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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 $G : \mathbb{R}^p \rightarrow \mathbb{R}$ such that

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

- 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 $b \in \mathbb{R}^p \implies$ **Single index model**:

$$Y = g(b^t X) + \xi$$

where ξ 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, \dots, X_n be n points in \mathbb{R}^p divided into h classes C_j , $j = 1, \dots, h$.

- **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 $b^t X$ 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

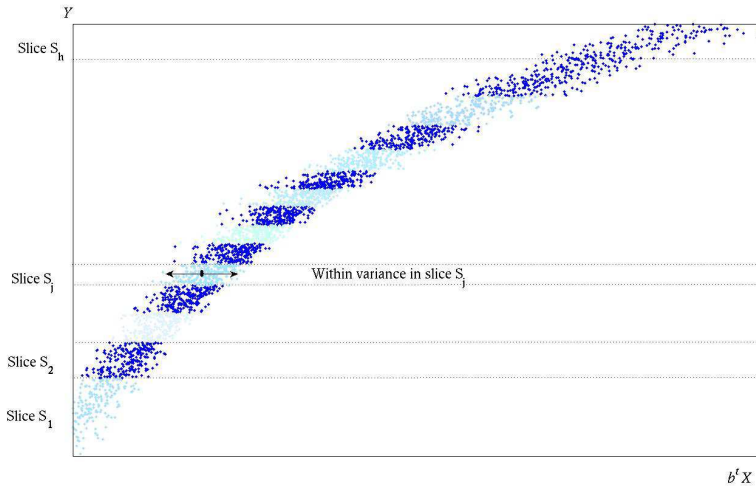
Idea:

- 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



1.6 Estimation procedure

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

$$\hat{b} = \underset{b}{\operatorname{argmax}} b^t \hat{\Gamma} b \quad \text{such that} \quad b^t \hat{\Sigma} b = 1. \quad (1)$$

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

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

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

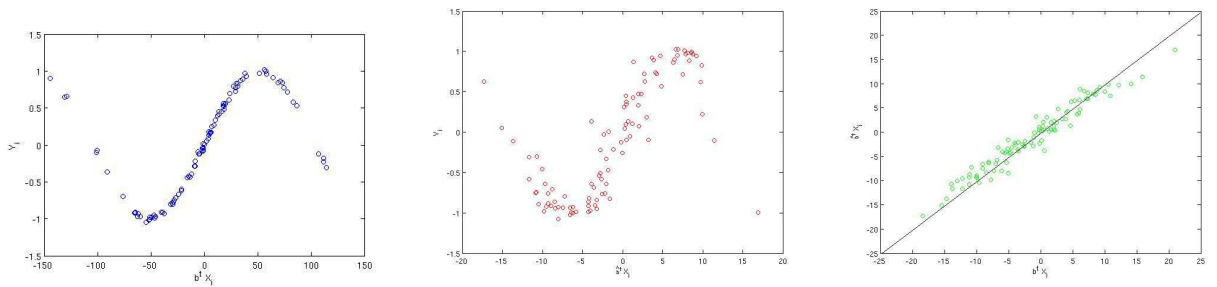
Simulated data.

- Sample $\{(X_1, Y_1), \dots, (X_n, Y_n)\}$ of size $n = 100$ with $X_i \in \mathbb{R}^p$ and $Y_i \in \mathbb{R}$, $i = 1, \dots, n$.
- $X_i \sim \mathcal{N}_p(0, \Sigma)$ where $\Sigma = Q \Delta Q^t$ with
 - $\Delta = \operatorname{diag}(p^\theta, \dots, 2^\theta, 1^\theta)$,
 - θ controls the decreasing rate of the eigenvalue screeplot,

- Q is an orientation matrix drawn from the uniform distribution on the set of orthogonal matrices.

