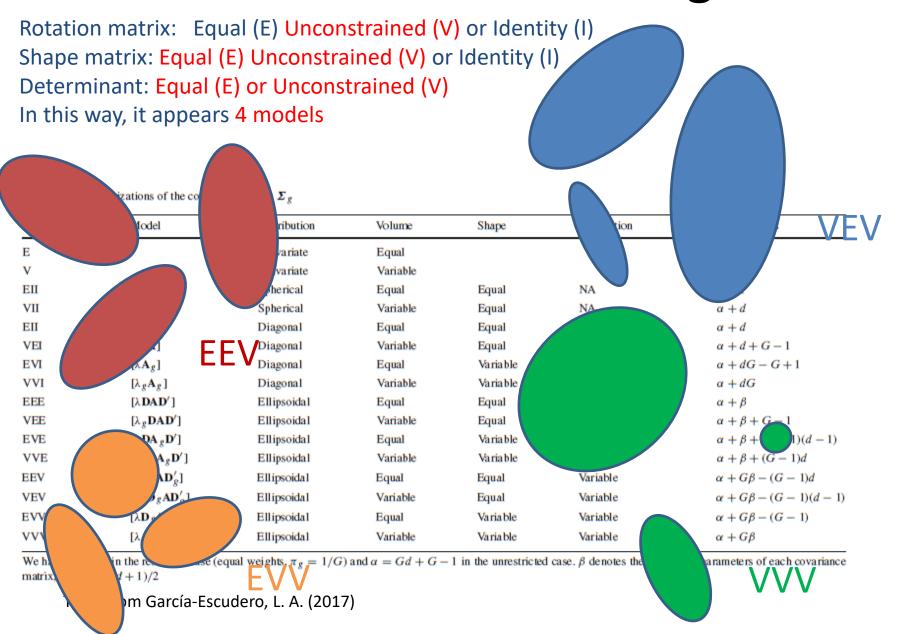
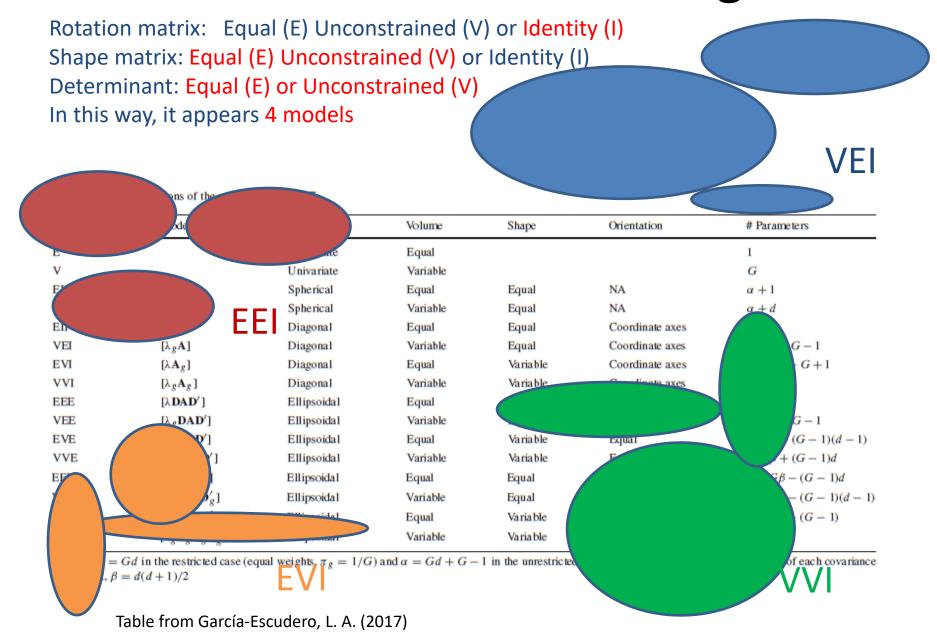


Table from

arcía-Escudero, L. A. (2017)



