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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

$$Y = G(X) + \xi$$

where $\xi$ 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 $b \in \mathbb{R}^p \implies$ **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**
  \[
  \Sigma = \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})(X_i - \bar{X})^t, \quad \text{where} \quad \bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i.
  \]

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

- $\hat{\Sigma} = \hat{B} + \hat{W}$

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

1.4 SIR

**Idea:**

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

**In practice:**

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

![Graph showing linear regression illustration](image)

1.6 Estimation procedure

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

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

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.

- $Y_i = g(b^tX_i) + \xi$ 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 $p = 10$

![Graphs showing results with $\theta = 2$, dimension $p = 10$.](image)

- **Blue**: $Y_i$ versus the projections $b^tX_i$ on the true direction $b$.
- **Red**: $Y_i$ versus the projections $\hat{b}^tX_i$ on the estimated direction $\hat{b}$.
- **Green**: $\hat{b}^tX_i$ versus $b^tX_i$.

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

![Graphs showing results with $\theta = 2$, dimension $p = 50$.](image)

- **Blue**: $Y_i$ versus the projections $b^tX_i$ on the true direction $b$.
- **Red**: $Y_i$ versus the projections $\hat{b}^tX_i$ on the estimated direction $\hat{b}$.
- **Green**: $\hat{b}^tX_i$ versus $b^tX_i$.

### 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 $(\Omega \Sigma + I_p)^{-1} \Omega \hat{\Gamma}$.

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

$$\Rightarrow$$ The inversion of $\hat{\Sigma}$ is replaced by the inversion of $\Omega \Sigma + I_p$.

$$\Rightarrow$$ For a well-chosen $a \text{ priori}$ matrix $\Omega$, 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 [Chiaramonte et al, 2002]:

$$\Omega = \sum_{j=1}^{d} \frac{1}{\hat{\delta}_j} \hat{q}_j \hat{q}_j^\top,$$

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:

$$\Omega = \frac{1}{\tau} \sum_{j=1}^{d} \hat{q}_j \hat{q}_j^\top.$$

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

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

• PCA+Tikhonov:

$$\Omega = \frac{1}{\tau} \sum_{j=1}^{d} \hat{\delta}_j \hat{q}_j \hat{q}_j^\top.$$

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 $b$.  

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2.7 Influence of the regularization parameter

\( \log \tau \) 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 CO\(_2\).

3.4 Estimated CO\(_2\) maps

Grain size of CO\(_2\) 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.
  http://www.hmwu.idv.tw/KSIR/

• **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


