Regularization methods for Sliced Inverse Regression

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Joint work with Caroline Bernard-Michel and Laurent Gardes
1 Sliced Inverse Regression (SIR)

2 Inverse regression without regularization

3 Inverse regression with regularization

4 Validation on simulations

5 Real data study
1. Sliced Inverse Regression (SIR)

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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

Slice $S_1$

Slice $S_2$

Slice $S_j$

Within variance in slice $S_j$

$Y$

$b'X$
SIR : Estimation procedure

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

\[
\hat{b} = \arg\max_b b^t \hat{\Gamma} b \quad \text{u.c.} \quad b^t \hat{\Sigma} b = 1. \tag{1}
\]

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 \( \{(X_1, Y_1), \ldots, (X_n, Y_n)\} \) of size \( n = 100 \) where \( X_i \in \mathbb{R}^p \) with \( p = 50 \) and \( Y_i \in \mathbb{R} \), for \( i = 1, \ldots, n \).
- \( X_i \sim \mathcal{N}_p(0, \Sigma) \) with \( \Sigma = Q \Delta Q^t \) where
  - \( \Delta = \text{diag}(p^\theta, \ldots, 2^\theta, 1^\theta) \),
  - \( Q \) is a matrix drawn from the uniform distribution on the set of orthogonal matrices.

\[ \implies \text{The condition number of } \Sigma \text{ is } p^\theta. \] (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 \( b = 5^{-1/2} Q(1, 1, 1, 1, 1, 0, \ldots, 0)^t \),
  - \( \xi \sim \mathcal{N}_1(0, 9.10^{-4}) \)
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 $\hat{b}^t X_i$. 
Outline

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

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

where $c = (c_1, \ldots, c_h)^t$ is unknown and $s(.) = (s_1(.), \ldots, s_h(.))^t$. 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 $\Sigma = \text{cov}(X)$. 
Notations

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

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

with $\bar{s} = \frac{1}{n} \sum_{i=1}^{n} s(Y_i)$.

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

$$M = \frac{1}{n} \sum_{i=1}^{n} (s(Y_i) - \bar{s})(X_i - \bar{X})^t.$$
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 $\hat{\Sigma}^{-1} M^t W^{-1} M$,
- **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.
In the particular case of **piecewise constant basis functions**

\[ s_j(.) = \mathbb{I}\{. \in S_j\}, \quad j = 1, \ldots, h, \]

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 \( \hat{\Sigma}^{-1} \hat{\Gamma} \).

\[ \implies \text{SIR method.} \]
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Introduction of a prior information on the projection of $X$ on $b$ appearing in the inverse regression model

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

- $(1 + \rho)^{-1/2}$ 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.

\( \Rightarrow \) The inversion of \( \hat{\Sigma} \) is replaced by the inversion of \( \Omega \hat{\Sigma} + I_p \).
\( \Rightarrow \) 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 $d \in \{1, \ldots, p\}$ 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.
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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Validation on simulations

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

- Ridge and Tikhonov: significant improvement if \( \tau \) is large,
- PCA+SIR: reasonable results compared to SIR,
- PCA+ridge and PCA+Tikhonov: small sensitivity to \( \tau \).
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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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$_2$).
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 $G(X) = g(b^t X)$.
- $b$ is estimated by SIR/GRSIR, $g$ is estimated by a nonparametric one-dimensional regression.
Functional relationship between reduced spectra $\hat{b}^t X$ on the first GRSIR (PCA+ridge prior) direction and $Y$, the grain size of CO$_2$. 
Estimated CO$_2$ maps

Grain size of CO$_2$ estimated by SIR (left) and GRSIR (right) on an hyperspectral image observed on Mars during orbit 61.

