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# Regularization methods for Sliced Inverse Regression

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*February 2008*

Joint work with Caroline Bernard-Michel and Laurent Gardes

# Outline

- 1 Sliced Inverse Regression (SIR)
- 2 Inverse regression without regularization
- 3 Inverse regression with regularization
- 4 Validation on simulations
- 5 Real data study

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[Li, 1991]

- Infer the conditional distribution of a response r.v.  $Y \in \mathbb{R}$  given a predictor  $X \in \mathbb{R}^p$ .
- When  $p$  is large, curse of dimensionality.
- **Sufficient dimension reduction** aims at replacing  $X$  by its projection onto a subspace of smaller dimension without loss of information on the distribution of  $Y$  given  $X$ .
- The **central subspace** is the smallest subspace  $S$  such that, conditionally on the projection of  $X$  on  $S$ ,  $Y$  and  $X$  are independent.

How to estimate a basis of the central subspace?

## SIR : Basic principle

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

$$Y = g(b^t X) + \xi \quad \text{where } \xi \text{ is independent of } X.$$

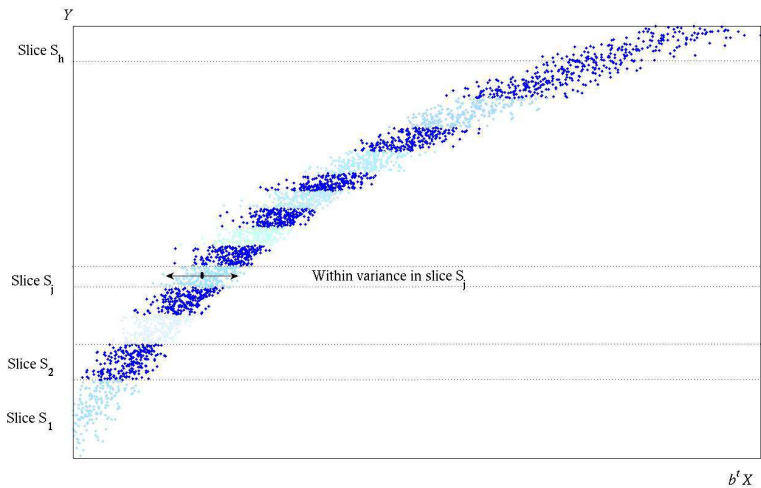
**Idea :**

- 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 range of  $Y$  is partitioned into  $h$  slices  $S_j$ .
- **Minimize the within slice variance of  $b^t X$**  under the normalization constraint  $\text{var}(b^t X) = 1$ .
- Equivalent to **maximizing the between slice variance** under the same constraint.

# SIR : Illustration



## SIR : Estimation procedure

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

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

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

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

with  $n_j$  is proportion of observations in slice  $S_j$ . The optimization problem (1) has an explicit solution :  $\hat{b}$  is the eigenvector of  $\hat{\Sigma}^{-1} \hat{\Gamma}$  associated to its largest eigenvalue.



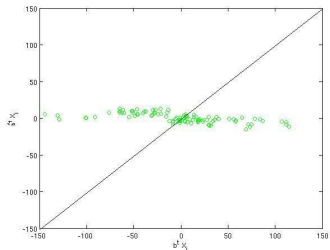
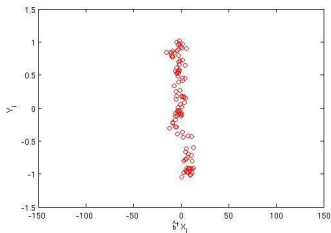
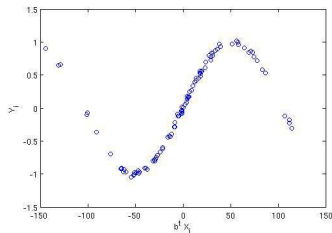
**Problem :**  $\hat{\Sigma}$  can be singular, or at least ill-conditioned, in several situations.