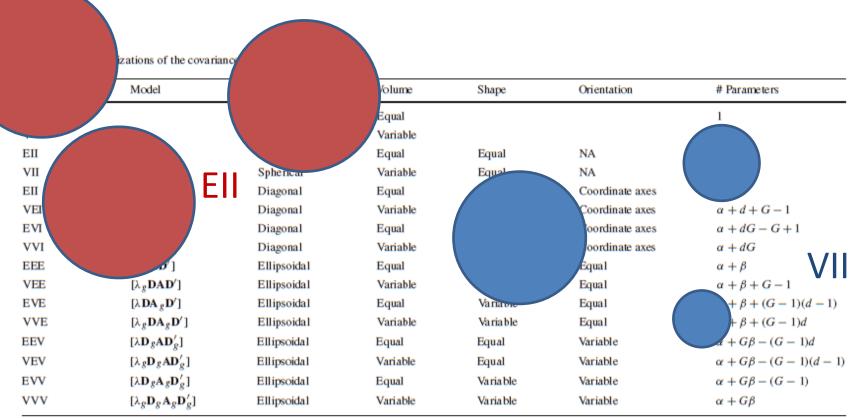


Rotation matrix: Equal (E) Unconstrained (V) or Identity (I)

Shape matrix: Equal (E) Unconstrained (V) or Identity (I)

Determinant: Equal (E) or Unconstrained (V)

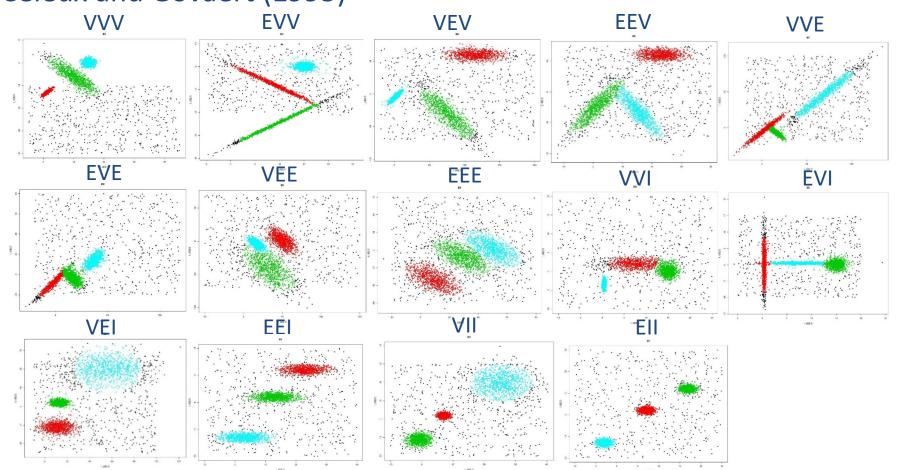
In this way, it appears 2 models



We have  $\alpha = Gd$  in the restricted case (equal weights,  $\pi_g = 1/G$ ) and  $\alpha = Gd + G - 1$  in the unrestricted case.  $\beta$  denotes the number of parameters of each covariance matrix, i.e.,  $\beta = d(d+1)/2$ 

## **TCLUST Parsimonious modelling**

Trimming & constraints for estimating 14 Parsimonious models from Celeux and Govaert (1995)

