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► **To cite this version:**

Raphaël Coudret, Stéphane Girard, Jerome Saracco. A new sliced inverse regression method for multivariate response regression. 2012. hal-00714981v1

HAL Id: hal-00714981

<https://inria.hal.science/hal-00714981v1>

Preprint submitted on 6 Jul 2012 (v1), last revised 5 Oct 2013 (v3)

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A new sliced inverse regression method for multivariate response regression

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Abstract

We consider a semiparametric regression model of a q -dimensional multivariate response y on a p -dimensional covariate x . In this paper, a new approach is proposed based on sliced inverse regression for estimating the effective dimension reduction (EDR) space without requiring a prespecified parametric model. The convergence at rate \sqrt{n} of the estimated EDR space is shown. We discuss the choice of the dimension of the EDR space. The numerical performance of the proposed multivariate SIR method is illustrated on a simulation study. Moreover, we provide a way to cluster components of y related to the same EDR space. One can thus apply properly multivariate SIR on each cluster instead of blindly applying multivariate SIR on all components of y . An application to hyperspectral data is provided.

Keywords: dimension reduction, semiparametric regression model, multivariate response, sliced inverse regression.

1 Introduction

In analyzing large datasets, multivariate response regression analysis with a p -dimensional vector of regressors has been extensively studied in the literature. The reduction of the dimension of the regressors' space is a major concern in this framework. When the response variable is univariate, the issue has been addressed by Li (1991) via the notion of EDR (effective dimension reduction) space. The EDR directions (which form a basis of this subspace) are used to project the p -dimensional covariate x on a K -dimensional linear subspace (with $K < p$) first for displaying and then for studying its relationship with the response variable y . When the dimension of y is one, it is easy to view the link between the projected predictors and the response variable. The notion of EDR space was also clarified by Cook and his collaborators in their numerous papers introducing the notions of central subspace and central mean subspace, see for details Cook (1998) or Cook and Li (2002). Li (1991) introduced sliced inverse regression (SIR) which is a well-known method to estimate the EDR space. The link function can be estimated with a smoothing method such as kernel estimator or smoothing splines approach for instance.

In this paper, a q -dimensional response variable y is considered. Hence, we deal with a high dimensional regression framework which is not a linear one or a prespecified parametric one. The

underlying idea of the dimension reduction of the explanatory variable x without loss of information is to identify the linear combinations $\beta'_1 x, \dots, \beta'_K x$ such that

$$y \perp x | (\beta'_1 x, \dots, \beta'_K x), \quad (1)$$

where \perp denotes independence, $K(\leq p)$ is as small as possible and the p -dimensional vectors β_k are linearly independent. Let $\mathcal{B} = [\beta_1, \dots, \beta_K]$ denote the $p \times K$ matrix of the β_k 's. Statement (1) means that $y|x$ and $y|\mathcal{B}'x$ share the same distribution for all values of x . A straightforward consequence is that the p -dimensional covariate x can be replaced by the K -dimensional predictor $\mathcal{B}'x$ without loss of regression information. The goal of dimension reduction is achieved for $K < p$. As it is mentioned in Li (1991) or Cook (1994), statement (1) is equivalent to $y \perp x | P_{\mathcal{B}}x$, where $P_{\mathcal{B}}$ denotes the projection operator on $\text{Span}(\mathcal{B})$ which is the linear subspace of \mathbb{R}^p spanned by the columns of \mathcal{B} . In addition, $\text{Span}(\mathcal{B})$ can be viewed as the EDR space. From a regression model point of view, one can mention that the corresponding underlying model is the following semiparametric one

$$y = f(\mathcal{B}'x, \varepsilon), \quad (2)$$

where $f : \mathbb{R}^{K+r} \rightarrow \mathbb{R}^q$ is an arbitrary and unknown link function, ε is a r -dimensional random error variable independent of x (with $r \geq 1$). Let $y^{(j)}$ (resp. $\varepsilon^{(j)}$) stand for the j th component of y (resp. of ε). For instance, such a model could be sometimes written in the following specific way:

$$\begin{cases} y^{(1)} = f_1(\mathcal{B}'x, \varepsilon^{(1)}) \\ \vdots \\ y^{(q)} = f_q(\mathcal{B}'x, \varepsilon^{(q)}) \end{cases}$$

in which the link functions f_j are unknown real-valued functions. It is also possible to consider the slightly more restrictive model suggested by Li, Aragon, Shedden, and Agnan (2003) with an additive error term:

$$y = g(\mathcal{B}'x) + \varepsilon,$$

where g is an unknown link function taking its values in \mathbb{R}^q .

The vectors β_k are not individually identifiable neither in model (2), nor in the more restrictive ones. Thus, the main objective is to estimate a basis of the K -dimensional EDR space. Many numerical methods have been introduced to achieve this goal. Let us mention three of them which are relatively simple and easy to implement: SIR introduced by Duan and Li (1991) for the single index model ($K = 1$) and Li (1991) for the multiple indices model ($K > 1$), principal Hessian directions (see for instance Li (1992) or Cook (1998)), and sliced average variance estimation (see for details Cook (2000), Prendergast (2007) or Shao, Cook, and Weisberg (2009)). In this paper,

we shall only focus on the SIR approach which is based on a property of the first moment of the inverse distribution of x given y .

