

## Session 6: Robust inference

### Winter course, CMStatistics 2016

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## Outline of the course

- 1. General notions of robustness
- 2. Robustness for univariate data
- 3. Robust multivariate methods
- 4. Robust regression
- 5. Robust principal component analysis
- 6. Inference
- 7. Multivariate and functional depth
- 8. High dimensional data and sparsity
- 9. Cellwise outliers

## Inference: Outline

- 1 Robust regression
- 2 Robust inference
- 3 Fast and robust bootstrap
- 4 Robust multivariate location and scatter
- 5 Inference for robust PCA
- 6 Inference for robust multivariate regression
- 7 Robust bootstrap tests in regression
- 8 Robust multigroup inference
- 9 Robust model selection
- 10 Software

## Regression model

- Dataset  $\mathcal{Z}_n = \{(y_1, \mathbf{x}_1), \dots, (y_n, \mathbf{x}_n)\} \subset \mathbb{R}^{p+1}$ .
- Linear regression model:

$$y_i = \mathbf{x}_i' \boldsymbol{\beta} + \varepsilon_i$$

- $E(\varepsilon_i) = 0$  and  $\text{Var}(\varepsilon_i) = \sigma^2$
- Residuals  $r_i(\hat{\boldsymbol{\beta}}) = y_i - \mathbf{x}_i' \hat{\boldsymbol{\beta}} \quad i = 1, \dots, n$

## Regression S-estimators

### Regression S-estimator

$$\hat{\beta}_S = \underset{\beta}{\operatorname{argmin}} \hat{\sigma}(\beta)$$

where  $\hat{\sigma}(\beta)$  is given by

$$\frac{1}{n} \sum_{i=1}^n \rho_0 \left( \frac{r_i(\beta)}{\hat{\sigma}(\beta)} \right) = \delta_0$$

with  $\rho_0$  a smooth bounded  $\rho$ -function.

## Regression MM estimates

### Regression MM-estimators

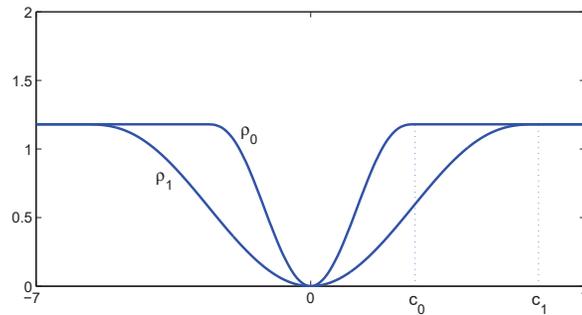
- 1 Compute an initial regression S-estimator  $\hat{\beta}_S$  with high breakdown value, and its corresponding scale estimate  $\hat{\sigma}_S = \hat{\sigma}(\hat{\beta}_S)$ .
- 2 Compute a regression M-estimator with fixed scale  $\hat{\sigma}_S$  and initial estimate  $\hat{\beta}_S$  but now using a bounded  $\rho$ -function with high efficiency.

$$\hat{\beta}_{MM} = \underset{\beta}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^n \rho_1 \left( \frac{r_i(\beta)}{\hat{\sigma}_S} \right)$$

Combines robustness and efficiency

## Example: loss functions

Tukey biweight  $\rho$  function for 50% breakdown point, and 95% efficiency:



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## Inference for robust estimators

- Reflect precision of parameter estimates
- Reflect existence and strength of observed effects
- Take into account that observed data contains outliers  
→ Inference should be robust!

## Inference for robust estimators

- Parametric inference: based on asymptotic distribution
  - ▶ Derived under ideal, outlier-free assumptions
  - ▶ No robustness guaranteed
- Bootstrap inference: less assumptions, but
  - ▶ High computational cost
  - ▶ Loss of robustness
- Computationally feasible and robust bootstrap inference?

→ Fast and Robust Bootstrap

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## MM estimating equations

The estimates  $\hat{\beta}_{MM}$ ,  $\hat{\sigma}_S$  and  $\hat{\beta}_S$  satisfy the equations

$$\begin{aligned} \hat{\beta}_{MM} &= \left[ \sum_{i=1}^n w_i^1 \mathbf{x}_i \mathbf{x}_i' \right]^{-1} \sum_{i=1}^n w_i^1 \mathbf{x}_i y_i \quad \text{with } w_i^1 = \frac{\psi_1(r_i(\hat{\beta}_{MM})/\hat{\sigma}_S)}{r_i(\hat{\beta}_{MM})}, \\ \hat{\sigma}_S &= \sum_{i=1}^n v_i (y_i - \hat{\beta}_S' \mathbf{x}_i) \quad \text{with } v_i = \frac{\hat{\sigma}_S \rho_0((r_i(\hat{\beta}_S)/\hat{\sigma}_S))}{n\delta_0 \tilde{r}_i(\hat{\beta}_S)}, \\ \hat{\beta}_S &= \left[ \sum_{i=1}^n w_i^0 \mathbf{x}_i \mathbf{x}_i' \right]^{-1} \sum_{i=1}^n w_i^0 \mathbf{x}_i y_i \quad \text{with } w_i^0 = \frac{\psi_0(r_i(\hat{\beta}_S)/\hat{\sigma}_S)}{r_i(\hat{\beta}_S)}, \end{aligned}$$

## Bootstrap sample MM estimating equations

- A bootstrap sample  $\mathcal{Z}_n^* = \{(\mathbf{x}_1^*, y_1^*), \dots, (\mathbf{x}_n^*, y_n^*)\}$  consists of  $n$  observations drawn from  $\mathcal{Z}_n$  with replacement.
- The MM-estimates  $\hat{\beta}_{MM}^*$  and  $\hat{\sigma}_S^*$  for a **bootstrap** sample  $\mathcal{Z}_n^*$  satisfy the equations

$$\begin{aligned}\hat{\beta}_{MM}^* &= \left[ \sum_{i=1}^n w_i^{1*} \mathbf{x}_i^* \mathbf{x}_i^{*'} \right]^{-1} \sum_{i=1}^n w_i^{1*} \mathbf{x}_i^* y_i^* \quad \text{with } w_i^{1*} = \frac{\psi_1(r_i(\hat{\beta}_{MM}^*)/\hat{\sigma}_S^*)}{r_i(\hat{\beta}_{MM}^*)}, \\ \hat{\sigma}_S^* &= \sum_{i=1}^n v_i^* (y_i^* - \hat{\beta}_S^* \mathbf{x}_i^*) \quad \text{with } v_i^* = \frac{\hat{\sigma}_S^* \rho_0((r_i(\hat{\beta}_S^*)/\hat{\sigma}_S^*))}{n\delta_0 \tilde{r}_i(\hat{\beta}_S^*)}, \\ \hat{\beta}_S^* &= \left[ \sum_{i=1}^n w_i^{0*} \mathbf{x}_i^* \mathbf{x}_i^{*'} \right]^{-1} \sum_{i=1}^n w_i^{0*} \mathbf{x}_i^* y_i^* \quad \text{with } w_i^{0*} = \frac{\psi_0(r_i(\hat{\beta}_S^*)/\hat{\sigma}_S^*)}{r_i(\hat{\beta}_S^*)},\end{aligned}$$

## First order approximation for a bootstrap sample

For a **bootstrap** sample  $\mathcal{Z}_n^* = \{(\mathbf{x}_1^*, y_1^*), \dots, (\mathbf{x}_n^*, y_n^*)\}$  calculate the estimates

$$\begin{aligned}\tilde{\beta}_{MM}^* &= \left[ \sum_{i=1}^n \tilde{w}_i^{1*} \mathbf{x}_i^* \mathbf{x}_i^{*'} \right]^{-1} \sum_{i=1}^n \tilde{w}_i^{1*} \mathbf{x}_i^* y_i^* \quad \text{with } \tilde{w}_i^{1*} = \frac{\psi_1(r_i(\hat{\beta}_{MM})/\hat{\sigma}_S)}{r_i(\hat{\beta}_{MM})}, \\ \tilde{\sigma}_S^* &= \sum_{i=1}^n \tilde{v}_i^* (y_i^* - \hat{\beta}_S \mathbf{x}_i^*) \quad \text{with } \tilde{v}_i^* = \frac{\hat{\sigma}_S \rho_0((r_i(\hat{\beta}_S)/\hat{\sigma}_S))}{n\delta_0 \tilde{r}_i(\hat{\beta}_S)}, \\ \tilde{\beta}_S^* &= \left[ \sum_{i=1}^n \tilde{w}_i^{0*} \mathbf{x}_i^* \mathbf{x}_i^{*'} \right]^{-1} \sum_{i=1}^n \tilde{w}_i^{0*} \mathbf{x}_i^* y_i^* \quad \text{with } \tilde{w}_i^{0*} = \frac{\psi_0(r_i(\hat{\beta}_S)/\hat{\sigma}_S)}{r_i(\hat{\beta}_S)},\end{aligned}$$

Note that  $\hat{\beta}_{MM}$ ,  $\hat{\sigma}_S$  and  $\hat{\beta}_S$  are not recalculated!

