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An introduction to SIR: A statistical method for dimension reduction in multivariate regression

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1 Sliced Inverse Regression (SIR)

1.1 Multivariate regression

Let $Y \in \mathbb{R}$ and $X \in \mathbb{R}^p$. The goal is to estimate $G: \mathbb{R}^p \to \mathbb{R}$ such that

$$Y = G(X) + \xi \text{ where } \xi \text{ is independent of } X.$$

• Unrealistic when $p$ is large (*curse of dimensionality*).

• **Dimension reduction**: Replace $X$ by its projection on a subspace of lower dimension without loss of information on the distribution of $Y$ given $X$.

• **Central subspace**: smallest subspace $S$ such that, conditionally on the projection of $X$ on $S$, $Y$ and $X$ are independent.

1.2 Dimension reduction

• Assume (for the sake of simplicity) that $\dim(S) = 1$ *i.e.* $S = \text{span}(b)$, with $b \in \mathbb{R}^p \implies \textbf{Single index model}:

$$Y = g(b'X) + \xi$$

where $\xi$ is independent of $X$.

• The estimation of the $p$-variate function $G$ is replaced by the estimation of the univariate function $g$ and of the direction $b$.

• **Goal of SIR** [Li, 1991]: Estimate a basis of the central subspace. (*i.e. $b$ in this particular case.*)
1.3 Reminder

Let $X_1, \ldots, X_n$ be $n$ points in $\mathbb{R}^p$ divided into $h$ classes $C_j$, $j = 1, \ldots, h$.

- **Empirical covariance matrix**

\[ \hat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})(X_i - \bar{X})^t, \text{ where } \bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i. \]

- **Within-class covariance matrix** “mean of covariances”

\[ \hat{W} = \sum_{j=1}^{h} \frac{n_j}{n} \hat{\Sigma}_j, \]

where $\hat{\Sigma}_j$ is the empirical covariance matrix of class $j$ and $n_j = \text{card}(C_j)$.

- **Between-class covariance matrix** “covariance of means”

\[ \hat{B} = \sum_{i=1}^{n} \frac{n_j}{n} (\bar{X}_j - \bar{X})(\bar{X}_j - \bar{X})^t, \text{ where } \bar{X}_j = \frac{1}{n_j} \sum_{X_i \in C_j} X_i. \]

\[ \hat{\Sigma} = \hat{B} + \hat{W} \]

- Let $b'X$ the projection of the random vector on the axis $b$. Then, $\text{var}(b'X) = b'\text{cov}(X)b$.

1.4 SIR

**Idea:**

- Find the direction $b$ such that $b'X$ best explains $Y$.
- Conversely, when $Y$ is fixed, $b'X$ should not vary.
- Find the direction $b$ minimizing the variations of $b'X$ given $Y$.

**In practice:**

- The support of $Y$ is divided into $h$ slices $S_j$.
- **Minimization of the within-slice variance of $b'X$** under the constraint $\text{var}(b'X) = 1$.
- Equivalent to maximizing the between-slice variance under the same constraint.
1.5 Illustration

![Image of scatter plot with slices and within variance indicated]

1.6 Estimation procedure

Given a sample \( \{(X_1, Y_1), \ldots, (X_n, Y_n)\} \), the direction \( b \) is estimated by

\[
\hat{b} = \arg\max_b b'\hat{\Gamma}b \text{ such that } b'\hat{\Sigma}b = 1.
\]  

(1)

where \( \hat{\Sigma} \) is the empirical covariance matrix and \( \hat{\Gamma} \) is the between-slice covariance matrix defined by

\[
\hat{\Gamma} = \sum_{j=1}^{h} \frac{n_j}{n}(\bar{X}_j - \bar{X})(\bar{X}_j - \bar{X})', \quad \bar{X}_j = \frac{1}{n_j} \sum_{Y_i \in S_j} X_i,
\]

where \( n_j \) is the number of observations in the slice \( S_j \).

The optimization problem (1) has a closed-form solution: \( \hat{b} \) is the eigenvector of \( \hat{\Sigma}^{-1}\hat{\Gamma} \) associated to the largest eigenvalue.