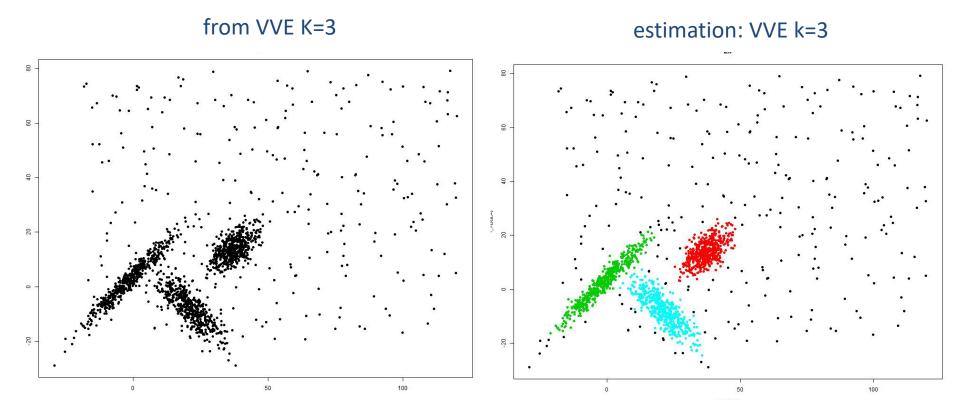


Trimmed & constrained Estimation applied to artificial data from the corresponding model  $\alpha$  + contamination  $\alpha$  = 15% c=25

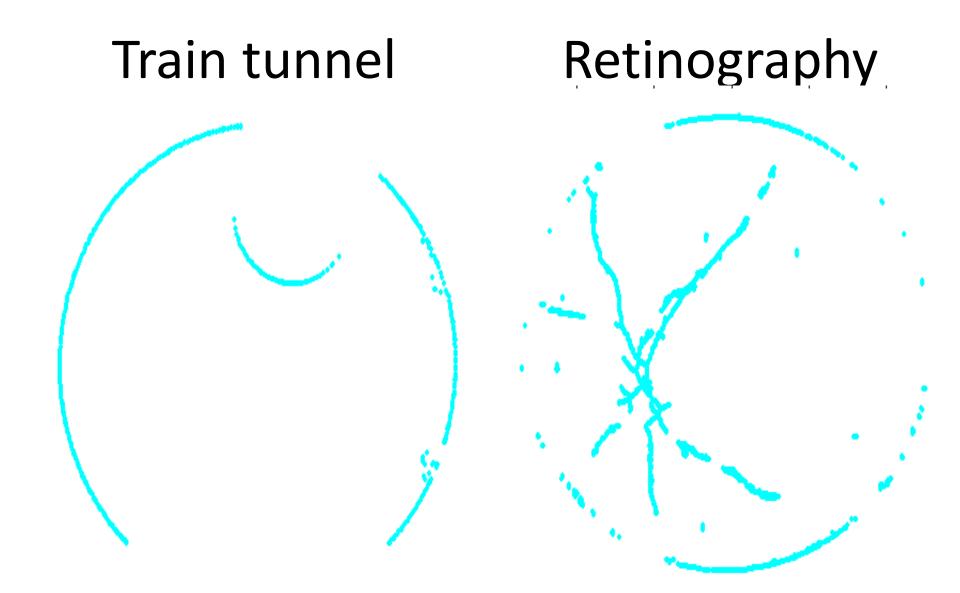
## **TCLUST Parsimonious modelling**

Trimming & constraints for estimating 14 Parsimonious models from Celeux and Govaert (1995)

BIC penalized TCLUST estimation  $\alpha$ = 15% applied to artificial data from VVE model Search in 14 models for k=1,2,3,4,5



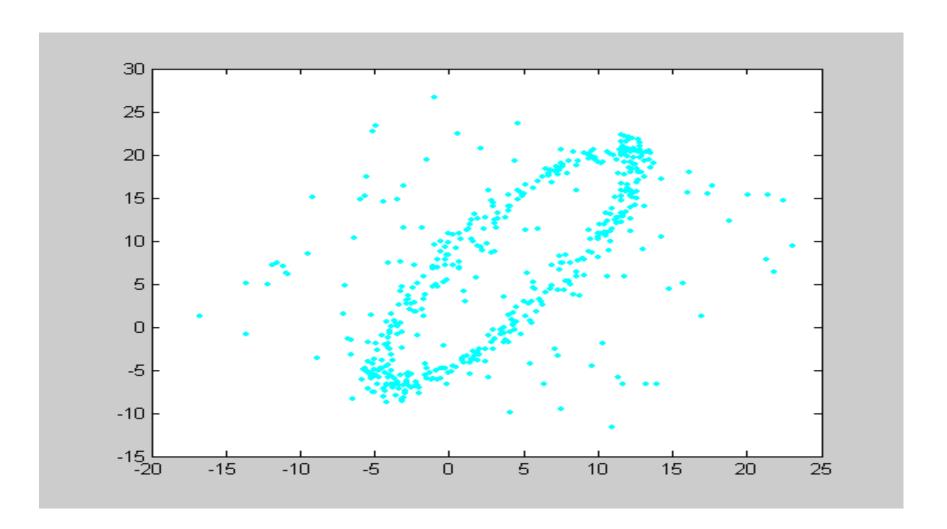
García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)