## Linear correction: FRB estimates

The first order approximations  $\tilde{\beta}_{MM}^*$ ,  $\tilde{\sigma}_S^*$  and  $\tilde{\beta}_S^*$  **underestimate** the sampling variability!

⇒ apply a **linear correction**:

- Put  $\hat{\Theta} = (\hat{\beta}_{MM}, \hat{\sigma}_S, \hat{\beta}_S)$ , then we have functions  $\mathbf{g}_n$ , such that

$$\mathbf{g}_n(\hat{\Theta}) = \hat{\Theta}$$

- Taylor expansion about estimands  $\Theta$ :

$$\hat{\Theta} = \mathbf{g}_n(\Theta) + \nabla \mathbf{g}_n(\Theta)(\hat{\Theta} - \Theta) + R$$

- With  $R$  small, rewrite:

$$(\hat{\Theta} - \Theta) \approx [\mathbf{I} - \nabla \mathbf{g}_n(\Theta)]^{-1}(\mathbf{g}_n(\Theta) - \Theta)$$

- Taking bootstrap equivalents:

$$(\hat{\Theta}^* - \hat{\Theta}) \approx [\mathbf{I} - \nabla \mathbf{g}_n(\hat{\Theta})]^{-1}(\mathbf{g}_n^*(\hat{\Theta}) - \hat{\Theta})$$

## Properties of fast and robust bootstrap

Fast and robust bootstrap distribution (Salibian-Barrera and Zamar, 2002)

The fast and robust bootstrap estimates for  $\hat{\Theta} = (\hat{\beta}_{MM}, \hat{\sigma}_S, \hat{\beta}_S)$  are given by

$$\hat{\Theta}_{FRB}^* = \hat{\Theta} + [\mathbf{I} - \nabla \mathbf{g}_n(\hat{\Theta})]^{-1}(\tilde{\Theta}^* - \hat{\Theta})$$

where  $\tilde{\Theta}^* = (\tilde{\beta}_{MM}^*, \tilde{\sigma}_S^*, \tilde{\beta}_S^*) = \mathbf{g}_n^*(\hat{\Theta})$

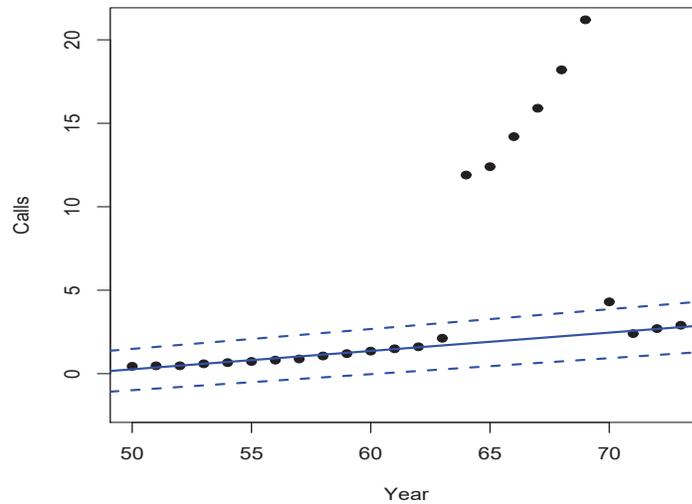
**Consistency:** Under regularity conditions the FRB distribution and the sample distribution of the estimators converge to the same limiting distribution.

**Computational efficiency:** The FRB estimates are solutions of a system of linear equations.

**Robustness:** The FRB estimates use the weights of the MM/S-estimates at the original sample. FRB quantiles have maximal breakdown point.

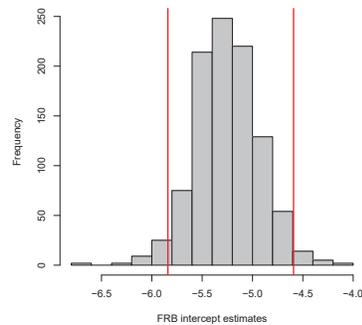
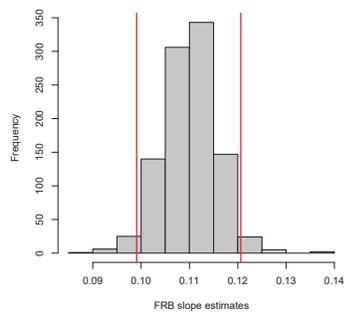
## Example: Telephone data

95% confidence bands based on FRB



## Robust inference: Telephone data

Yearly number of international calls from Belgium, from 1950 to 1973



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## Multivariate location and scatter model

- Dataset  $\mathcal{X}_n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subset \mathbb{R}^p$ .
- Multivariate location and scatter model:

$$\mathbf{x}_i = \boldsymbol{\mu} + \Sigma^{1/2} \boldsymbol{\varepsilon}_i \quad i = 1, \dots, n$$

- $E(\boldsymbol{\varepsilon}_i) = \mathbf{0}$  and  $\text{Cov}(\boldsymbol{\varepsilon}_i) = I_p$
- Distances  $d_i(\boldsymbol{\mu}, \Sigma) = \sqrt{(\mathbf{x}_i - \boldsymbol{\mu})' \Sigma^{-1} (\mathbf{x}_i - \boldsymbol{\mu})}$   $i = 1, \dots, n$

## Multivariate S-estimates

### S-estimator of location and scatter

$$(\hat{\boldsymbol{\mu}}_S, \hat{\Sigma}_S) = \underset{\boldsymbol{\mu}, \Sigma}{\operatorname{argmin}} |\Sigma|$$

over all  $\boldsymbol{\mu} \in \mathbb{R}^p$  and symmetric positive definite  $\Sigma$  that satisfy

$$\frac{1}{n} \sum_{i=1}^n \rho_0(d_i(\boldsymbol{\mu}, \Sigma)) = \delta$$

with  $\rho_0$  a smooth *bounded*  $\rho$ -function.

## Multivariate MM-estimates

### MM-estimator of location and scatter

- 1 Denote  $\hat{\sigma}^2 = |\hat{\Sigma}_S|^{1/p}$ , the S-estimate of the generalized scale.
- 2 The MM-estimator for location and shape  $(\hat{\boldsymbol{\mu}}_{MM}, \hat{\Gamma}_{MM})$  minimizes

$$\frac{1}{n} \sum_{i=1}^n \rho_1 \left( \frac{\sqrt{(\mathbf{x}_i - \boldsymbol{\mu})' \Gamma^{-1} (\mathbf{x}_i - \boldsymbol{\mu})}}{\hat{\sigma}} \right) \quad (1)$$

among all  $\boldsymbol{\mu} \in \mathbb{R}^p$  and symmetric positive definite  $\Gamma$  with  $|\Gamma| = 1$ .

The MM-estimator for the covariance matrix is then  $\hat{\Sigma}_{MM} = \hat{\sigma}^2 \hat{\Gamma}_{MM}$ .