1.7 Illustration

Simulated data.

- Sample \( \{(X_1, Y_1), \ldots, (X_n, Y_n)\} \) of size \( n = 100 \) with \( X_i \in \mathbb{R}^p \) and \( Y_i \in \mathbb{R}, \)
  \( i = 1, \ldots, n. \)
- \( X_i \sim \mathcal{N}_p(0, \Sigma) \) where \( \Sigma = Q\Delta Q' \) with
  - \( \Delta = \text{diag}(p^\theta, \ldots, 2^\theta, 1^\theta), \)
  - \( \theta \) controls the decreasing rate of the eigenvalue screeplot,
- $Q$ is an orientation matrix drawn from the uniform distribution on the set of orthogonal matrices.

• $Y_i = g(b^t X_i) + \xi$ where
  - $g$ is the link function $g(t) = \sin(\pi t/2)$,
  - $b$ is the true direction $b = 5^{-1/2}Q(1, 1, 1, 1, 0, \ldots, 0)^t$,
  - $\xi \sim \mathcal{N}_i(0, 9.10^{-4})$

1.8 Results with $\theta = 2$, dimension $p = 10$

1.9 Results with $\theta = 2$, dimension $p = 50$

1.10 Explanation
Problem : $\hat{\Sigma}$ may be singular or at least ill-conditioned in several situations.

• Since $\text{rank}(\hat{\Sigma}) \leq \min(n - 1, p)$, if $n \leq p$ then $\hat{\Sigma}$ is singular.
• Even if \( n \) and \( p \) are of the same order, \( \hat{\Sigma} \) is ill-conditioned, and its inversion yields numerical problems in the estimation of the central subspace.

• The same phenomenon occurs if the coordinates of \( X \) are strongly correlated.

In the previous example, the condition number of \( \Sigma \) was \( p^0 \).

2 Regularization of SIR

2.1 Regularized SIR

• We propose to compute \( \hat{b} \) as the eigenvector associated to the largest eigenvalue of \((\Omega \hat{\Sigma} + I_p)^{-1}\hat{\Omega} \Gamma\).

• \( \Omega \) describes which directions in \( \mathbb{R}^p \) are more likely to contain \( b \).

\[ \implies \text{The inversion of } \hat{\Sigma} \text{ is replaced by the inversion of } \Omega \hat{\Sigma} + I_p. \]

\[ \implies \text{For a well-chosen } a \text{ priori} \text{ matrix } \Omega, \text{ numerical problems disappear.} \]

2.2 Links with existing methods

• Ridge [Zhong et al, 2005]: \( \Omega = \tau^{-1} I_p \). No privileged direction for \( b \) in \( \mathbb{R}^p \).
  \( \tau > 0 \) is a regularization parameter.

• PCA+SIR [Chiaromonte et al, 2002]:

\[ \Omega = \sum_{j=1}^{d} \frac{1}{\hat{\delta}_j} \hat{q}_j \hat{q}_j^T, \]

where \( d \in \{1, \ldots, p\} \) is fixed, \( \hat{\delta}_1 \geq \cdots \geq \hat{\delta}_d \) are the \( d \) largest eigenvalues of \( \hat{\Sigma} \) and \( \hat{q}_1, \ldots, \hat{q}_d \) are the associated eigenvectors.

2.3 Three new methods

• PCA+ridge:

\[ \Omega = \frac{1}{\tau} \sum_{j=1}^{d} \hat{q}_j \hat{q}_j^T. \]

In the eigenspace of dimension \( d \), all the directions are \( a \text{ priori} \) equivalent.

• Tikhonov: \( \Omega = \tau^{-1} \hat{\Sigma} \). The directions with large variance are the most likely to contain \( b \).

• PCA+Tikhonov:

\[ \Omega = \frac{1}{\tau} \sum_{j=1}^{d} \hat{\delta}_j \hat{q}_j \hat{q}_j^T. \]

In the eigenspace of dimension \( d \), the directions with large variance are the most likely to contain \( b \).
2.4 Recall of SIR results with $\theta = 2$ and $p = 50$

Blue: Projections $b'X_i$ on the true direction $b$ versus $Y_i$,
Red: Projections $\hat{b}'X_i$ on the estimated direction $\hat{b}$ versus $Y_i$,
Green: $b'X_i$ versus $\hat{b}'X_i$.