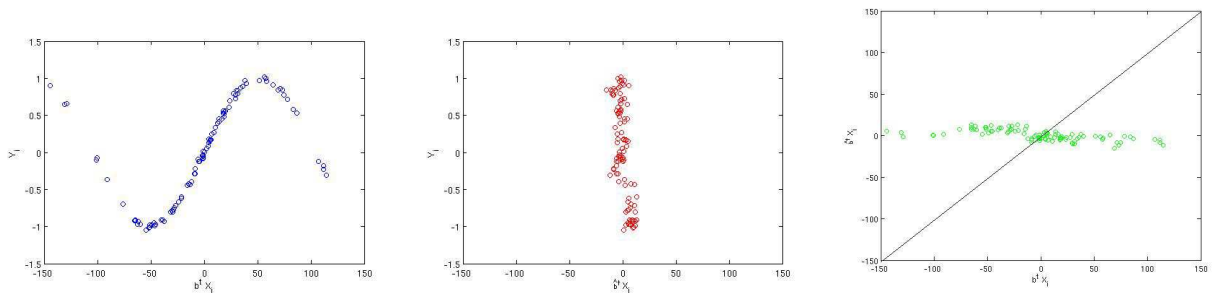
- $Y_i = g(b^t X_i) + \xi$ where
 - g is the link function $g(t) = \sin(\pi t/2)$,
 - b is the true direction $b = 5^{-1/2}Q(1, 1, 1, 1, 0, \dots, 0)^t$,
 - $\xi \sim \mathcal{N}_1(0, 9.10^{-4})$

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



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

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



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

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 Σ was p^θ .

2 Regularization of SIR

2.1 Regularized SIR

- We propose to compute \hat{b} as the eigenvector associated to the largest eigenvalue of $(\Omega\hat{\Sigma} + I_p)^{-1}\Omega\hat{\Gamma}$.
- Ω describes which directions in \mathbb{R}^p are more likely to contain b .

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

⇒ For a well-chosen *a priori* matrix Ω , 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 $d \in \{1, \dots, p\}$ is fixed, $\hat{\delta}_1 \geq \dots \geq \hat{\delta}_d$ are the d largest eigenvalues of $\hat{\Sigma}$ and $\hat{q}_1, \dots, \hat{q}_d$ are the associated eigenvectors.

2.3 Three new methods

- PCA+ridge:

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

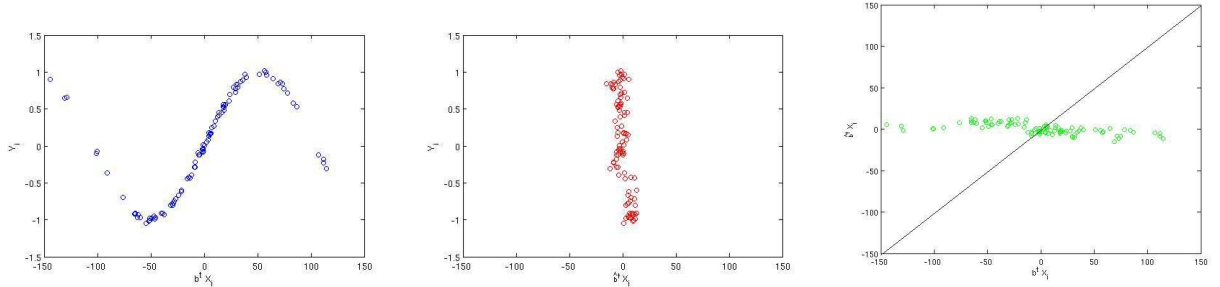
In the eigenspace of dimension d , all the directions are *a priori* equivalent.

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

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

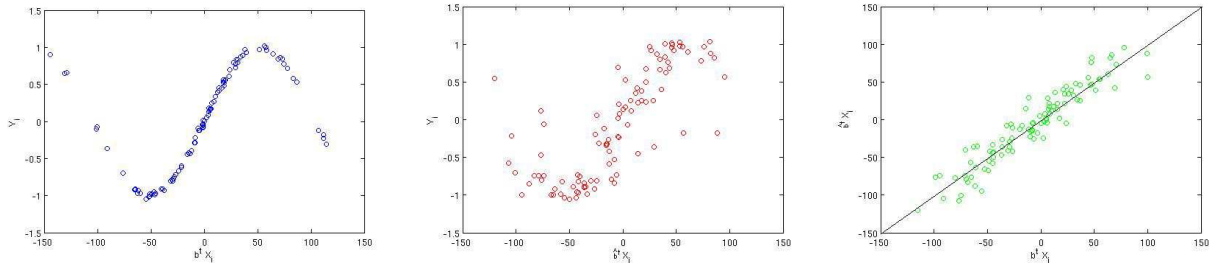
In the eigenspace of dimension d , the directions with large variance are the most likely to contain b .