García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)

### ellipse

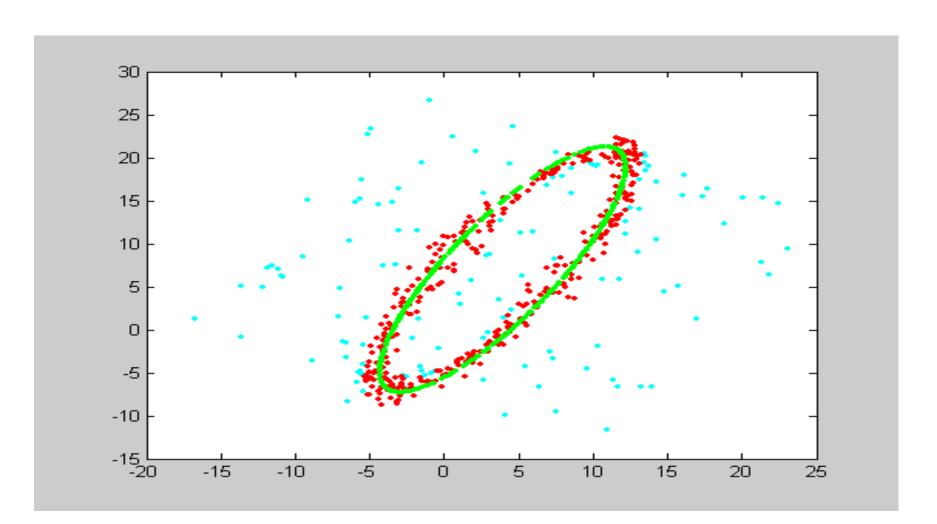
contamination=0.20



García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)

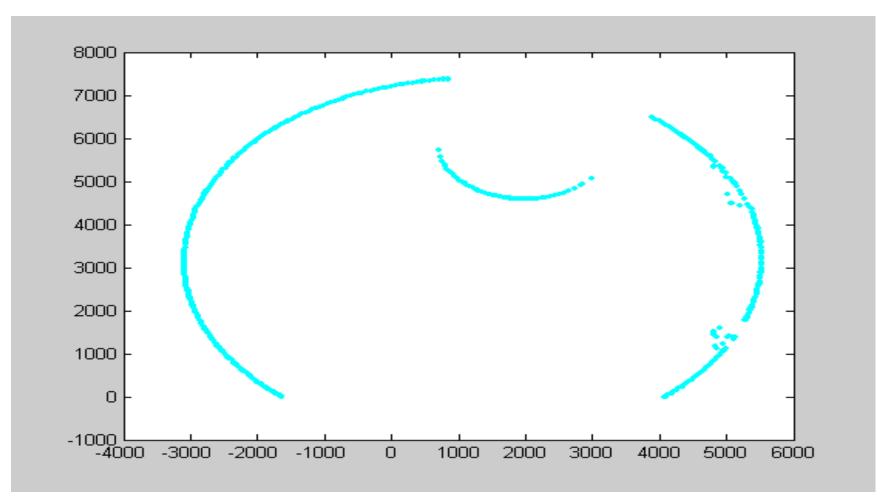
### ellipse

contamination=0.20 trimming level =0.25



García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)