- Since  $\text{rank}(\hat{\Sigma}) \leq \min(n - 1, p)$ , if  $n \leq p$  then  $\hat{\Sigma}$  is singular.
- Even when  $n$  and  $p$  are of the same order,  $\hat{\Sigma}$  is ill-conditioned, and its inversion introduces numerical instabilities in the estimation of the central subspace.
- Similar phenomena occur when the coordinates of  $X$  are highly correlated.

**Experimental set-up.**

- A sample  $\{(X_1, Y_1), \dots, (X_n, Y_n)\}$  of size  $n = 100$  where  $X_i \in \mathbb{R}^p$  with  $p = 50$  and  $Y_i \in \mathbb{R}$ , for  $i = 1, \dots, n$ .
  - $X_i \sim \mathcal{N}_p(0, \Sigma)$  with  $\Sigma = Q\Delta Q^t$  where
    - $\Delta = \text{diag}(p^\theta, \dots, 2^\theta, 1^\theta)$ ,
    - $Q$  is a matrix drawn from the uniform distribution on the set of orthogonal matrices.
- $\implies$  The condition number of  $\Sigma$  is  $p^\theta$ . (Here,  $\theta = 2$ ).
- $Y_i = g(b^t X_i) + \xi$  where
    - $g$  is the link function  $g(t) = \sin(\pi t/2)$ ,
    - $b$  is the true direction  $b = 5^{-1/2}Q(1, 1, 1, 1, 1, 0, \dots, 0)^t$ ,
    - $\xi \sim \mathcal{N}_1(0, 9.10^{-4})$

# SIR : Numerical experiment (2/2)



**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  $\hat{b}^t X_i$ .

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# Single-index inverse regression model

Model introduced in [Cook, 2007].

$$X = \mu + c(Y)Vb + \varepsilon, \quad (2)$$

where

- $\mu$  and  $b$  are non-random  $\mathbb{R}^p$ - vectors,
- $\varepsilon \sim \mathcal{N}_p(0, V)$ , independent of  $Y$ ,
- $c: \mathbb{R} \rightarrow \mathbb{R}$  is a nonrandom coordinate function.

**Consequence :** The conditional expectation of  $X - \mu$  given  $Y$  is a degenerated random vector located in the direction  $Vb$ .

## Maximum Likelihood estimation (1/3)

- **Projection estimator of the coordinate function.**  $c(\cdot)$  is expanded as a linear combination of  $h$  basis functions  $s_j(\cdot)$ ,

$$c(\cdot) = \sum_{j=1}^h c_j s_j(\cdot) = s^t(\cdot)c,$$

where  $c = (c_1, \dots, c_h)^t$  is unknown and  $s(\cdot) = (s_1(\cdot), \dots, s_h(\cdot))^t$ . Model (2) can be rewritten as

$$X = \mu + s^t(Y)cVb + \varepsilon, \quad \varepsilon \sim \mathcal{N}_p(0, V),$$

- Definition : **Signal to Noise Ratio in the direction  $b$ .**

$$\rho = \frac{b^t \Sigma b - b^t V b}{b^t V b},$$

where  $\Sigma = \text{cov}(X)$ .

## Maximum Likelihood estimation (2/3)

### Notations

- $W$  : the  $h \times h$  empirical covariance matrix of  $s(Y)$  defined by

$$W = \frac{1}{n} \sum_{i=1}^n (s(Y_i) - \bar{s})(s(Y_i) - \bar{s})^t \quad \text{with} \quad \bar{s} = \frac{1}{n} \sum_{i=1}^n s(Y_i).$$

- $M$  : the  $h \times p$  matrix defined by

$$M = \frac{1}{n} \sum_{i=1}^n (s(Y_i) - \bar{s})(X_i - \bar{X})^t,$$

## Maximum Likelihood estimation (3/3)

If  $W$  and  $\hat{\Sigma}$  are regular, then the ML estimators are :

- **Direction** :  $\hat{b}$  is the eigenvector associated to the largest eigenvalue  $\hat{\lambda}$  of  $\hat{\Sigma}^{-1}M^tW^{-1}M$ ,
- **Coordinate** :  $\hat{c} = W^{-1}M\hat{b}/\hat{b}^t\hat{V}\hat{b}$ ,
- **Location parameter** :  $\hat{\mu} = \bar{X} - \bar{s}^t\hat{c}\hat{V}\hat{b}$ ,
- **Covariance matrix** :  $\hat{V} = \hat{\Sigma} - \hat{\lambda}\hat{\Sigma}\hat{b}\hat{b}^t\hat{\Sigma}/\hat{b}^t\hat{\Sigma}\hat{b}$ ,
- **Signal to Noise Ratio** :  $\hat{\rho} = \hat{\lambda}/(1 - \hat{\lambda})$ .