2.4 Recall of SIR results with $\theta = 2$ and $p = 50$



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

2.5 Regularized SIR results (PCA+Ridge)



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

2.6 Validation on simulations

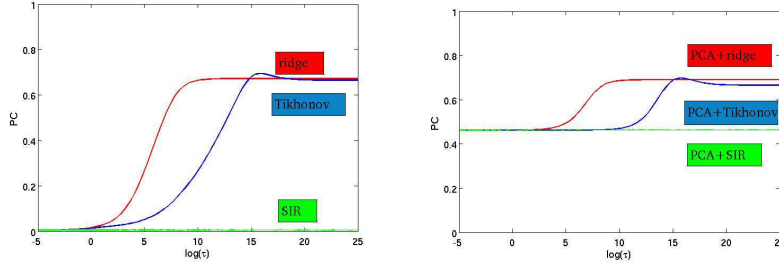
Proximity criterion between the true direction b and the estimated ones $\hat{b}^{(r)}$ on $N = 100$ replications:

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

- $0 \leq PC \leq 1$,
- 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

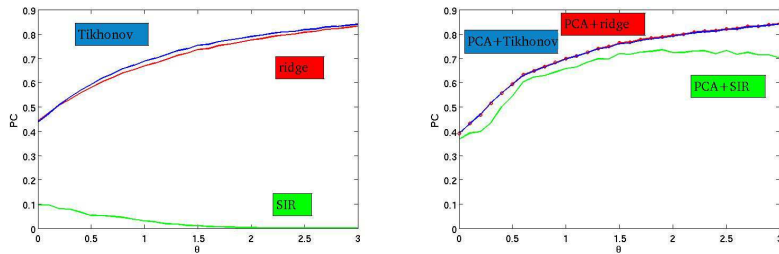
$\log \tau$ versus PC. The “cut-off” dimension and the condition number are fixed ($d = 20$ and $\theta = 2$).



- **Ridge** and **Tikhonov**: significant improvement if τ is large,
- **PCA+SIR**: reasonable results compared to **SIR**,
- **PCA+ridge** and **PCA+Tikhonov**: small sensitivity to τ .

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

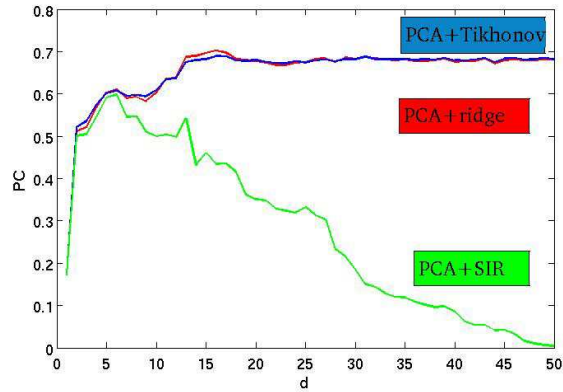
θ versus PC. The “cut-off” dimension is fixed to $d = 20$. The optimal regularization parameter is used for each value of θ .



- 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

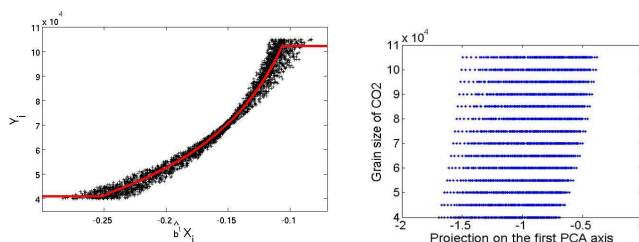
Forward problem.

- 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. \implies **Learning database.**

Inverse problem.

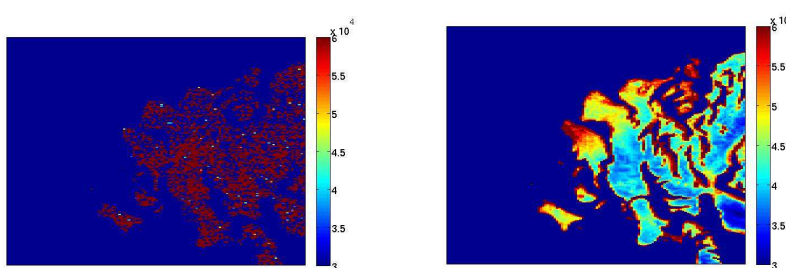
- Estimate the functional relationship $Y = G(X)$.
- Dimension reduction assumption $G(X) = g(b^t X)$.
- b is estimated by (regularized) SIR, g is estimated by a nonparametric one-dimensional regression.

3.3 Estimated function g



Estimated function g between the projected spectra $\hat{b}^t X$ 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 $b^t X$ is replaced by a kernel.
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