Combines robustness and efficiency

## Multivariate MM estimating equations

The estimates  $\hat{\boldsymbol{\mu}}_{MM}$ ,  $\hat{\Gamma}_{MM}$ ,  $\hat{\boldsymbol{\mu}}_S$ , and  $\hat{\Sigma}_S$  satisfy the equations

$$\begin{aligned}\hat{\boldsymbol{\mu}}_{MM} &= \left( \sum_{i=1}^n \frac{\psi_1(d_{i,MM}/\hat{\sigma})}{d_{i,MM}} \right)^{-1} \left( \sum_{i=1}^n \frac{\psi_1(d_{i,MM}/\hat{\sigma})}{d_{i,MM}} \mathbf{x}_i \right) \\ \hat{\Gamma}_{MM} &= G \left( \sum_{i=1}^n \frac{\psi_1(d_{i,MM}/\hat{\sigma})}{d_{i,MM}} (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_{MM})(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_{MM})' \right) \\ \hat{\boldsymbol{\mu}}_S &= \left( \sum_{i=1}^n \frac{\psi_0(d_{i,S})}{d_{i,S}} \right)^{-1} \left( \sum_{i=1}^n \frac{\psi_0(d_{i,S})}{d_{i,S}} \mathbf{x}_i \right) \\ \hat{\Sigma}_S &= \frac{1}{n\delta} \left( \sum_{i=1}^n p \frac{\psi_0(d_{i,S})}{d_{i,S}} (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_S)(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_S)' + \left( \sum_{i=1}^n v_i \right) \hat{\Sigma}_S \right)\end{aligned}$$

where  $G(A) = |A|^{-1/p} A$ ,  $v_i = \rho_0(d_{i,S}) - \psi_0(d_{i,S})d_{i,S}$ ,  $\hat{\sigma} = |\hat{\Sigma}_S|^{1/p}$  and  $d_{i,MM}^2 = (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_{MM})' \hat{\Gamma}_{MM}^{-1} (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_{MM})$ ,  $d_{i,S}^2 = (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_S)' \hat{\Sigma}_S^{-1} (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_S)$ .

## First order approximation for a bootstrap sample

$$\begin{aligned}\tilde{\boldsymbol{\mu}}_{MM}^* &= \left( \sum_{i=1}^n \frac{\psi_1(\tilde{d}_{i,MM}^*/\hat{\sigma})}{\tilde{d}_{i,MM}^*} \right)^{-1} \left( \sum_{i=1}^n \frac{\psi_1(\tilde{d}_{i,MM}^*/\hat{\sigma})}{\tilde{d}_{i,MM}^*} \mathbf{x}_i^* \right) \\ \tilde{\Gamma}_{MM}^* &= G \left( \sum_{i=1}^n \frac{\psi_1(\tilde{d}_{i,MM}^*/\hat{\sigma})}{\tilde{d}_{i,MM}^*} (\mathbf{x}_i^* - \hat{\boldsymbol{\mu}}_{MM})(\mathbf{x}_i^* - \hat{\boldsymbol{\mu}}_{MM})' \right) \\ \tilde{\boldsymbol{\mu}}_S^* &= \left( \sum_{i=1}^n \frac{\psi_0(\tilde{d}_{i,S}^*)}{\tilde{d}_{i,S}^*} \right)^{-1} \left( \sum_{i=1}^n \frac{\psi_0(\tilde{d}_{i,S}^*)}{\tilde{d}_{i,S}^*} \mathbf{x}_i^* \right) \\ \tilde{\Sigma}_S^* &= \frac{1}{n\delta} \left( \sum_{i=1}^n p \frac{\psi_0(\tilde{d}_{i,S}^*)}{\tilde{d}_{i,S}^*} (\mathbf{x}_i^* - \hat{\boldsymbol{\mu}}_S)(\mathbf{x}_i^* - \hat{\boldsymbol{\mu}}_S)' + \left( \sum_{i=1}^n \tilde{v}_i \right) \hat{\Sigma}_S \right)\end{aligned}$$

where  $G(A) = |A|^{-1/p} A$ ,  $\tilde{v}_i = \rho_0(\tilde{d}_{i,S}^*) - \psi_0(\tilde{d}_{i,S}^*)\tilde{d}_{i,S}^*$ ,  $\hat{\sigma} = |\hat{\Sigma}_S|^{1/p}$  and  $(\tilde{d}_{i,MM}^*)^2 = (\mathbf{x}_i^* - \hat{\boldsymbol{\mu}}_{MM})' \hat{\Gamma}_{MM}^{-1} (\mathbf{x}_i^* - \hat{\boldsymbol{\mu}}_{MM})$ ,  $(\tilde{d}_{i,S}^*)^2 = (\mathbf{x}_i^* - \hat{\boldsymbol{\mu}}_S)' \hat{\Sigma}_S^{-1} (\mathbf{x}_i^* - \hat{\boldsymbol{\mu}}_S)$ .

## Properties of fast and robust bootstrap

### Fast and robust bootstrap distribution (Salibián-Barrera et al., 2006)

The fast and robust bootstrap estimates for  $\hat{\Theta} = (\hat{\boldsymbol{\mu}}_{MM}, \hat{\Gamma}_{MM}, \hat{\boldsymbol{\mu}}_S, \hat{\Sigma}_S)$  are given by

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where  $\tilde{\Theta}^* = (\tilde{\boldsymbol{\mu}}_{MM}^*, \tilde{\Gamma}_{MM}^*, \tilde{\boldsymbol{\mu}}_S^*, \tilde{\Sigma}_S^*)$ .

- Consistency:** Under regularity conditions the FRB distribution and the sample distribution of the estimators converge to the same limiting distribution.
- Computational efficiency:** The FRB estimates are solutions of a system of linear equations.
- Robustness:** The FRB estimates use the weights of the MM/S-estimates at the original sample. FRB quantiles have maximal breakdown point.

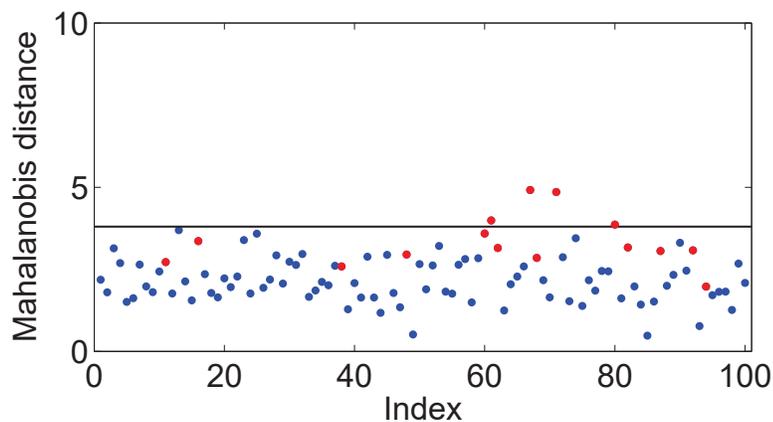
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## Example: Forged Swiss bank notes data

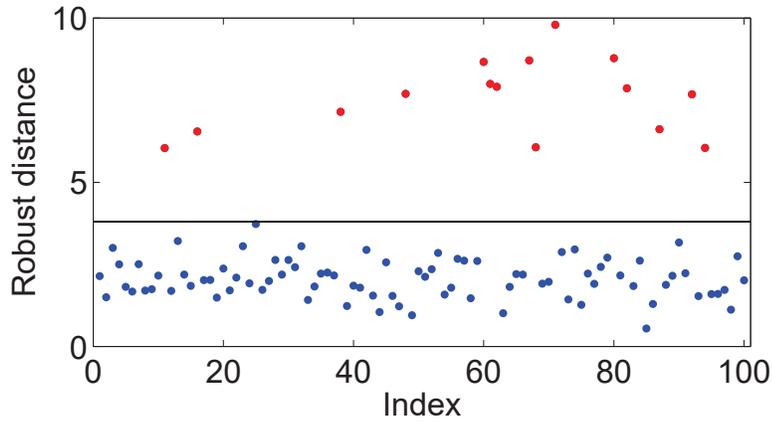
- $n = 100$  forged Swiss bank notes
- 6 variables:
  - ▶ V1: length of the bill
  - ▶ V2: height of the bill, measured on the left
  - ▶ V3: height of the bill, measured on the right
  - ▶ V4: distance of inner frame to the lower border
  - ▶ V5: distance of inner frame to the upper border
  - ▶ V6: length of diagonal

## Outliers?



Mahalanobis distances:  $MD(x_i) = [(x_i - \bar{x}_n)' S_n^{-1} (x_i - \bar{x}_n)]^{1/2}$