The inversion of  $\hat{\Sigma}$  is still necessary.



## SIR : A particular case

In the particular case of **piecewise constant basis functions**

$$s_j(\cdot) = \mathbb{I}\{\cdot \in S_j\}, \quad j = 1, \dots, h,$$

standard calculations show that

$$M^t W^{-1} M = \hat{\Gamma}$$

and thus the ML estimator  $\hat{b}$  of  $b$  is the eigenvector associated to the largest eigenvalue of  $\hat{\Sigma}^{-1} \hat{\Gamma}$ .

$\implies$  SIR method.

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## Gaussian prior

Introduction of a prior information on the projection of  $X$  on  $b$  appearing in the inverse regression model

$$(1 + \rho)^{-1/2} (s(Y) - \bar{s})^t c b \sim \mathcal{N}(0, \Omega).$$

- $(1 + \rho)^{-1/2}$  is introduced for normalization purposes, permitting to preserve the interpretation of the eigenvalue in terms of signal to noise ratio.
- $\Omega$  describes which directions in  $\mathbb{R}^p$  are the most likely to contain  $b$ .

## Gaussian regularized estimators

If  $W$  and  $\Omega\hat{\Sigma} + I_p$  are regular, the ML estimators are

- **Direction** :  $\hat{b}$  is the eigenvector associated to the largest eigenvalue  $\hat{\lambda}$  of  $(\Omega\hat{\Sigma} + I_p)^{-1}\Omega M^t W^{-1}M$ ,
- **Coordinate** :  $\hat{c} = W^{-1}M\hat{b}/((1 + \eta(\hat{b}))\hat{b}^t\hat{V}\hat{b})$ , with  $\eta(\hat{b}) = \hat{b}^t\Omega^{-1}\hat{b}/\hat{b}^t\hat{\Sigma}\hat{b}$ ,
- $\hat{\mu}$ ,  $\hat{V}$  and  $\hat{\rho}$  are unchanged.

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

$\implies$  For a properly chosen prior matrix  $\Omega$ , the numerical instabilities in the estimation of  $b$  disappear.

## Gaussian regularized SIR (1/2)

**GRSIR** : In the particular case of piecewise constant basis functions, the ML estimator  $\hat{b}$  of  $b$  is the eigenvector associated to the largest eigenvalue of  $(\Omega\hat{\Sigma} + I_p)^{-1}\Omega\hat{\Gamma}$ .

### 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 the 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.

## Three new methods

- PCA+ridge :

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

No privileged direction in the  $d$ -dimensional eigenspace.

- Tikhonov :  $\Omega = \tau^{-1} \hat{\Sigma}$ . Directions with large variance are most likely.
- PCA+Tikhonov :

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

In the  $d$ -dimensional eigenspace, directions with large variance are most likely.

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**Experimental set-up** : Same as previously.

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

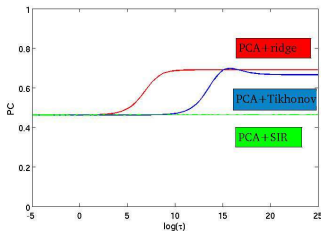
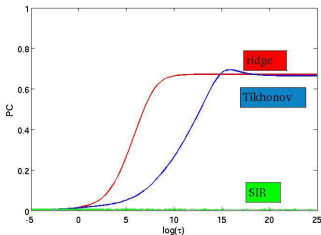
$$PC = \frac{1}{N} \sum_{r=1}^N (b^t \hat{b}^{(r)})^2$$

- $0 \leq PC \leq 1$ ,
- 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 approximatively collinear with  $b$ .



