PCA by Projection Pursuit
The Package \textit{pcaPP}

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Joint work with . . .

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Agenda

• Principal components
• Robust approaches
• The implementation
• Supporting methods
• Covariance estimation by PCAs

Principal Component Analysis (PCA)
Principal Component Analysis (PCA)

Outliers
### Outliers

![Outliers diagram](image)

### The Classical Approach

- **PCA by decomposition of the covariance matrix**
  
  \[ \hat{\Sigma} = \Gamma \Lambda \Gamma^t \]
  
  \[ Y = (X - 1\bar{x}^t) \Gamma \]

- Robustness due to robust covariance estimates.
  
  - package *rrcov*: covMCD, covMest
  
  - package *robustbase*: covGK, covOGK

### PCA by Projection Pursuit

- No covariance estimation necessary

- Especially for high dimensional data

- Procedure
  
  - Define a data center (mean, median, l1median, …)
  
  - Search for promising directions by maximizing a spread estimation (sd, mad, qn) of the data projected onto these directions
  
  - Reduce the amount of candidate directions

### Defining the Data Center

![Defining the Data Center diagram](image)
Maximizing Spread

$s = 0.64$

$MAD = 0.26$

$s = 0.65$

$MAD = 0.25$

$s = 0.66$

$MAD = 0.35$
Maximizing Spread

\[ s = 0.66, \quad \text{MAD} = 0.43 \]

Maximizing Spread

\[ s = 0.67, \quad \text{MAD} = 0.52 \]

Maximizing Spread

\[ s = 0.67, \quad \text{MAD} = 0.63 \]
Maximizing Spread

\[ s = 0.66 \]
\[ \text{MAD} = 0.7 \]

Maximizing Spread

\[ s = 0.65 \]
\[ \text{MAD} = 0.69 \]

Maximizing Spread

\[ s = 0.65 \]
\[ \text{MAD} = 0.67 \]

Maximizing Spread

\[ s = 0.64 \]
\[ \text{MAD} = 0.61 \]
Maximizing Spread

\[ s = 0.63 \]

\[ \text{MAD} = 0.64 \]

\[ s = 0.62 \]

\[ \text{MAD} = 0.66 \]

\[ s = 0.62 \]

\[ \text{MAD} = 0.59 \]
Maximizing Spread

\[ s = 0.62 \]
\[ \text{MAD} = 0.54 \]

PCAproj

PCAproj

PCAproj

PCAproj
**Candidate Directions:**
- each data point
- additionally random directions through center
- additional directions by linear combinations of data points
- update algorithm (based on eigenvalues)

**Grid Algorithm:**
Optimization is done on a regular grid in the plane.
- select two variables
- optimization on the grid
- select other variables
- ...

**Implementation**
- Implementation in C
- Wrapping functions
  - `PCAproj(x, k = 2, method = c("sd", "mad", "qn"), CalcMethod = c("eachobs", "lincomb", "sphere"), nmax = 1000, update = TRUE, scores = TRUE, maxit = 5, maxhalf = 5, control, ...)
  - `PCAgrid(x, k = 2, method = c("sd", "mad", "qn"), maxiter = 10, splitcircle = 10, scores = TRUE, anglehalving = TRUE, fact2dim = 10, control, ...)`
Common Parameters

- \( x \): Data matrix (data frame)
- \( k \): Number of principal components
- \( \text{method} \): Spread estimator for projection pursuit
- \( \text{scores} \): Return scores-matrix?
- \( \text{control} \): Control-structure
- ... Passed to ScaleAdv

PCAproj - Individual Parameters

- \( \text{CalcMethod} \): "eachobs","lincomb" or "sphere"
- \( \text{nmax} \): Max directions to search in each step (for "lincomb" or "sphere")
- \( \text{update} \): Perform update steps?
  - \( \text{maxhalf} \): Maximum number of steps for angle halving
  - \( \text{maxit} \): Maximum number of iterations

PCAgrid - Individual Parameters

- \( \text{splitcircle} \): Number of directions
- \( \text{anglehalving} \): Perform anglehalving
- \( \text{fact2dim} \): Behavior in 2 dimensional case.
- \( \text{maxiter} \): Maximum number of iterations.

Return Structure

- (S3) class \text{pcaPP} derived from \text{princomp}:
  - \( \text{sdev} \): Spread of principal components
  - \( \text{loadings} \): Matrix containing the loadings
  - \( \text{center} \): Center applied to the data matrix
  - \( \text{scale} \): Scale applied to the data matrix
  - \( \text{n.obs} \): Number of observations
  - \( \text{scores} \): Matrix containing the scores
  - \( \text{call} \): Function call
Additional Functions

- \texttt{l1median(X, MaxStep = 200, ItTol = 10^{-8})}
  Robust center estimator

- \texttt{qn(x)}
  Robust scale estimator

- \texttt{ScaleAdv(x, center = mean, scale = sd)}
  Advanced scaling method (takes functions or vectors as input values)

Robust Covariance Estimation

- Robust covariance estimation based on PCs
  \[ \hat{\Sigma} = \hat{\Gamma} \hat{\Lambda} \hat{\Gamma}^t \]

- \texttt{covPCAproj(x, control)}

- \texttt{covPCAGrid(x, control)}

- \texttt{covPC(x, k, method)} (under construction ...)

Example

```r
> library(pcaPP)
> data(swiss)
> result = PCAproj(swiss, k = 6, method = "mad")
> summary(result)
```

Importance of components:

<table>
<thead>
<tr>
<th>Comp. 1</th>
<th>Comp. 2</th>
<th>Comp. 3</th>
<th>Comp. 4</th>
<th>Comp. 5</th>
<th>Comp. 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard deviation</td>
<td>44.1005199</td>
<td>41.0302723</td>
<td>17.0911415</td>
<td>6.92022550</td>
<td>4.619893062</td>
</tr>
<tr>
<td>Proportion of Variance</td>
<td>0.4859749</td>
<td>0.4206639</td>
<td>0.07299087</td>
<td>0.01196649</td>
<td>0.005333229</td>
</tr>
<tr>
<td>Cumulative Proportion</td>
<td>0.4859749</td>
<td>0.9066387</td>
<td>0.97962962</td>
<td>0.99159611</td>
<td>0.996929342</td>
</tr>
</tbody>
</table>

```

Example

```r
screeplot(result)
```

Scree-plot
Example

```r
biplot(result)
```

Covariance Estimation

```r
> library (covrob)
> covswiss.mad <- covrob (swiss, method="covPCAproj", control = list
(k=6,method="mad"))
> covswiss.sd <- covrob (swiss, method="covPCAproj", control = list
(k=6,method="sd"))
> plot (covswiss.mad, covswiss.sd)
```