## Multivariate outlier detection

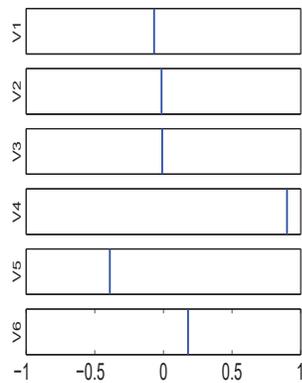


⇒ group of 15 outliers

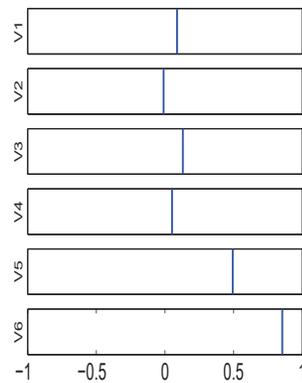
## PCA

### Classical PC estimates

weights in 1st PC

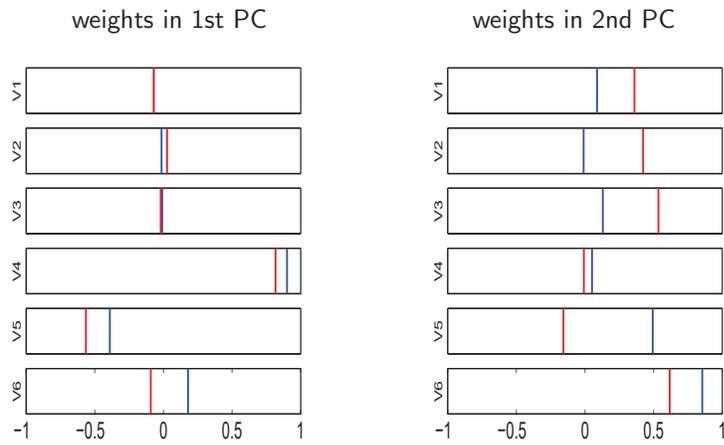


weights in 2nd PC



## Robust PCA with MM-estimates

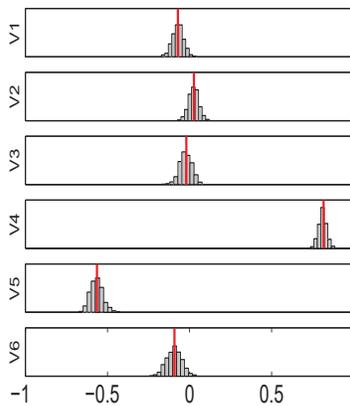
Classical + robust (MM) PC estimates



## Forged Swiss bank notes data

Histograms of FRB estimates of the weights

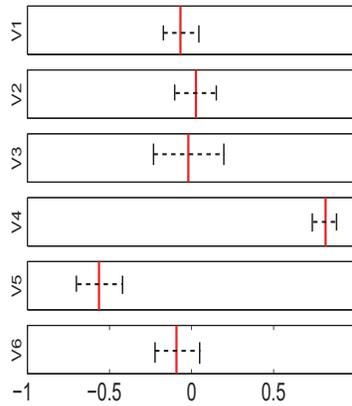
weights in first PC



→ Accuracy of loadings in the first PC

## Forged Swiss bank notes data

FRB confidence intervals for the weights in first PC



## Forged Swiss bank notes data

Stability of PCA based on MM-estimates?

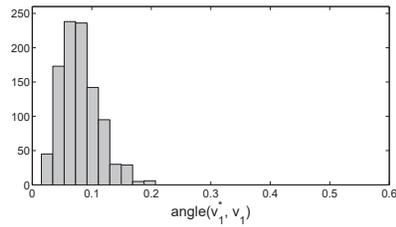
→ Investigate sampling distribution of angles between  $\hat{v}_1$  and true component  $v_1$ :  
**distribution of  $\text{acos}(|v_1' \hat{v}_1|)$**

▷ can be estimated through bootstrap values  $\text{acos}(|\hat{v}_1' \hat{v}_1^*|)$  ◁

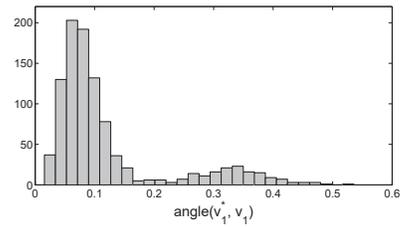
## Forged Swiss bank notes data

angles between  $\hat{v}_1^*$  and  $\hat{v}_1$  ( $\in [0, \pi/2]$ )

FRB



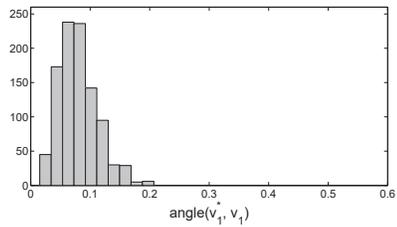
classical bootstrap



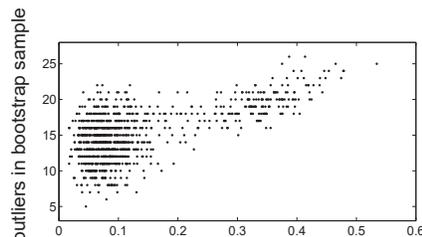
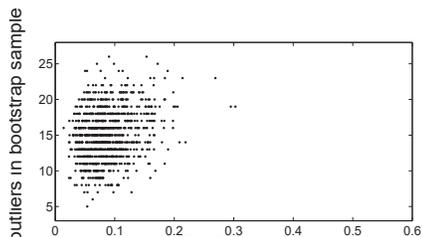
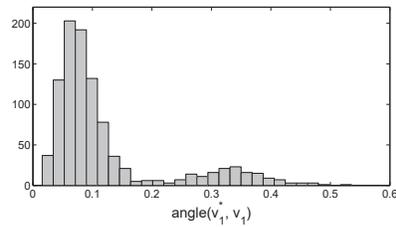
## Forged Swiss bank notes data

angles between  $\hat{v}_1^*$  and  $\hat{v}_1$  ( $\in [0, \pi/2]$ )

FRB



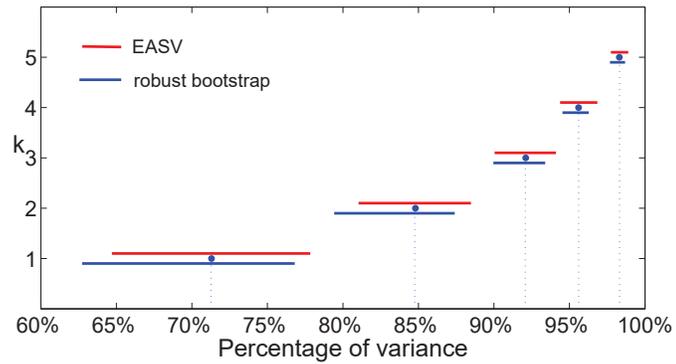
classical bootstrap



## Forged Swiss bank notes data

Percentage of variance explained

95% confidence intervals: **robust bootstrap** and **asymptotic normality**



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## Example: School data

- Explain scores on 3 different tests from 70 school sites by means of 5 explanatory variables
- Responses: reading ( $y_1$ ), mathematics ( $y_2$ ), and selfesteem ( $y_3$ ) score
- Predictors: education level of mother ( $x_1$ ), highest occupation of a family member ( $x_2$ ), parent counseling index ( $x_3$ ), number of teachers ( $x_4$ ), parental visits index ( $x_5$ )
- Model:

$$y_1 = \beta_{11} + \beta_{21}x_1 + \beta_{31}x_2 + \beta_{41}x_3 + \beta_{51}x_4 + \beta_{51}x_5 + \epsilon_1$$

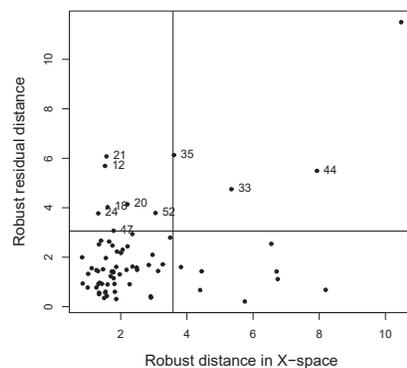
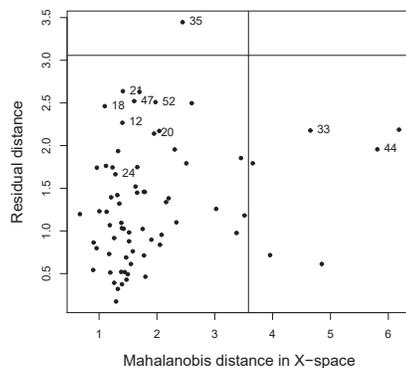
$$y_2 = \beta_{12} + \beta_{22}x_1 + \beta_{32}x_2 + \beta_{42}x_3 + \beta_{52}x_4 + \beta_{52}x_5 + \epsilon_2$$

$$y_3 = \beta_{13} + \beta_{23}x_1 + \beta_{33}x_2 + \beta_{43}x_3 + \beta_{53}x_4 + \beta_{53}x_5 + \epsilon_3$$