# Influence of the regularization parameter

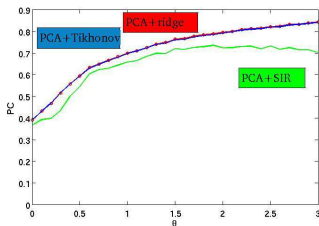
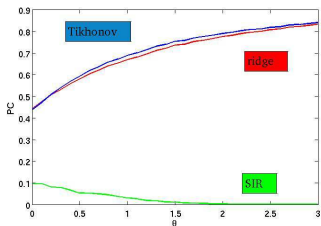
$\log \tau$  versus PC. The “cut-off” dimension and the condition number are fixed ( $d = 20$  and  $\theta = 2$ ).



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

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

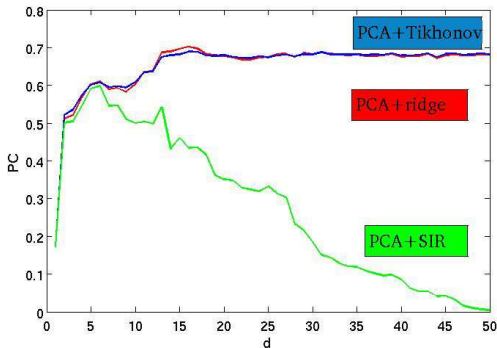
$\theta$  versus PC. The “cut-off” dimension is fixed to  $d = 20$ . The optimal regularization parameter is used for each value of  $\theta$ .



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

## 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.

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# 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  $\text{CO}_2$ ).

# An inverse problem

## Forward problem.

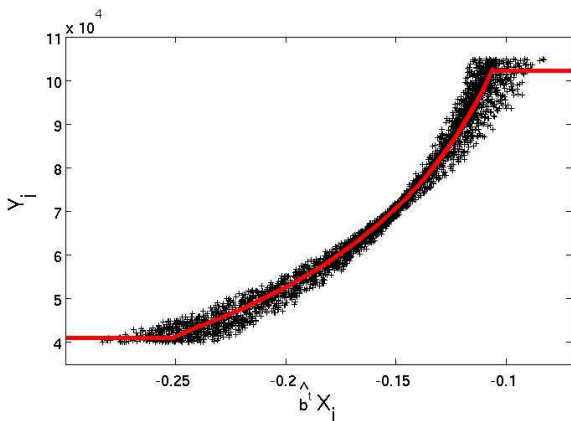
- Physical modeling of individual spectra with a surface reflectance model.
- Starting from a physical parameter  $Y$ , simulate  $X = F(Y)$ .
- Generation of  $n = 12,000$  synthetic spectra with the corresponding parameters.

⇒ Learning database.

## Inverse problem.

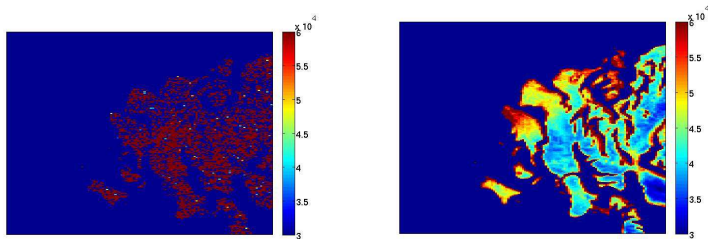
- Estimate the functional relationship  $Y = G(X)$ .
- Dimension reduction assumption  $G(X) = g(b^t X)$ .
- $b$  is estimated by SIR/GRSIR,  $g$  is estimated by a nonparametric one-dimensional regression.

# Estimated functional relationship



Functional relationship between reduced spectra  $\hat{b}^t X$  on the first GRSIR (PCA+ridge prior) direction and  $Y$ , the grain size of  $\text{CO}_2$ .

## Estimated CO<sub>2</sub> maps



Grain size of CO<sub>2</sub> estimated by SIR (left) and GRSIR (right) on an hyperspectral image observed on Mars during orbit 61.



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