A New Robust Partial Least Squares Regression Method

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Introduction
  Motivation
  Robust PLS Methods

PLSKurSD
  PLS Algorithm
  Computing Robust Variance Covariance Matrix

Experimental Results
  Monte Carlo Simulation
  A Service Quality Application

Conclusions and Future work
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  Future work
Why robust methods?

"... just which robust methods you use is not important, what is important is that you use some." J. W. Tukey (1979)

Fundamental Continuity Concept

- Small changes in the data result in only small changes in estimate.
Outliers are atypical observations that are “well” separated from the bulk of the data. Covariance matrix and means vector are very sensitive to outliers in data.

- 1-D (relatively easy to detect).
- 2-D (*harder* to detect).
- Higher-D (*very hard* to detect).
Literature review

- **Wakeling and Macfie (1992)**. First PLSR robustification. Algorithm with weighted regressions for PLS1 and PLS2.
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- **Hubert and Vandem Brandem (2003)**. PLS Robustification based on the SIMPLS algorithm.
Data and General Considerations

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- Optimal number of PLS component through *leave-one-out cross* validation.
We analyze the case $q=1$.

Population loading vector computed as in Helland (1988).

Optimal number of PLS component through *leave-one-out* cross validation.

One-step robustification comes from using the robust covariance matrix.
PLS Algorithm

The population loading vectors given by Helland (1988):

1. $w_1 \propto \delta_{y,x}$
2. $w_{a+1} \propto \delta_{y,x} - \sum_x W_a(W_a^T \sum_x W_a)^{-1}W_a^T \delta_{y,x}$

Where $W_a$, $1 < a \leq A$ are the loading vectors $W_i$ and $A$ the selected numbers of PLS components.

$W_a = [w_1, w_2, ..., w_a]$
Then the population regression vector (non robust) is given by:

\[
\beta_a = W_a (W_a^T \sum_x W_a)^{-1} W_a^T \delta_{y,x}
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The proposed global Robust algorithm come from using the covariance matrix $\tilde{S}_{[y,x]}$ obtained from the original data being in this case $w_1$ a normalization of $\tilde{\delta}_{y,x}$ and:

$$w_{a+1} \propto \tilde{\delta}_{y,x} - \tilde{S}_x W_a( W_a^T \tilde{S}_x W_a )^{-1} W_a^T \tilde{\delta}_{y,x}$$
Outliers detection and computation of $\tilde{S}$

The algorithm Peña and Prieto(2005) works in three steps after data are scaled and centered:

$$\tilde{x}_i = S^{-1/2}(x_i - \bar{x}), \quad i = 1, \ldots, n.$$  

STEP 1: finding directions maximizing and minimizing the kurtosis, projecting the data and identifying outliers.
Outliers detection and computation of $\tilde{S}$

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- **STEP 1**: finding directions maximizing and minimizing the kurtosis, projecting the data and identifying outliers.
- **STEP 2**: generating random directions and stratifying the sample and identifying outliers again.
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- **STEP 1**: finding directions maximizing and minimizing the kurtosis, projecting the data and identifying outliers.
- **STEP 2**: generating random directions and stratifying the sample and identifying outliers again.
- **STEP 3**: check the suspicious observations by using the Mahalanobis distance and repit until no more outliers are found.
Step I: Searching kurtosis directions

The direction that maximizes (minimizes) the coefficient of kurtosis is obtained as the solution of the optimization problem:

\[ d_j = \arg \max_{d} \left( \min_{d} \right) \frac{1}{n} \sum_{i=1}^{n} \left( d' \tilde{x}_i^{(j)} \right)^4 \]

\[ \text{s.t.} \quad d' d = 1. \]

The sample points are projected onto a lower dimension subspace, orthogonal to the directions \( d_j \).
Step 1: Searching kurtosis directions

Why kurtosis directions?

Because it is possible to study the presence of outliers on the kurtosis values and to use this moment coefficient to identify them.

- Symmetric and and a small proportion of outliers generated with asymmetric contamination increase the coefficient on the observed data.
Step I: Searching kurtosis directions

Why kurtosis directions?

Because it is possible to study the presence of outliers on the kurtosis values and to use this moment coefficient to identify them.