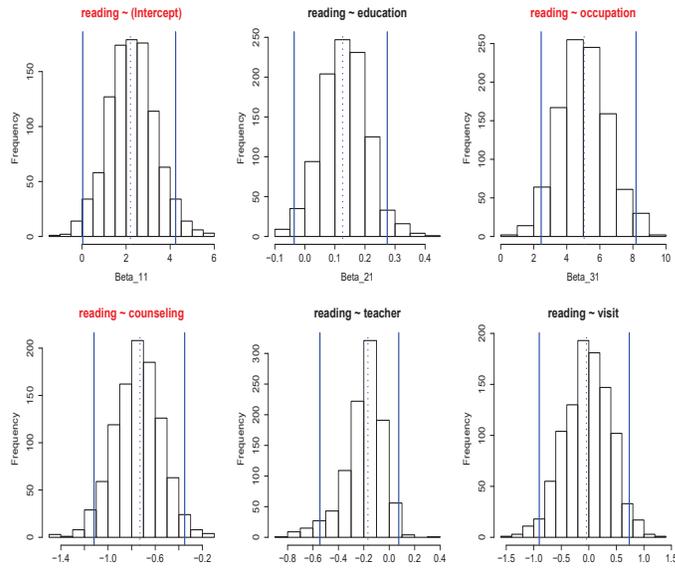
The errors  $\epsilon = (\epsilon_1, \epsilon_2, \epsilon_3)'$  have center zero and some positive definite scatter matrix  $\Sigma$

## Multivariate regression example: School data

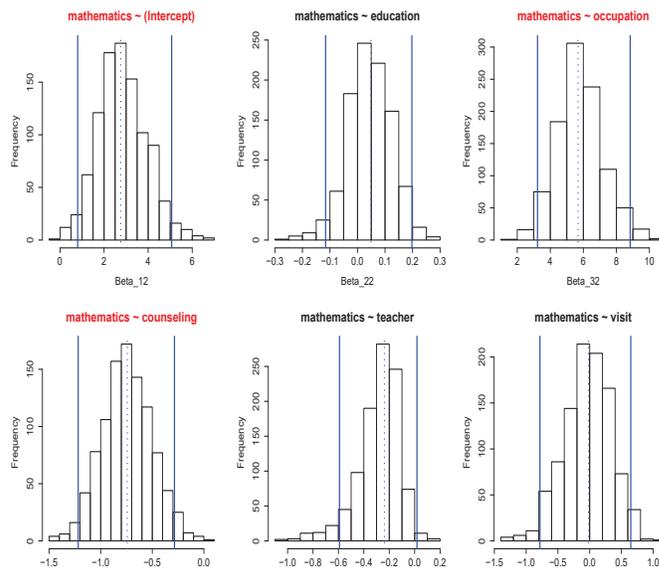
Diagnostic plot: Outlier detection



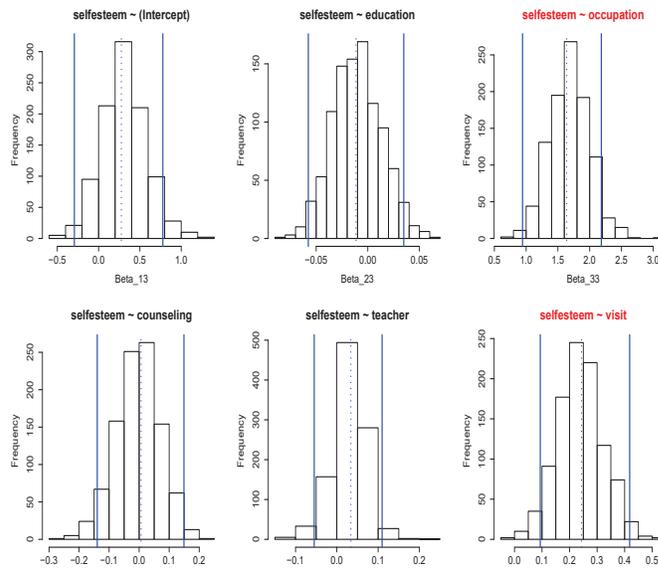
## Example: School data



## Example: School data



## Example: School data



## Inference: Outline

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## Tests for the regression model

- Linear regression model:

$$y_i = \mathbf{x}'_i \boldsymbol{\beta} + \varepsilon_i$$

- Denote  $\boldsymbol{\beta} = ((\boldsymbol{\beta}^{(1)})', (\boldsymbol{\beta}^{(2)})')'$  with  $\boldsymbol{\beta}^{(1)} \in \mathbb{R}^q$  and  $\boldsymbol{\beta}^{(2)} \in \mathbb{R}^{p-q}$
- Test for a linear hypothesis

$$H_0: \boldsymbol{\beta}_0^{(2)} = \mathbf{0}$$

$$H_a: \boldsymbol{\beta}_0^{(2)} \neq \mathbf{0}$$

## Classical approach: the F-test

- $\hat{\boldsymbol{\beta}}_{LS}, \hat{\sigma}_{LS}$ : least squares estimates in the full model
- $\hat{\boldsymbol{\beta}}_{LS,r}, \hat{\sigma}_{LS,r}$ : least squares estimates in the reduced model under  $H_0$

$$F = \frac{(\text{SSE}(\hat{\boldsymbol{\beta}}_{LS,r}) - \text{SSE}(\hat{\boldsymbol{\beta}}_{LS})) / (p - q)}{\text{SSE}(\hat{\boldsymbol{\beta}}_{LS}) / (n - p)}$$

- Under  $H_0$ :  $F \sim F_{p-q, n-p}$  if errors are normal
- Under  $H_0$ :  $(p - q)F \sim \chi_{p-q}^2$  asymptotically

$$(p - q)F \approx n \left( \frac{\hat{\sigma}_{LS,r}^2 - \hat{\sigma}_{LS}^2}{\hat{\sigma}_{LS}^2} \right)$$

## Robust test statistic

Let  $\hat{\sigma}_S$  and  $\hat{\sigma}_{S,r}$  be the scale estimates corresponding to the S/MM-estimates in the full and reduced model.

Consider the test statistic

$$L_n = n \left( \frac{\hat{\sigma}_{S,r}^2 - \hat{\sigma}_S^2}{\hat{\sigma}_S^2} \right)$$

## Asymptotic null distribution

### Asymptotic null distribution (Salibián-Barrera et al., 2016)

Asymptotically the distribution of the test statistic  $L_n$  under  $H_0$  is given by

$$\frac{2DB}{H} L_n \xrightarrow{\mathcal{D}} \chi_{p-q}^2$$

with

$$B = E(\psi_0(u)u)$$

$$D = E(\psi_0'(u))$$

$$H = E(\psi_0^2(u))$$

## Robust test

- The asymptotic approximation of the null distribution
  - ▶ Only holds well for large samples
  - ▶ Is worse for contaminated data
- Can we estimate the null distribution by fast and robust bootstrap?

## Fast and robust bootstrap test

- For the full model, set  $\hat{\Theta} = (\hat{\sigma}_S, \hat{\beta}_S)$  and  $\tilde{\Theta}^* = (\tilde{\sigma}_S^*, \tilde{\beta}_S^*)$ , then

$$\hat{\Theta}_{FRB}^* = \hat{\Theta} + [\mathbf{I} - \nabla \mathbf{g}_n(\hat{\Theta})]^{-1}(\tilde{\Theta}^* - \hat{\Theta})$$

- For the reduced model, set  $\hat{\Theta}_r = (\hat{\sigma}_{S,r}, \hat{\beta}_{S,r})$  and  $\tilde{\Theta}_r^* = (\tilde{\sigma}_{S,r}^*, \tilde{\beta}_{S,r}^*)$ , then

$$\hat{\Theta}_{r,FRB}^* = \hat{\Theta}_r + [\mathbf{I} - \nabla \mathbf{g}_{rn}(\hat{\Theta}_r)]^{-1}(\tilde{\Theta}_r^* - \hat{\Theta}_r)$$

- However, the distribution of

$$\tilde{L}_n^* = n \left( \frac{(\hat{\sigma}_{S,r,FRB}^*)^2 - (\hat{\sigma}_{S,FRB}^*)^2}{(\hat{\sigma}_{S,FRB}^*)^2} \right)$$

is **inconsistent** because it converges at a faster rate  $(1/n)$ !