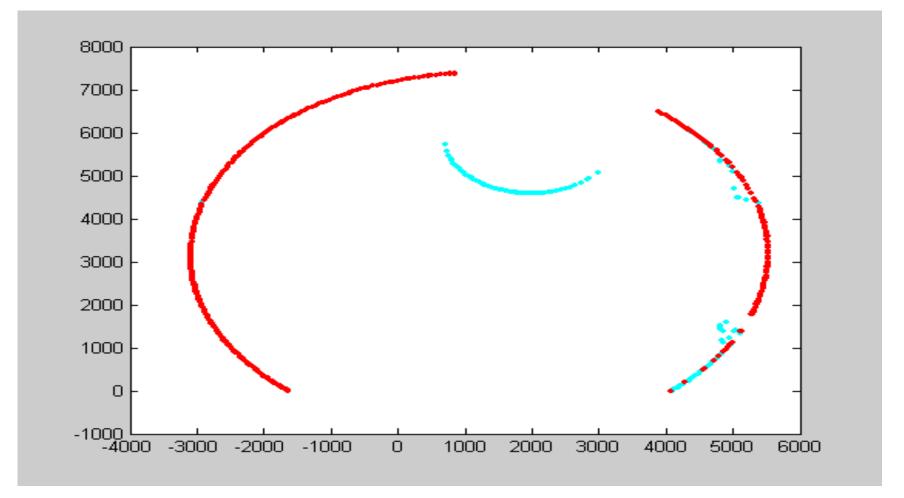
# High speed train tunnel (ellipse)



García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)

### High speed train tunnel (ellipse)

trimming level =0.25

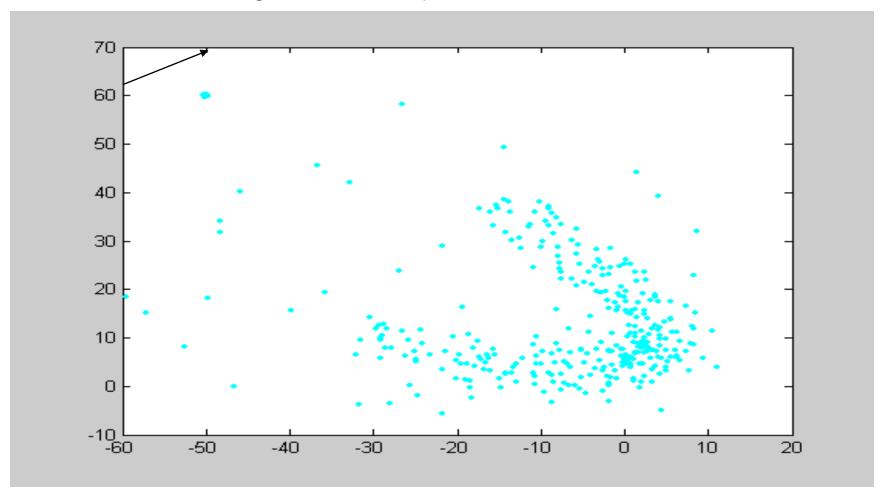


trimming level =0.25

García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)

#### Parabola

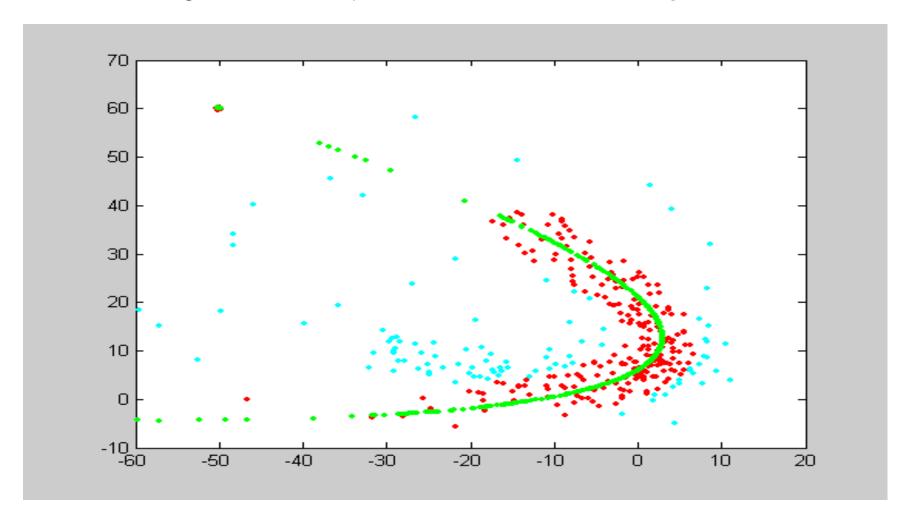
background noise=0.08 pointwise contamination=0.16