- Symmetric and a small proportion of outliers generated with asymmetric contamination increase the coefficient on the observed data.
- A large proportion of outliers generated by asymmetric contamination can make the kurtosis coefficient very small.
Step II: Searching random directions

- Chosen two observations \textit{randomly} from the sample and compute the direction $\hat{d}_i$ defined by these two observations.
Step II: Searching random directions

- Chosen two observations randomly from the sample and compute the direction $\hat{d}_l$ defined by these two observations.
- The observations are then projected onto this direction, to obtain the values $\hat{z}_i = \hat{d}_l^T \hat{x}_i$
Step II: Searching random directions

- Chosen two observations *randomly* from the sample and compute the direction $\hat{d}_l$ defined by these two observations.
- The observations are then projected onto this direction, to obtain the values $\hat{z}_i^l = \hat{d}_l^T \hat{x}_i$
- Then the sample is partitioned into $K$ groups of size $n/K$, where $K$ is a prespecified number, based on the ordered values of the projections $\hat{z}_i^l$, so that group $k, 1 \leq k \leq K$, contains those observations $i$ satisfying:

$$\hat{z}_i^l(\lfloor (k-1)n/K \rfloor + 1) \leq \hat{z}_i^l \leq \hat{z}_i^l(\lfloor kn/K \rfloor)$$
Step II: Searching random directions

- From each group $k$, $1 \leq k \leq K$, a subsample of $p$ observations is chosen without replacement, the orthogonal direction is computed and the corresponding projections.

Why random directions?

- Because it is necessary a procedure that detect outliers when the proportion of contamination is between .2 and .3 and the contamination distribution has the same variance as the original distribution. (case when kurtosis fails)
Step III: Deleting outliers and computing $\tilde{S}$

A *Mahalanobis* distance is computed for all observations labeled as outliers in the preceding steps. Being $U$ the set of all observations not labeled as outliers:

$$\tilde{m} = \frac{1}{|U|} \sum_{i \in U} x_i$$

$$\tilde{S} = \frac{1}{|U| - 1} \sum_{i \in U} (x_i - \tilde{m})(x_i - \tilde{m})'$$

$$v_i = (x_i - \tilde{m})^T \tilde{S}^{-1} (x_i - \tilde{m})$$

Those observations $i \in U$ such that $v_i < \xi^2_{p-1,0.99}$ are considered not to be outliers and are included in $U$. 
Simulation Study

- Comparative of methods $PLS$ (Helland, 1988), $PLS-SD$ (Gil and Romera, 1998), $RSIMPLS$ (Hubert and Branden 2003) and $PLSKurSD$ (González, Peña and Romera).
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- Four types of outliers were generated: bad leverage points, vertical outliers, orthogonal outliers and very concentrated outliers.
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- Three measures for comparing the methods.
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- Four types of outliers were generated: bad leverage points, vertical outliers, orthogonal outliers and very concentrated outliers.
- Three measures for comparing the methods.
- Simulations have been done in a personal computer Pentium III 650 MH with 128 Mb of internal memory. Code implemented in Matlab.
Simulation Study. Bilinear model

\[ T \sim N_A(0_A, \Sigma_t) \text{ with } A < p \]
\[ X = TI_{A,p} + N_p(0_p, 0.1I_p) \]
\[ Y = TQ + N_q(0_q, I_q) \]

\((I_{A,p})_{i,j} = 1 \text{ for } i = j \text{ and } (I_{A,p})_{i,j} \neq 1.\) Q is a matrix of dimensions \(A \times p\) with \((A_{i,j}) = 1 \forall i,j\) The simulation is done with a known values of \(A = A_{opt}\) and generating randomly a number \(n_e\) of outliers.

<table>
<thead>
<tr>
<th>q</th>
<th>n</th>
<th>p</th>
<th>A</th>
<th>(\sigma_t)</th>
<th>(\sigma_t)</th>
<th>Contamination</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>100</td>
<td>5</td>
<td>2</td>
<td>diag(4,2)</td>
<td>1</td>
<td>10% and 30% Out.</td>
</tr>
</tbody>
</table>

Table: Simulation study
Simulation Study. Outliers

- **Bad leverage regression points:**
  \[ T_\varepsilon \sim N_A(10_A, \sigma_t) \]
  \[ X_\varepsilon = T_\varepsilon I_{A,p} + N_p(0_p, 0.1I_p) \]
Simulation Study. Outliers