## FRB estimate of the null distribution

- Consider a test statistic  $L_n = h_n(\hat{\alpha}_n)$
- We now need that

$$h_n^*(\hat{\alpha}_{n,FRB}^*) = h_n^*(\hat{\alpha}_n^*) + o_p(1/n)$$

- Taylor expansion of  $h_n^*(\hat{\alpha}_{n,FRB}^*)$ :

$$h_n^*(\hat{\alpha}_{n,FRB}^*) = h_n^*(\hat{\alpha}_n^*) + \nabla h_n^*(\hat{\alpha}_n^*)(\hat{\alpha}_{n,FRB}^{R*} - \hat{\alpha}_n^*) + o_P(n^{-1})$$

- $\hat{\alpha}_{n,FRB}^* - \hat{\alpha}_n^* = O_P(n^{-1})$

⇒ we need that

$$\nabla h_n^*(\hat{\alpha}_n^*) = o_P(1)$$

## Test statistics for FRB

- Rewrite the test statistics  $L_n$  as

$$L_n = n \left( \frac{\hat{\sigma}_{S,r}^2 - \hat{\sigma}_S^2}{\hat{\sigma}_S^2} \right) = n \left( \frac{\hat{\sigma}^2(\hat{\beta}_{S,r}) - \hat{\sigma}^2(\hat{\beta}_S)}{\hat{\sigma}^2(\hat{\beta}_S)} \right) = h_n(\hat{\beta}_{S,r}, \hat{\beta}_S)$$

- $\nabla h_n^*(\hat{\beta}_{S,r}^*, \hat{\beta}_S^*) = o_P(1)$
- Set

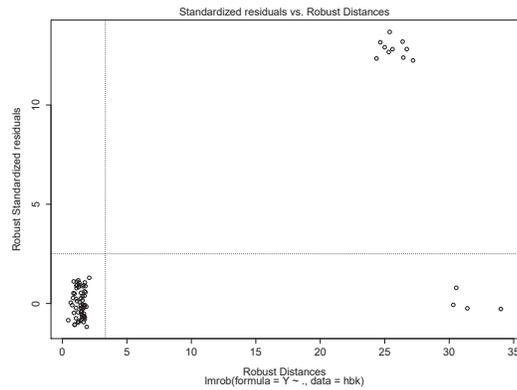
$$L_{n,FRB}^* = h_n^*(\hat{\beta}_{S,r,FRB}^*, \hat{\beta}_{S,FRB}^*)$$

⇒ The distribution of  $L_{n,FRB}^*$  consistently estimates the null distribution of the test statistic  $L_n$ .

- Limited extra computational cost

## Example: Hawkins-Bradu-Kass data

Cases 1–10 are bad leverage points, cases 11–14 are good leverage points, and the remainder is regular ( $n = 75$ ,  $p = 3$ ).



## Example: Hawkins-Bradu-Kass data

Model:  $y = \beta_{01}x_{i1} + \beta_{02}x_{i2} + \beta_{03}x_{i3} + \beta_{04} + \epsilon_i$

$H_0 : \beta_{01} = \beta_{03} = 0$

	F-test	$L_n$ (asyp)	$L_{n,FRB}$
Full data	0.00035	0.786	0.564
Regular data	0.252		

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## Multigroup model

- Observations  $\mathbf{x}_{ji} \in \mathbb{R}^p$  with  $j = 1, \dots, k$ ;  $i = 1, \dots, n_j$
- For each group  $j$ :

$$\mathbf{x}_{ji} = \boldsymbol{\mu}_j + \Sigma^{1/2} \boldsymbol{\varepsilon}_{ji} \quad i = 1, \dots, n_j$$

- $E(\boldsymbol{\varepsilon}_{ji}) = 0$  and  $\text{Cov}(\boldsymbol{\varepsilon}_{ji}) = I_p$
- Distances  $d_{ji}(\boldsymbol{\mu}_j, \Sigma) = \sqrt{(\mathbf{x}_{ji} - \boldsymbol{\mu}_j)' \Sigma^{-1} (\mathbf{x}_{ji} - \boldsymbol{\mu}_j)}$

## $k$ -sample S-estimators

### $k$ -sample S-estimators (He and Fung, 2000)

The S-estimator of the  $k$  locations  $\hat{\boldsymbol{\mu}}_{S,1}, \dots, \hat{\boldsymbol{\mu}}_{S,k}$  and common scatter  $\hat{\Sigma}_S^{(k)}$  minimize  $|\Sigma|$  subject to

$$\frac{1}{n} \sum_{j=1}^k \sum_{i=1}^{n_j} \rho_0(d_{ji} \boldsymbol{\mu}_j, \Sigma) = \delta$$

among all  $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_k \in \mathbb{R}^p$  and symmetric positive definite  $\Sigma$ .

## $k$ -sample MM-estimators

### $k$ -sample MM-estimators (Van Aelst and Willems, 2011)

- 1 Put  $(\hat{\sigma}_S^{(k)})^2 = |\hat{\Sigma}_S^{(k)}|^{1/p}$ , the S-estimate of the generalized scale
- 2 the MM-estimator of the  $k$  locations  $\hat{\boldsymbol{\mu}}_{MM,1}, \dots, \hat{\boldsymbol{\mu}}_{MM,k}$  and common shape  $\hat{\Gamma}_{MM}^{(k)}$  minimize

$$\frac{1}{n} \sum_{j=1}^k \sum_{i=1}^{n_j} \rho_1 \left( \frac{\sqrt{(\mathbf{x}_{ji} - \boldsymbol{\mu}_j)^t \Gamma^{-1} (\mathbf{x}_{ji} - \boldsymbol{\mu}_j)}}{\hat{\sigma}_S^{(k)}} \right)$$

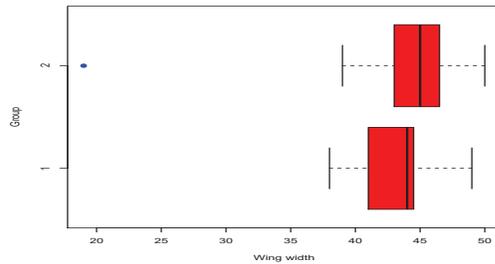
among all  $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_k \in \mathbb{R}^p$  and symmetric positive definite  $\Gamma$  with  $|\Gamma| = 1$ .  
The MM-estimator of the common covariance matrix is then

$$\hat{\Sigma}_{MM}^{(k)} = (\hat{\sigma}_S^{(k)})^2 \hat{\Gamma}_{MM}^{(k)}$$

## Example: robust LDA

### Biting flies data

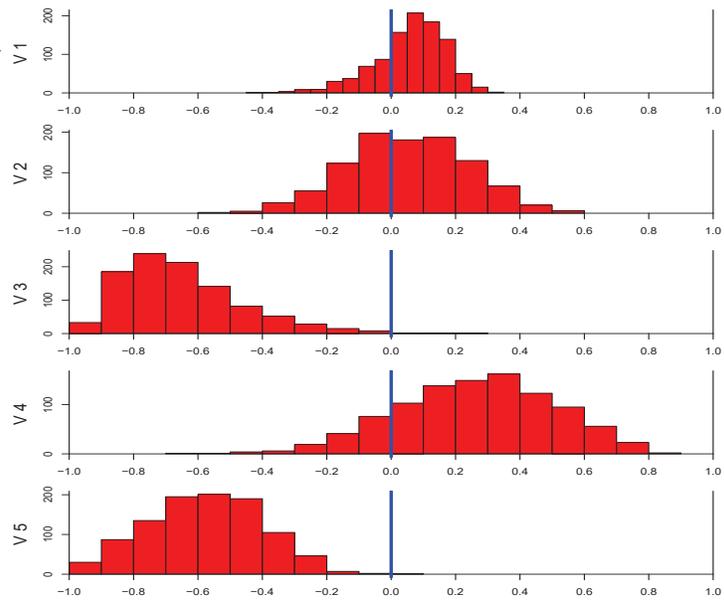
- Two groups of 35 flies (Leptoconops torrens and Leptoconops carteri)
- Measurements of
  - ▶ wing length
  - ▶ wing width
  - ▶ third palp length
  - ▶ third palp width
  - ▶ fourth palp length



## Biting Flies: LDA

- Robust LDA
- Simultaneous two-sample MM-estimates
- FRB inference for the canonical variate
- Variable selection using backward elimination
- Selection criterion: Significance of the discriminant coordinate coefficients

