Robustness under missing data: a comparison with special attention to inference

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Problem statement

Goal: Evaluate different robust regression methods in inference when missing data are present

Procedure: Simulations

Framework: Let $X \in \mathbb{R}^{n \times p}$ be the design matrix containing n observations and p predictor variables. Let $\beta \in \mathbb{R}^p$ be the vector of regression coefficients.

The dependent variable $y \in \mathbb{R}^n$ is defined according to the linear model as

$$y = X\beta + \varepsilon$$

where ε is a vector from \mathbb{R}^n with entries independent and identically distributed with $\mathbb{E}[\varepsilon] = 0$ and $Var[\varepsilon] = \sigma^2$.



Comparison of robust linear regressions in inference

Comparison criteria:

- Bias of the regression coefficients
- Standard error of the regression coefficients
- Mean Squared Prediction Error

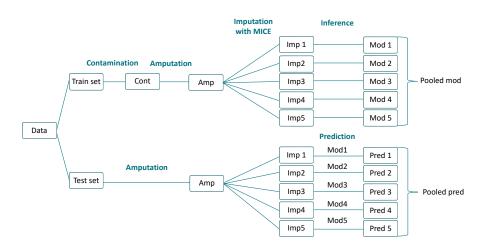


Simulation procedure

- Generate the starting train and test sets
- Contaminate the train set
- Ampute the train set and the test set by deleting a selection of values
- Impute the train set using MICE to obtain 5 complete imputed train sets
- Impute the test set using the same models as created in the previous step to obtain 5 complete imputed test sets
- Fit a linear model on the 5 train sets to get 5 models and pool the results → inference performance
- $oldsymbol{\circ}$ Predict the response variable for the 5 test sets with the 5 fitted models from the previous step and pool the results \to prediction performance



Overview of the simulation procedure





Generation of the train and test sets

The simulation setup follows the one proposed by Öllerer, Alfons and Croux [10]:

- p = 15 variables; n = 300 observations for the train set and n = 100 for the test set
- Regression coefficients: $\beta_j = j/p$ for $j = 1, \dots, p$
- Correlation:
 - Independent case: $\Sigma = I_p$ the covariance matrix, $\sigma^2 = 0.5^2$ the error variance
 - Dependent case: $\Sigma_{ij} = 0.5^{|i-j|}$, $\sigma^2 = 0.81^2$
- Generate X according to $\mathcal{N}_p(0,\Sigma)$
- Generate ε according to $\mathcal{N}(0,\sigma^2)$
- Define $y_i = x_i'\beta + \varepsilon_i$ for i = 1, ..., n



Contamination of the train set

Cellwise contamination

- Dense cluster: $x_{ij}^{cont} \sim \mathcal{N}(50,1)$
- Dispersed outliers: $x_{ii}^{cont} \sim \mathcal{N}(0, 100^2)$
- Wide cluster: $x_{ii}^{cont} \sim \mathcal{N}(50, 10^2)$

Rowwise contamination

- Dense cluster: $x_i^{cont} \sim \mathcal{N}_p(50, \Sigma)$
- Dispersed outliers: $x_i^{cont} \sim \mathcal{N}_p(0, 100^2 \Sigma)$
- Wide cluster: $x_i^{cont} \sim \mathcal{N}_p(50, 10^2 \Sigma)$

• Response contamination

- Vertical outliers: $\varepsilon_i^{cont} \sim \mathcal{N}(50, \sigma^2)$
- \rightarrow Percentage of contamination : 0%, 5% or 10%.

Dense cluster



Dispersed outliers

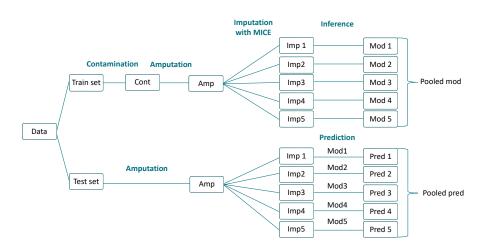


Wide cluster





Overview of the simulation procedure





Imputation methods – Robust against rowwise outliers

• S-estimators [6]

$$\hat{eta}_{\mathcal{S}} = \arg \min_{eta \in \mathbb{R}^p} s(r_1(eta), \dots, r_n(eta))$$

where $s(r_1, \ldots, r_n)$ is a solution of $\frac{1}{n} \sum_{i=1}^n \rho(r_i/s) = \delta$, $\delta = \mathbb{E}_{\phi}[\rho]$ and (r_1, \ldots, r_n) are the residuals.

