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Stéphane Girard. An introduction to SIR: A statistical method for dimension reduction in multivariate regression. 2014. hal-01058721

**HAL Id: hal-01058721**

**<https://hal.science/hal-01058721v1>**

Preprint submitted on 27 Aug 2014

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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  $\xi$  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  $X_1, \dots, X_n$  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

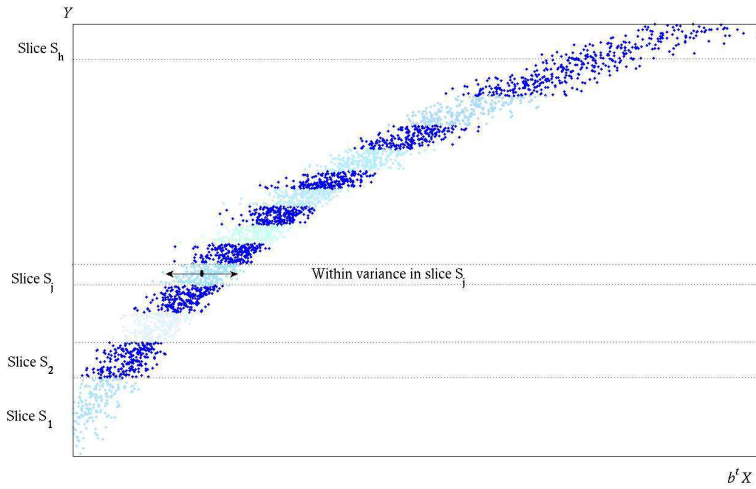
**Idea:**

- 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

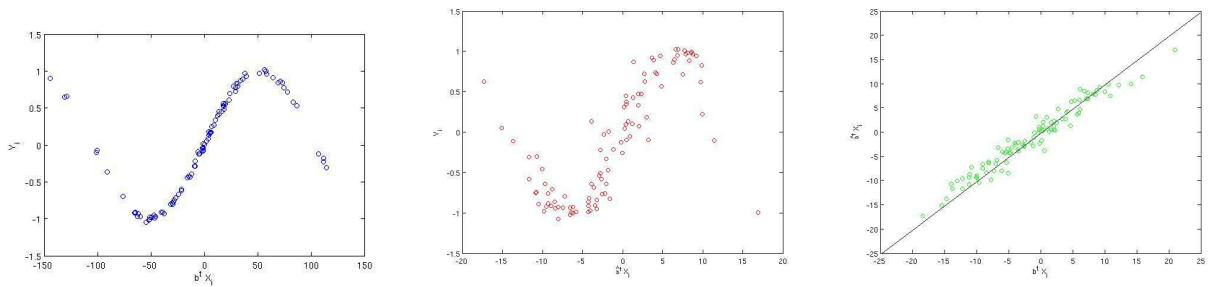
### Simulated data.

- 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
  - $\Delta = \operatorname{diag}(p^\theta, \dots, 2^\theta, 1^\theta)$ ,
  - $\theta$  controls the decreasing rate of the eigenvalue screeplot,

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

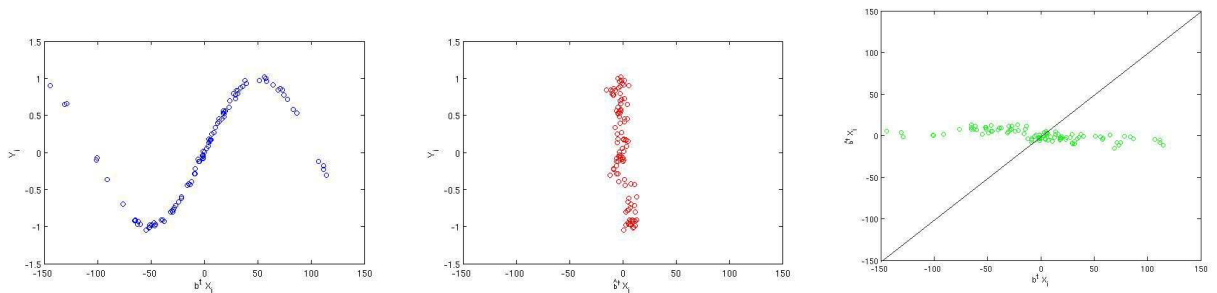
- $Y_i = g(b^t X_i) + \xi$  where
  - $g$  is the link function  $g(t) = \sin(\pi t/2)$ ,
  - $b$  is the true direction  $b = 5^{-1/2}Q(1, 1, 1, 1, 0, \dots, 0)^t$ ,
  - $\xi \sim \mathcal{N}_1(0, 9.10^{-4})$