## Biting Flies: FRB



## Biting Flies: Backward elimination

	Variable				
Model	1	2	3	4	5
1	0.490	0.817	0.006	0.296	0.002
2	0.306	-	0.016	0.216	0.000
3	-	-	0.016	0.096	0.000
4	-	-	0.006	-	0.000

## One-way MANOVA model

- Observations  $\mathbf{x}_{ji} \in \mathbb{R}^p$  with  $j = 1, \dots, k; i = 1, \dots, n_j$
- For each group  $j$ :

$$\mathbf{x}_{ji} = \boldsymbol{\mu}_j + \Sigma^{1/2} \boldsymbol{\varepsilon}_{ji} \quad i = 1, \dots, n_j$$

- $E(\boldsymbol{\varepsilon}_{ji}) = 0$  and  $\text{Cov}(\boldsymbol{\varepsilon}_{ji}) = I_p$
- MANOVA test:

$$H_0 : \boldsymbol{\mu}_1 = \dots = \boldsymbol{\mu}_k$$

$$H_a : \boldsymbol{\mu}_r \neq \boldsymbol{\mu}_s \text{ for at least one } r \neq s$$

## Classical test: Wilk's Lambda

$$\Lambda_n = \frac{|\sum_{j=1}^k \sum_{i=1}^{n_j} (\mathbf{x}_{ji} - \bar{\mathbf{x}}_j)(\mathbf{x}_{ji} - \bar{\mathbf{x}}_j)^t|}{|\sum_{j=1}^k \sum_{i=1}^{n_j} (\mathbf{x}_{ji} - \bar{\mathbf{x}})(\mathbf{x}_{ji} - \bar{\mathbf{x}})^t|}$$

- LRT assuming that  $F_j = N(\boldsymbol{\mu}_j, \Sigma)$
- Asymptotic  $\chi_{p(k-1)}^2$  distribution
- Sensitive to outliers

## A robust one-way MANOVA test statistic

Based on the one-sample and  $k$ -sample S-estimates, consider the test statistic

$$\begin{aligned}\Lambda_n &= \frac{|\hat{\Sigma}_S^{(k)}|}{|\hat{\Sigma}_S^{(1)}|} \equiv \frac{\hat{\sigma}_S^{(k)}}{\hat{\sigma}_S^{(1)}} = \frac{\hat{\sigma}(\hat{\boldsymbol{\mu}}_{S,1}, \dots, \hat{\boldsymbol{\mu}}_{S,k}, \hat{\Gamma}_S^{(k)})}{\hat{\sigma}(\hat{\boldsymbol{\mu}}_S, \hat{\Gamma}_S^{(1)})} \\ &= h_n(\hat{\boldsymbol{\mu}}_{S,1}, \dots, \hat{\boldsymbol{\mu}}_{S,k}, \hat{\Gamma}_S^{(k)}, \hat{\boldsymbol{\mu}}_S, \hat{\Gamma}_S^{(1)})\end{aligned}$$

The distribution of

$$\Lambda_{n,FRB}^* = h_n^*(\hat{\boldsymbol{\mu}}_{S,1,FRB}^*, \dots, \hat{\boldsymbol{\mu}}_{S,k,FRB}^*, \hat{\Gamma}_{S,FRB}^{(k)*}, \hat{\boldsymbol{\mu}}_{S,FRB}^*, \hat{\Gamma}_{S,FRB}^{(1)*})$$

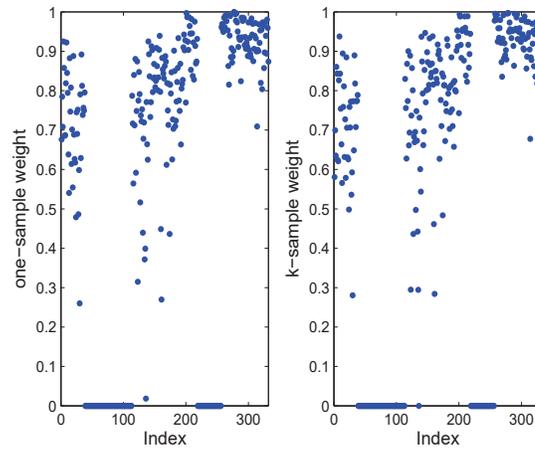
consistently estimates the null distribution of the test statistic  $\Lambda_n$ .

## Example: Oslo transect data

Oslo transect data

- 360 samples of different plant species collected along a transect running through Oslo, Norway.
- Factor lithology which consists of four levels ( $k = 4$ )
- Three elements: P, K and Zn ( $p = 3$ )

## MM-estimator weights (90% efficiency)



## MANOVA results

	Clas	$\Lambda_{n,FRB}$	$S\Lambda_n^{2a}$	$S\Lambda_n^{2b}$	$MMA_n^a$	$MMA_n^b$
$p$	.704	.016	.015	.014	.018	.019

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## Selecting a linear regression model

- Dataset  $\mathcal{Z}_n = \{(y_i, x_{i1}, \dots, x_{ip}) = (y_i, \mathbf{x}_i); i = 1, \dots, n\} \subset \mathbb{R}^{p+1}$
- $X_1, \dots, X_p$  are the candidate regressors
- The full model:  $y_i = \mathbf{x}_i' \boldsymbol{\beta} + \varepsilon_i \quad i = 1, \dots, n$
- An estimate  $\hat{\boldsymbol{\beta}}$  may become unstable if there are
  - ▶ several noise variables among the candidate regressors
  - ▶ highly correlated predictors (multicollinearity)
- Model selection can improve the unstable coefficient estimates
  - ▶ Trade (a little) bias for (a large) variability reduction!
  - ▶ Enhance interpretability: most relevant effects

## Submodels

- Dataset  $\mathcal{Z}_n = \{(y_i, x_{i1}, \dots, x_{ip}); i = 1, \dots, n\} \subset \mathbb{R}^{p+1}$ .
- Let  $\alpha \subset \{1, \dots, p\}$  denote the predictors included in a submodel
- The corresponding submodel is:

$$y_i = \mathbf{x}'_{\alpha i} \boldsymbol{\beta}_\alpha + \varepsilon_{\alpha i} \quad i = 1, \dots, n.$$

A selected model is considered a good model if

- It is parsimonious
  - It fits the data well
  - It yields good predictions for similar data
- Use selection criteria!

## Final prediction error

- Final prediction error  $FPE(\alpha) = \frac{1}{\sigma^2} \sum_{i=1}^n E \left[ (z_i - \mathbf{x}'_{\alpha i} \hat{\boldsymbol{\beta}}_\alpha)^2 \right]$
- Based on LS,  $FPE(\alpha)$  can be estimated by

$$\widehat{FPE}(\alpha) = \frac{RSS(\alpha)}{\hat{\sigma}_{LS}^2} + 2d(\alpha)$$

- $\hat{\sigma}_{LS}$  is the residual scale estimate in the "full" model  $\alpha_f$ .  
Usually,  $\alpha_f = \{1, \dots, p\}$

## Robust FPE

- Final prediction error  $FPE(\alpha) = \frac{1}{\sigma^2} \sum_{i=1}^n E \left[ (z_i - \mathbf{x}'_{\alpha i} \hat{\beta}_\alpha)^2 \right]$
- Robust final prediction error:

$$RFPE(\alpha) = \sum_{i=1}^n E \left[ \rho \left( \frac{z_i - \mathbf{x}'_{\alpha i} \hat{\beta}_\alpha}{\sigma} \right) \right]$$

with  $\rho$  a bounded loss function

- An estimate of  $RFPE(\alpha)$  is given by

$$\widehat{RFPE}(\alpha) = \sum_{i=1}^n \rho(r_i(\hat{\beta}_\alpha)/\hat{\sigma}_n) + p(\alpha) \frac{\sum_{i=1}^n \psi^2(r_i(\hat{\beta}_\alpha)/\hat{\sigma}_n)}{\sum_{i=1}^n \psi'(r_i(\hat{\beta}_\alpha)/\hat{\sigma}_n)}$$

- $\hat{\sigma}_n$  is the robust scale estimate of a 'full' model  $\alpha_f$ .  
Usually,  $\alpha_f = \{1, \dots, p\}$

## Bootstrap based selection criteria

- The (conditional) expected prediction error:

$$PE(\alpha) = E \left[ \frac{1}{n} \sum_{i=1}^n (z_i - \mathbf{x}'_{\alpha i} \hat{\beta}_\alpha)^2 \middle| y, X \right],$$