• MM-estimators [9]

 $\hat{\beta}_{MM}$ is any solution of

$$\sum_{i=1}^{n} \rho' \left(\frac{r_i(\beta)}{s(r_1(\beta_S), \ldots, r_n(\beta_S))} \right) x_i = 0$$

which verifies $S(\beta_{MM}) \leq S(\beta_S)$ where $S(\beta) = \sum_{i=1}^n \rho\left(\frac{r_i(\beta)}{s(r_1(\beta_S), \dots, r_n(\beta_S))}\right)$

• Least trimmed squares [4, 5]

For a fixed h with $\left[\frac{n+p+2}{2}\right] \le h \le n$,

$$\hat{\beta}_{LTS} = \underset{\hat{\beta}}{\operatorname{argmin}} \sum_{i=1}^{h} (r^2)_{i:n}$$

where $(r^2)_{1:n} \leq \ldots \leq (r^2)_{n:n}$ are the ordered squared residuals



Imputation methods - Robust against cellwise outliers

• Shooting-S [10]

Combine the coordinate descent algorithm with regression S-estimation to obtain the following objective function, $\forall j \in \{1, \dots, p\}$:

$$\begin{split} \hat{\beta}_j &= \underset{\beta \in \mathbb{R}}{\text{arg min }} \hat{\sigma}_j(\beta) \\ \text{with } \frac{1}{n} \sum_{i=1}^n \rho \left(\frac{\tilde{y}_i^{(j)} - x_{ij}\beta}{\hat{\sigma}_j(\beta)} \right) = \delta \\ \text{and } w_{ik} &= w \left(\frac{|\tilde{y}_i^{(j)} - x_{ik}\hat{\beta}_k|}{\hat{\sigma}_k(\hat{\beta}_k)} \right) \end{split} \quad \text{and } \hat{x}_{ik} = \frac{\tilde{y}_i^{(k)}}{\hat{\beta}_k} \end{split}$$

- Cellwise robust M regression (CRM) [2]
 - Center and scale the data
 - ② Use a starting robust regression estimator (MM) to flag observations as casewise outliers if their absolute standard residuals exceed z_{0.95}. Apply SPADIMO to separate cellwise and casewise outliers. Cellwise outliers are deleted and then imputed
 - 3 Apply an IRLS procedure to improve efficiency of the estimates



Inference methods

- S-estimators
- MM-estimators
- Least trimmed squares

- Shooting-S estimator
- Cellwise robust M regression
- Linear regression (classical)

But How to compute the standard deviation of the regression parameters ?

- ightarrow For LTS and the classical regression : given in the output
- \rightarrow Other methods: use bootstrap samples \Rightarrow Fast and robust bootstrap [7]
 - Already computed and implented in R for S and MM-estimators
 - Need to be adapted for CRM and Shooting-S



Fast and robust bootstrap (FRB) [7]

Let $\hat{\theta}_n \in \mathbb{R}^p$ be the robust parameter estimates of interest and Z_n be a sample. FRB can be used if $\hat{\theta}_n$ can be represented as a solution of fixed-point equations :

$$\hat{\theta}_n = g_n(\hat{\theta}_n)$$

where g_n generally depends on the sample Z_n . Given a boostrap sample Z_n^* , the recalculated estimates $\hat{\theta}_n^*$ then solves

$$\hat{\theta}_n^* = g_n^*(\hat{\theta}_n^*).$$

Instead of computing $\hat{\theta}_n^*$, we can compute the approximation

$$\hat{\theta}_n^{1*} := g_n^*(\hat{\theta}_n).$$

But $\hat{\theta}_n^{1*}$ underestimate the variability of $\hat{\theta}_n$. To remedy this, they define a linearly corrected version of $\hat{\theta}_n^{1*}$:

$$\hat{\theta}_n^{R*} := \hat{\theta}_n + [I + \nabla g_n(\hat{\theta}_n)]^{-1} (\hat{\theta}_n^{1*} - \hat{\theta}_n)$$



FRB applied to shooting-S

Note $\tilde{y}_i^{(j)} = y_i - \sum_{k \neq j} (w_{ik} x_{ik} + (1 - w_{ik}) \hat{x}_{ik}) \hat{\beta}_k$, the objective function of shooting-S, $\forall j \in \{1, \dots, p\}$, can be written as

$$\frac{1}{n} \sum_{i=1}^{n} \rho \left(\frac{\tilde{y}_{i}^{(j)} - x_{ij} \hat{\beta}_{j}}{\hat{\sigma}_{i}(\hat{\beta}_{i})} \right) = \delta \tag{1}$$

$$\frac{1}{n}\sum_{i=1}^{n}\rho'\left(\frac{\tilde{y}_{i}^{(j)}-x_{ij}\hat{\beta}_{j}}{\hat{\sigma}_{j}(\hat{\beta}_{j})}\right)x_{ij}=0$$
(2)