2.5 Regularized SIR results (PCA + Ridge)

Blue: Projections $b'X_i$ on the true direction $b$ versus $Y_i$,
Red: Projections $\hat{b}'X_i$ on the estimated direction $\hat{b}$ versus $Y_i$,
Green: $b'X_i$ versus $\hat{b}'X_i$.

2.6 Validation on simulations

**Proximity criterion** between the true direction $b$ and the estimated ones $\hat{b}^{(r)}$ on $N = 100$ replications:

$$PC = \frac{1}{N} \sum_{r=1}^{N} \cos^2(b, \hat{b}^{(r)})$$

- $0 \leq PC \leq 1$,
- a value close to 0 implies a low proximity: The $\hat{b}^{(r)}$ are nearly orthogonal to $b$,
- a value close to 1 implies a high proximity: The $\hat{b}^{(r)}$ are approximately collinear with $b$. 
2.7 Influence of the regularization parameter

\[
\log \tau \text{ versus PC. The “cut-off” dimension and the condition number are fixed (} \ d = 20 \text{ and } \theta = 2\).
\]

- Ridge and Tikhonov: significant improvement if \( \tau \) is large,
- PCA+SIR: reasonable results compared to SIR,
- PCA+ridge and PCA+Tikhonov: small sensitivity to \( \tau \).

2.8 Sensitivity with respect to the condition number of the covariance matrix

\( \theta \) versus PC. The “cut-off” dimension is fixed to \( d = 20 \). The optimal regularization parameter is used for each value of \( \theta \).

- Only SIR is very sensitive to the ill-conditioning,
- ridge and Tikhonov: similar results,
- PCA+ridge and PCA+Tikhonov: similar results.

2.9 Sensitivity with respect to the “cut-off” dimension

\( d \) versus PC. The condition number is fixed (\( \theta = 2 \)). The optimal regularization parameter is used for each value of \( d \).
• PCA+SIR: very sensitive to $d$.
• PCA+ridge and PCA+Tikhonov: stable as $d$ increases.

3 Application to real data

3.1 Estimation of Mars surface physical properties from hyperspectral images

Context:

• Observation of the south pole of Mars at the end of summer, collected during orbit 61 by the French imaging spectrometer OMEGA on board Mars Express Mission.
• 3D image: On each pixel, a spectra containing $p = 184$ wavelengths is recorded.
• This portion of Mars mainly contains water ice, CO$_2$ and dust.

Goal: For each spectra $X \in \mathbb{R}^p$, estimate the corresponding physical parameter $Y \in \mathbb{R}$ (grain size of CO$_2$).

3.2 An inverse problem

Forward problem.

• Physical modeling of individual spectra with a surface reflectance model.
• Starting from a physical parameter $Y$, simulate $X = F(Y)$.
• Generation of $n = 12,000$ synthetic spectra with the corresponding parameters. \(\Rightarrow\) Learning database.

Inverse problem.
• Estimate the functional relationship \( Y = G(X) \).
• Dimension reduction assumption \( G(X) = g(b'X) \).
• \( b \) is estimated by (regularized) SIR, \( g \) is estimated by a nonparametric one-dimensional regression.

### 3.3 Estimated function \( g \)

Estimated function \( g \) between the projected spectra \( b'X \) on the first axis of regularized SIR (PCA+ridge) and \( Y \), the grain size of CO₂.

### 3.4 Estimated CO₂ maps

Grain size of CO₂ estimated with SIR (left) and regularized SIR (right) on a hyperspectral image of Mars.

### 3.5 Extensions

- **Kernel SIR.** The usual dot product \( b'X \) is replaced by a kernel.
  
  

- **Sparse SIR.** Introduction of a \( L_1 \) penalty on \( b \) to obtain sparse axes.
  
3.6 References on this work


3.7 References on SIR


