Regularization methods for Sliced Inverse Regression

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Outline

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)

2. Inverse regression without regularization

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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 \( b \in \mathbb{R}^p \)

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

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

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

\[ \Rightarrow \text{The condition number of } \Sigma \text{ is } p^\theta. \] (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 \( b = 5^{-1/2}Q(1, 1, 1, 1, 0, \ldots, 0)^t \),
  - \( \xi \sim \mathcal{N}_1(0, 9.10^{-4}) \)
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 $\hat{b}^t X_i$. 
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Model introduced in [Cook, 2007].

\[ X = \mu + c(Y)Vb + \varepsilon, \]  

(2)

where

- $\mu$ and $b$ are non-random $\mathbb{R}^p$ vectors,
- $\varepsilon \sim \mathcal{N}_p(0, V)$, independent of $Y$,
- $c : \mathbb{R} \to \mathbb{R}$ 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.** \( c(.) \) 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 \( \Sigma = \text{cov}(X) \).
Maximum Likelihood estimation (2/3)

Notations

- $W$: the $h \times h$ empirical covariance matrix of $s(Y)$ defined by
  
  $$W = \frac{1}{n} \sum_{i=1}^{n} (s(Y_i) - \bar{s})(s(Y_i) - \bar{s})^t$$
  
  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 $\hat{\Sigma}^{-1}M^tW^{-1}M$,
- **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**: $\hat{V} = \hat{\Sigma} - \hat{\lambda}\hat{b}\hat{b}^t\hat{\Sigma}/\hat{b}^t\hat{\Sigma}\hat{b}$,
- **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**

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

standard calculations show that

\[ M^tW^{-1}M = \hat{\Gamma} \]

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

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

- $(1 + \rho)^{-1/2}$ 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 $b$. 
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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**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 $b$. 
$\log \tau$ 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, 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.

$\implies$ Learning database.

Inverse problem.
- Estimate the functional relationship $Y = G(X)$.
- Dimension reduction assumption $G(X) = g(b^t X)$.
- $b$ is estimated by 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 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.


References