Equations (1) and (2) can be rewritten as

$$\hat{\beta}_{j} = \left(\sum_{i=1}^{n} z_{ij} x_{ij}^{2}\right)^{-1} \sum_{i=1}^{n} z_{ij} x_{ij} \tilde{y}_{i}^{(j)}$$
(3)

$$\hat{\sigma}_j = \sum_{i=1}^n v_{ij} (\tilde{y}_i^{(j)} - x_{ij} \hat{\beta}_j) \tag{4}$$

where
$$z_{ik} = \frac{\rho'(r_{ik}/\hat{\sigma}_k)}{r_{ik}}$$
, $v_{ik} = \frac{\hat{\sigma}_k}{n\delta} \frac{\rho(r_{ik}/\hat{\sigma}_k)}{r_{ik}}$ and $r_{ik} = \tilde{y}_i^{(j)} - x_{ij}\hat{\beta}_j$.



FRB applied to cellwise robust M regression

Cellwise robust M regression:

- Center and scale the data
- ② Use a starting robust regression estimator (MM) to flag observations as casewise outliers if their absolute standard residuals exceed $z_{0.95}$.
 - Apply SPADIMO to separate cellwise and casewise outliers. Cellwise outliers are deleted and then imputed
- Apply an IRLS procedure to improve efficiency of the estimates

Output of the method:

- $\hat{\beta}$: The regression coefficients
 - ullet $ilde{X}$: The imputed design matrix
 - ullet Ω : A diagonal matrix containing the weights on the diagonal

Bootstrap procedure:

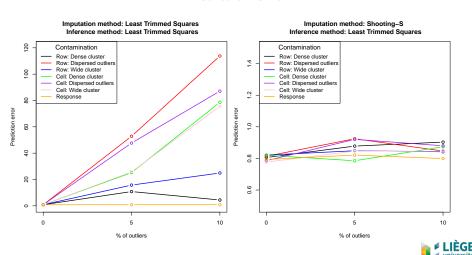
- ① Compute the clean and weighted sample : $y_{\omega}=\Omega y$ and $X_{\omega}=\Omega \tilde{X}$
- 2 Draw bootstrap samples $(X_{\omega}^*, y_{\omega}^*)$ from (X_{ω}, y_{ω})
- Sootstrap regression estimates are obtained by fitting a linear regression on that clean bootstrap sample:

$$y_{\omega}^* = X_{\omega}^* \hat{\beta}^*$$



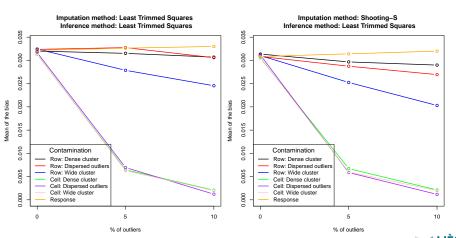
Preliminary results

Prediction error



Preliminary results

Bias



References

- [1] Michiel Debruyne, Sebastiaan Höppner, Sven Serneels, and Tim Verdonck. Outlyingness: Which variables contribute most? *Statistics and Computing*, 29(4):707–723, 2019.
- [2] Peter Filzmoser, Sebastiaan Höppner, Irene Ortner, Sven Serneels, and Tim Verdonck. Cellwise robust M regression. *Computational Statistics & Data Analysis*, 147:106944, 2020.
- [3] Roderick J. A. Little and Donald B. Rubin. *Statistical analysis with missing data*. Wiley series in probability and statistics. John Wiley, New York, NY, 2nd edition edition, 2002.
- [4] Peter Rousseeuw. Least Median of Squares Regression. *Journal of the American Statistical Association*, 79(388):871–880, 1984.
- [5] Peter Rousseeuw and Annick Leroy. Robust Regression and Outlier Detection. Wiley Series in Probability and Statistics. Wiley, 1987.

- [6] Peter Rousseeuw and Victor Yohai. Robust Regression by Means of S-Estimators. In Jürgen Franke, Wolfgang Härdle, and Douglas Martin, editors, Robust and Nonlinear Time Series Analysis, pages 256–272, New York, NY, 1984. Springer US.
- [7] Matías Salibián-Barrera, Stefan Van Aelst, and Gert Willems. Fast and robust bootstrap. *Statistical Methods and Applications*, 17:41–71, 2008.
- [8] Rianne Margaretha Schouten, Peter Lugtig, and Gerko Vink. Generating missing values for simulation purposes: a multivariate amputation procedure. *Journal of Statistical Computation and Simulation*, 88(15):2909–2930, 2018.
- [9] Victor Yohai. High Breakdown-Point and High Efficiency Robust Estimates for Regression. The Annals of statistics, 15(2):642–656, 1987.
- [10] Viktoria Öllerer, Aneas Alfons, and Christophe Croux. The shooting S-estimator for robust regression. *Computational statistics*, 31(3):829–844, 2016.