García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)

#### Parabola

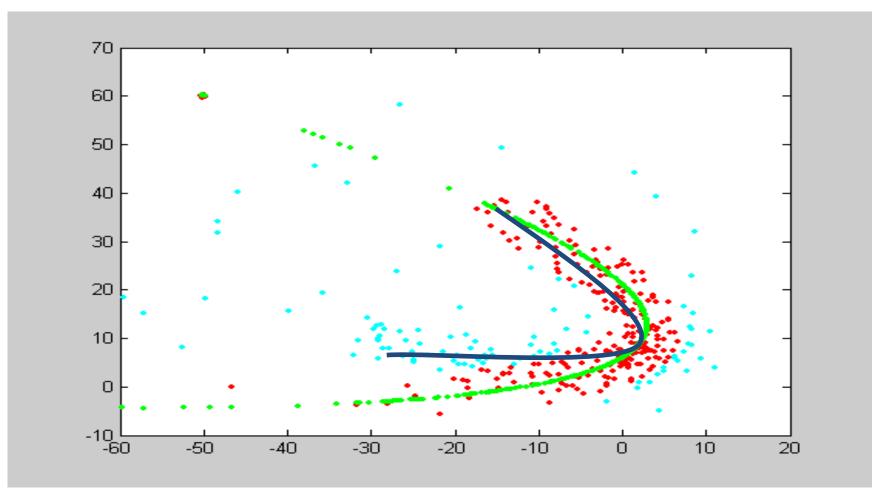
background noise=0.08 pointwise contamination=0.16 trimming level=0.25



García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)

#### Parabola

background noise=0.08 pointwise contamination=0.16 trimming level=0.25



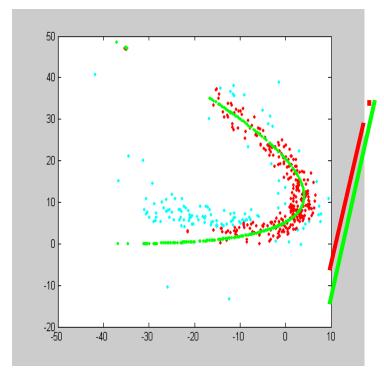
García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)

## Second trimming step

For avoiding the influence of pointwise contamination

This trimming is applied inside E step using the survival observations from the first trimming step

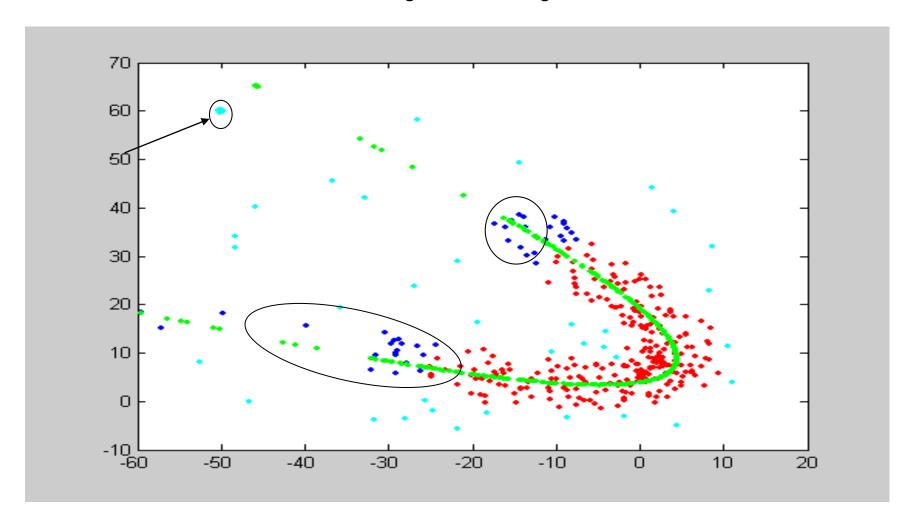
It is carried by using a  $\alpha_2\text{-trimmed}$  mean over the proyected points in an orthogonal direction to the main axe of the parabola