### 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  $\Sigma$  was  $p^\theta$ .

## 2 Regularization of SIR

### 2.1 Regularized SIR

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

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

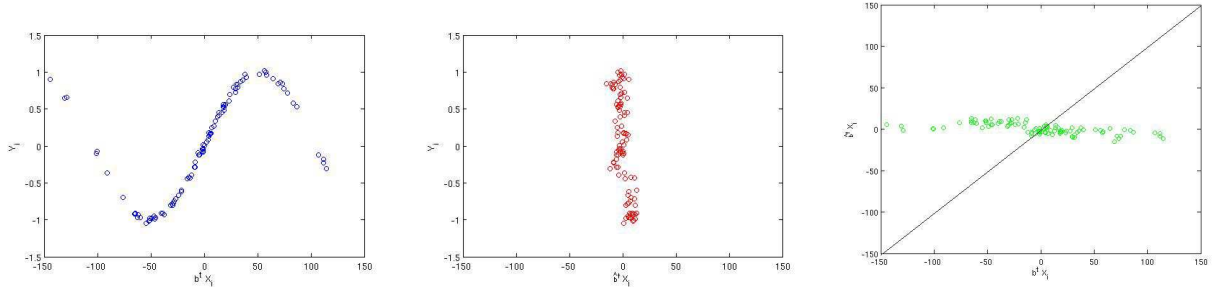
In the eigenspace of dimension  $d$ , all the directions are *a priori* equivalent.

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

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

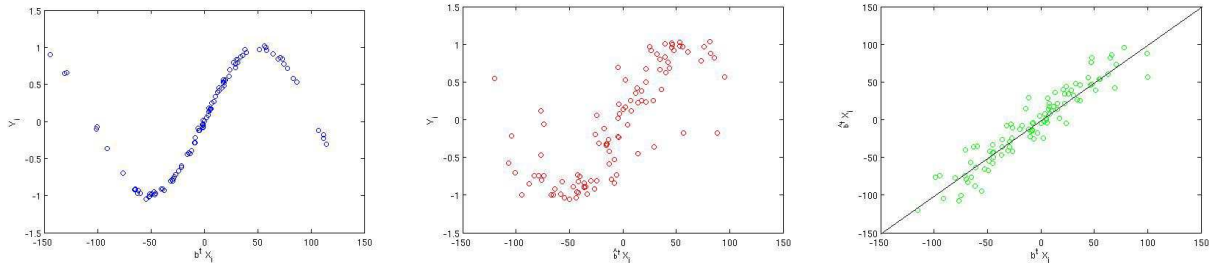
In the eigenspace of dimension  $d$ , the directions with large variance are the most likely to contain  $b$ .

## 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

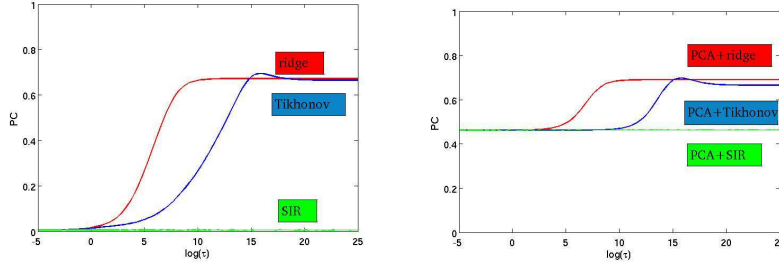
**Proximity criterion** between the true direction  $b$  and the estimated ones  $\hat{b}^{(r)}$  on  $N = 100$  replications:

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

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

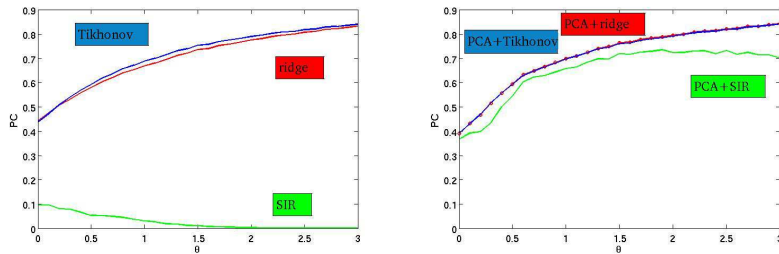
$\log \tau$  versus PC. The “cut-off” dimension and the condition number are fixed ( $d = 20$  and  $\theta = 2$ ).



- **Ridge** and **Tikhonov**: significant improvement if  $\tau$  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  $\theta$ .

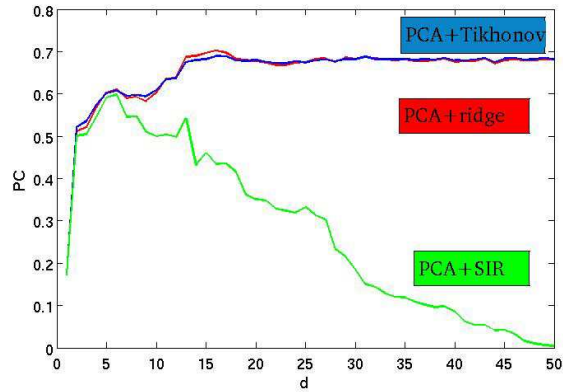


- Only **SIR** is very sensitive to the ill-conditioning,
- **ridge** and **Tikhonov**: similar results,
- **PCA+ridge** and **PCA+Tikhonov**: similar results.

## 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,  $\text{CO}_2$  and dust.

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

#### 3.2 An inverse problem

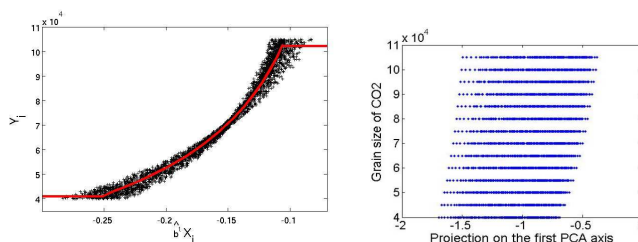
**Forward problem.**

- 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.**

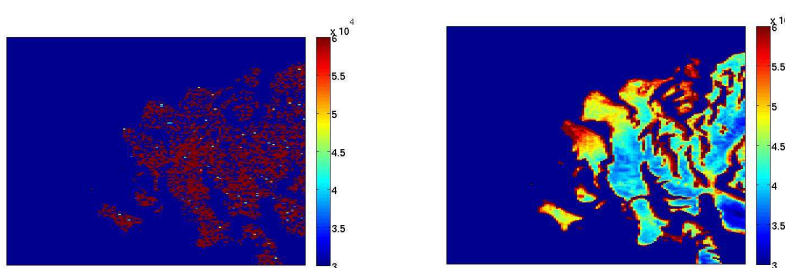
- Estimate the functional relationship  $Y = G(X)$ .
- Dimension reduction assumption  $G(X) = g(b^t X)$ .
- $b$  is estimated by (regularized) SIR,  $g$  is estimated by a nonparametric one-dimensional regression.

### 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  $\text{CO}_2$ .

### 3.4 Estimated $\text{CO}_2$ maps



Grain size of  $\text{CO}_2$  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.  
Wu, H. M. (2008). Kernel Sliced Inverse Regression with Applications to Classification, *Journal of Computational and Graphical Statistics*, **17**(3), 590–610.  
<http://www.hmwu.idv.tw/KSIR/>
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- [Chiaromonte et al, 2002]: Chiaromonte, F. and Martinelli, J. (2002). Dimension reduction strategies for analyzing global gene expression data with a response. *Mathematical Biosciences*, **176**, 123–144.