- Estimates of  $PE(\alpha)$  can be obtained by **bootstrap**
- A more advanced selection criterion takes both goodness-of-fit and PE into account:

$$PPE(\alpha) = \frac{1}{n} \sum_{i=1}^n (y_i - \mathbf{x}'_{\alpha i} \hat{\beta}_\alpha)^2 + f(n) p(\alpha) + E^* \left[ \frac{1}{n} \sum_{i=1}^n (z_i - \mathbf{x}'_{\alpha i} \hat{\beta}_\alpha)^2 \middle| y, X \right]$$

## Robust bootstrap selection criteria

Robust equivalents of the bootstrap based selection criteria:

$$\widehat{RPE}(\alpha) = \frac{\hat{\sigma}_n^2}{n} E^* \left[ \sum_{i=1}^n \rho \left( \frac{z_i - \mathbf{x}'_{\alpha i} \hat{\beta}_\alpha}{\hat{\sigma}_n} \right) \middle| y, X \right]$$

$$\widehat{PRPE}(\alpha) = \frac{\hat{\sigma}_n^2}{n} \left\{ \sum_{i=1}^n \rho \left( \frac{y_i - \mathbf{x}'_{\alpha i} \hat{\beta}_\alpha}{\hat{\sigma}_n} \right) + f(n) p(\alpha) \right\} + \widehat{RPE}(\alpha)$$

- $\rho$  is a bounded loss function
- $f(n)d(\alpha)$  is the penalty term with e.g.  $f(n) = 2 \log n$
- $\hat{\sigma}_n$  is the robust scale estimate of a 'full' model  $\alpha_f$ . Usually,  $\alpha_f = \{1, \dots, p\}$
- $E^*$  is a bootstrap estimate of the expected value

## FRB based selection criteria

$$\widehat{RPE}(\alpha) = \frac{\hat{\sigma}_n^2}{n} E_{FRB}^* \left[ \sum_{i=1}^n \rho \left( \frac{z_i - \mathbf{x}'_{\alpha i} \hat{\beta}_\alpha}{\hat{\sigma}_n} \right) \middle| y, X \right]$$

$$\widehat{PRPE}(\alpha) = \frac{\hat{\sigma}_n^2}{n} \left\{ \sum_{i=1}^n \rho \left( \frac{y_i - \mathbf{x}'_{\alpha i} \hat{\beta}_\alpha}{\hat{\sigma}_n} \right) + f(n) p(\alpha) \right\} + \widehat{RPE}(\alpha)$$

- $\rho$  is the MM loss function and  $\hat{\beta}_\alpha$  is the MM estimate
- $E_{FRB}^*$  is a bootstrap estimate of the expected value using FRB estimates of  $\beta_\alpha$  based on bootstrap samples of size  $m \leq n$

## Consistent model selection

Suppose a true model  $\alpha_0 \subset \{1, \dots, p\}$  exists and is included in the set  $\mathcal{A}$  of models considered.

If we select the model that minimizes  $\widehat{RPE}(\alpha)$  or  $\widehat{PRPE}(\alpha)$ , that is

$$\hat{\alpha}_{m,n} = \operatorname{argmin}_{\alpha \in \mathcal{A}} \widehat{RPE}(\alpha) \text{ and } \tilde{\alpha}_{m,n} = \operatorname{argmin}_{\alpha \in \mathcal{A}} \widehat{PRPE}(\alpha),$$

then, under appropriate regularity conditions, the model selection criteria are consistent in the sense that

$$\lim_{n \rightarrow \infty} P(\hat{\alpha}_{m,n} = \alpha_0) = 1 \text{ and } \lim_{n \rightarrow \infty} P(\tilde{\alpha}_{m,n} = \alpha_0) = 1.$$

Two conditions have practical consequences

- $m = o(n)$  ( $m$  out of  $n$  bootstrap)
- $f(n) = o(n/m)$

## Variable selection strategies

- 1 Choose a selection criterion
- 2 Follow a model selection strategy
  - ▶ All subsets → **too time consuming**
  - ▶ Backward elimination
  - ▶ Forward selection
  - ▶ Stepwise selection
- 3 Select optimal model(s)
- 4 Evaluate their performance

## Examples: backward elimination

- We compare the full model with models selected by backward elimination based on
  - ▶  $\widehat{RFPE}(\alpha)$
  - ▶  $\widehat{RPE}(\alpha)$
  - ▶  $\widehat{PRPE}(\alpha)$  with  $f(n) = \log(n)$
- For each of the models we report an adjusted robust  $R^2$
- To compare predictive power we consider the robust 5-fold CV MSPE (5% trimming)

## Example: Los Angeles Ozone Pollution Data

- 366 observations (different days) on 9 variables
- Response: temperature (degrees F) at El Monte, CA
- Covariates: Measurements of temperature, pressure, humidity, ozone, etc at other places in CA.
- We start from the full quadratic model ( $p = 45$ )

model	$p(\alpha)$	$RR_a^2$	5% Trimmed MSPE
Full	45	0.8660	10.78
RFPE	23	0.8174	10.66
RPE	10	0.7583	11.67
PRPE	7	0.7643	10.45

## Example: Diabetes data

- 442 observations on 16 variables.
- Response: Measure of disease progression after one year
- Covariates: 10 baseline variables (age, sex, BMI, , ...)
- We start from a quadratic model with some interactions ( $p = 65$ )

model	$p(\alpha)$	$RR_a^2$	5% Trimmed MSPE
Full	65	0.7731	4988.1
RFPE	16	0.6045	2231.2
RPE	11	0.5127	2657.2
PRPE	7	0.5302	2497.0

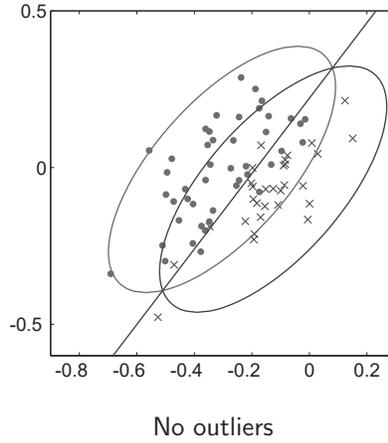
## Example: Linear discriminant analysis

### Hemophilia data

- 2 groups
- $n = 75$  training samples
  - ▶  $n_1 = 30$  controls
  - ▶  $n_2 = 45$  hemophilia A carriers
- 2 variables

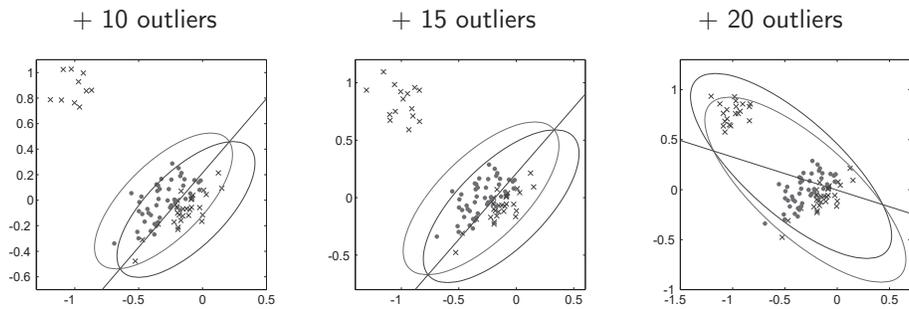
## Robust LDA based on S-estimates

Discriminant line and 97.5% tolerance ellipses



## Robust LDA based on S-estimates

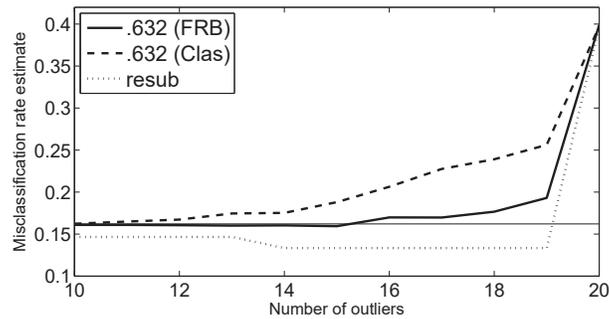
Discriminant line and 97.5% tolerance ellipses



## FRB error rates for LDA based on S-estimates

We use the 0.632 estimator to estimate the error rate:

$$\widehat{\text{err}}_{.632} = .632 \widehat{\text{err}}_{\text{boot}} + .368 \widehat{\text{err}}_{\text{resub}}$$



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## Software

Software for FRB inference: R package *FRB* described in Van Aelst and Willems (2013).

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