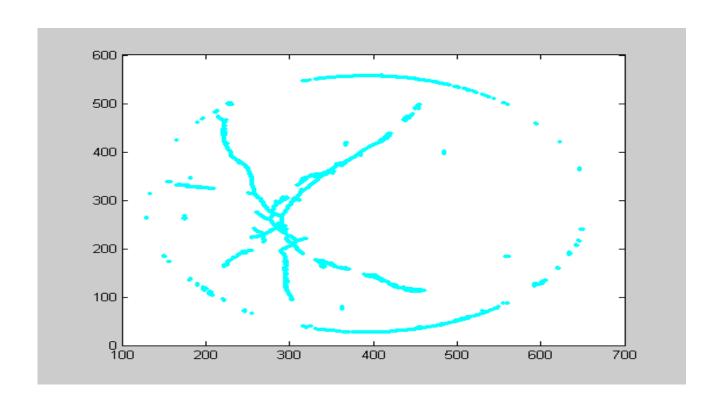
García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)

#### Parabola

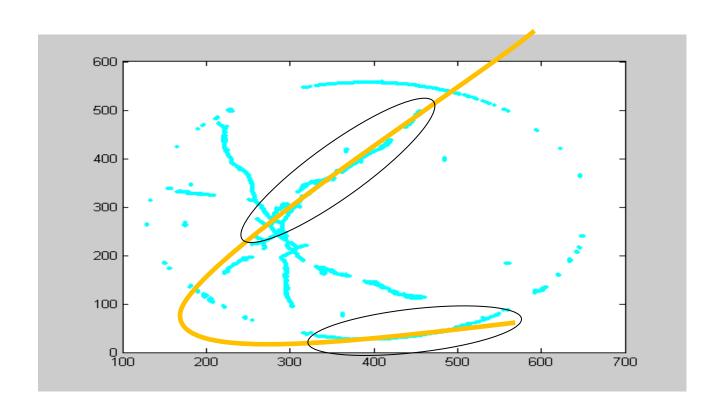
background noise=0.08 pointwise contamination=0.16 level of trimming1=0.25 trimming level=0.15



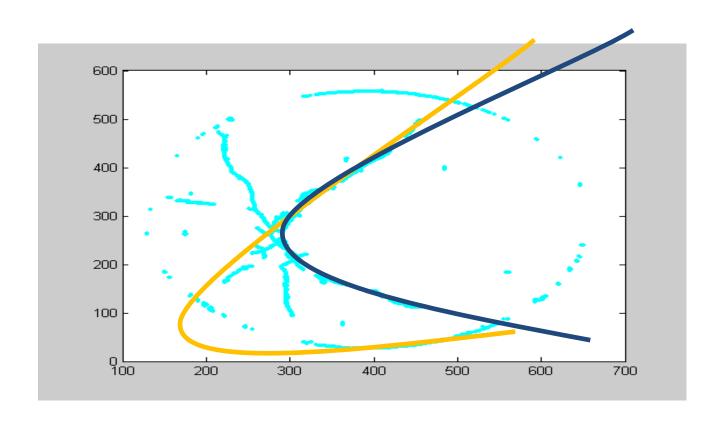
García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)



García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)



García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)



García-Escudero, M-I, Sánchez-Gutiérrez (CSDA, 2017)