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- **Vertical outliers:**
  \[ Y_\epsilon = TQ_A,q + N_q(10_q, 0.1l_q) \]
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- **Orthogonal outliers:**
  \[ X_\epsilon = T_\epsilon I_{A,p} + N_p((0_A, 10p-A), 0.1l_p) \]
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- **Very concentrated outliers:**
  \[ X_\varepsilon = T_\varepsilon I_{A,p} + N_p(10_p, 0.001I_p) \]
MC Simulation Study. Measures

- The experimental *slope* of each method $\beta^{(l)}$
  
  $\text{ang} \beta_1, A = \text{ang}(\beta, \hat{\beta}_{[y^c, X^c], A})$
MC Simulation Study. Measures

- The experimental slope of each method $\beta^{(l)}$

$$\text{ang} \beta_{1,A} = \text{ang}(\beta, \hat{\beta}_{[y^c,X^c],A})$$

- The mean squared error of the norms.

$$MSE_A(\hat{\beta}) = \frac{1}{m} \sum_{i=1}^{m} \| \hat{\beta}^{(l)}_A - \beta \|$$
MC Simulation Study. Measures

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- The mean squared error of the norms.
  
  $$\text{MSE}_A(\hat{\beta}) = \frac{1}{m} \sum_{i=1}^{m} \| \hat{\beta}^{(l)}_A - \beta \|$$

- A test set of $n_t$ observations with the original model and we compute:
  
  $$\text{RMSE}_A = \sqrt{\frac{1}{n_t} \sum_{i=1}^{n_t} (y_i - \hat{y}_{i,A})^2}$$

  Being $\hat{y}_{i,k}$ the predicted value of $y$ in the observation $i$. 

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MC Simulation Study. 10% contamination

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<thead>
<tr>
<th>Algorithm</th>
<th>No Contamination</th>
<th>10% Bad leverage points</th>
<th>10% Vertical outliers</th>
<th>10% Orthogonal outliers</th>
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</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean(Angle)</td>
<td>Norm(β)</td>
<td>MSE(σe)</td>
<td>Mean(Angle)</td>
<td>Norm(β)</td>
</tr>
<tr>
<td>PLS</td>
<td>0.06 (0.03)</td>
<td>0.01 (0.01)</td>
<td>0.16 (0.08)</td>
<td>1.13 (0.22)</td>
<td>1.23 (0.15)</td>
</tr>
<tr>
<td>PLS-SD</td>
<td>0.07 (0.03)</td>
<td>0.01 (0.01)</td>
<td>0.17 (0.09)</td>
<td>0.11 (0.06)</td>
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</tr>
<tr>
<td>PLS-KurSD</td>
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<td>0.01 (0.01)</td>
</tr>
<tr>
<td>RSIMPLS</td>
<td>0.08 (0.03)</td>
<td>0.01 (0.01)</td>
<td>0.17 (0.09)</td>
<td>0.08 (0.03)</td>
<td>0.02 (0.01)</td>
</tr>
</tbody>
</table>
### MC Simulation Study. 30% contamination

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<td>Norm((\beta))</td>
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<td>MSE((\sigma_e))</td>
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<td><strong>30% Bad leverage points</strong></td>
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</tr>
<tr>
<td>Mean(Angle)</td>
<td>1.36 (0.18)</td>
<td>0.61 (0.21)</td>
<td>0.10 (0.10)</td>
<td>1.29 (0.26)</td>
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<td>Norm((\beta))</td>
<td>1.39 (0.13)</td>
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<td>MSE((\sigma_e))</td>
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<td>0.24 (0.22)</td>
<td>2.19 (0.25)</td>
</tr>
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RENFE Data

- 17 independent variables that present some measures of the RENFE (Public Railroad system in Spain) service.
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  - Train cleanliness
  - Noise level...
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One dependent variable that corresponds with a measure of the global satisfaction of the customers with the service quality.
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- One dependent variable that corresponds with a measure of the global satisfaction of the customers with the service quality.

- All variables were requested to evaluate on a 0-9 scale.
The sample include 1499 questionnaires and are available in 
http://halweb.uc3m.es".

### Computational times

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The first principal component explains the 93.4% of the variability.

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Conclusions

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- PLSKurSD is resistant to outliers even with a big percent of contamination.

- PLSKurSD is very fast and is useful in large data sets.
Future work

- Extend the work to the case of several dependent variables.
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- To develop a Robust PLS with $p \gg n$. 
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- To develop a Robust PLS with $p \gg n$.
- To analyze in which cases a robustification of the regression is necessary.