From a theoretical point of view, the following linearity condition is required:

$$(LC) \quad \text{the conditional expectation } \mathbb{E}[b'x|\mathcal{B}'x] \text{ is linear in } \mathcal{B}'x \text{ for any } b \in \mathbb{R}^p.$$

One can observe that the linearity condition does not involve the response variable y and only concerns the distribution of the covariate x . Let us mention that, when the distribution of x is an elliptically symmetric distribution (such as a p -dimensional normal distribution), this condition is satisfied. [Cook and Nachtsheim \(1994\)](#) proposed a method based on the minimum volume ellipsoid to transform and weight the predictors in order to approximate ellipticity. [Kuentz and Saracco \(2010\)](#) recommended to cluster the predictor space so that the linearity condition approximately holds in the different partitions. To conclude this brief discussion on the linearity condition, using a Bayesian argument of [Hall and Li \(1993\)](#), we can infer that (LC) approximately holds for many high-dimensional datasets (that is when p is large).

The main goal of this paper is to propose a new SIR approach for estimating the K -dimensional EDR space which is common to the q components of the multivariate response variable. The paper is organized as follows. In [Section 2](#), we give a brief overview on usual univariate SIR and existing multivariate SIR methods. The population version of the new SIR approach for a multivariate response, named MSIR hereafter, is described in [Section 3.1](#). The corresponding sample version is introduced in [Section 3.2](#) and asymptotic results are provided in [Section 3.3](#). A weighted version of MSIR, named wMSIR hereafter, is proposed in [Section 3.4](#). The choice of the dimension K is discussed in [Section 3.5](#). Numerical results based on simulations are exhibited in [Section 4](#) in order to show the good behavior of MSIR and wMSIR approaches. Moreover, a practical method to investigate the possible existence of a common EDR space for all the components of y is proposed in [Section 5](#). This procedure is then applied to hyperspectral data in [Section 6](#). Finally, concluding remarks are given in [Section 7](#).

2 Brief review of univariate and multivariate SIR approaches

We first provide an overview of the SIR method when the response y is univariate. Then, some existing SIR methods for a multivariate response are briefly described. The aim of all these approaches is to estimate the EDR space.

2.1 Univariate SIR

In this section, we consider an univariate response (i.e. $q = 1$) satisfying regression model (2).

Inverse regression step. The basic principle of the SIR method is to reverse the roles of y and x , that is, instead of regressing the univariate variable y on the multivariate variable x , the covariable x is regressed on the response variable y .

Let T denote a monotone (but not necessarily strictly monotone) transformation of y . Let $\mu = \mathbb{E}(x)$ and $\Sigma = \mathbb{V}(x)$. Under model (2) and (LC), Li (1991) established the following geometric property: the centered inverse regression curve, $\mathbb{E}(x|T(y)) - \mu$ as y varies, is contained in the linear subspace of \mathbb{R}^p spanned by $\Sigma\mathcal{B}$. A straightforward consequence is that the covariance matrix

$$\Gamma := \mathbb{V}(\mathbb{E}(x|T(y)))$$

is degenerated in any direction Σ -orthogonal to $\text{Span}(\mathcal{B})$. Therefore, the eigenvectors associated with the K non-null eigenvalues of $\Sigma^{-1}\Gamma$ are some EDR directions.

Slicing step. Li (1991) proposed a transformation T , called “slicing”, which categorizes the response y into a new response with $H > K$ levels. The support of y is partitioned into H non-overlapping slices $s_1, \dots, s_h, \dots, s_H$. With such a transformation T , the subspace recovered through a slicing (based on the inverse $x|T(y)$ function) may fall short of the space recovered through y in its entirety (based on the $x|y$ function). However the main advantage of the slicing is that the matrix of interest is now written as

$$\Gamma = \sum_{h=1}^H p_h (m_h - \mu)(m_h - \mu)'$$

where $p_h = \mathbb{P}(y \in s_h)$ and $m_h = \mathbb{E}(x|y \in s_h)$.

Estimation process. In the usual statistical framework, when a sample $\{(x_i, y_i), i = 1, \dots, n\}$ is available, it is straightforward to estimate the matrices Σ and Γ , by substituting empirical versions of the moments for their theoretical counterparts, and therefore to obtain the estimation of the EDR directions. Li (1991) showed that each of these estimated EDR directions converges to an EDR direction at rate \sqrt{n} . Asymptotic normality of these estimated EDR directions has been obtained by Saracco (1997).

From a practical point of view, the choice of the slicing is discussed in Li (1991), Chen and Li (1998) or Saracco (2001). Since SIR theory makes no assumption about the slicing strategy, the user must choose the number H of slices and how to construct them. In practice, there are

naturally two possibilities: to fix the width of the slices or to fix the number of observations per slice. This second option is often preferred, and from the sample point of view, the slices are often chosen such that the number of observations in each slice is as close to each other as possible. Note that H must be greater than K in order to avoid an artificial reduction of dimension and must be lower than $\lfloor n/2 \rfloor$ in order to have at least two observations in each slice (where $\lfloor a \rfloor$ denotes the integer part of a). The choice of H is less sensitive than the choice of a smoothing parameter in nonparametric regression. This point is clearly illustrated in [Liquet and Saracco \(2012\)](#) with a graphical tool that allows the user to find simultaneously realistic values of the two parameters H and K , see [Section 3.5](#) for details on this method.

The SIR estimates based on the first inverse moment have been studied extensively, see for instance [Hsing and Carroll \(1992\)](#), [Zhu and Ng \(1995\)](#), [Saracco \(1999\)](#), [Prendergast \(2005\)](#), [Szretter and Yohai \(2009\)](#) among others for some asymptotic results. [Chen and Li \(1998\)](#) exhibited many features to popularize SIR. [Chavent, Kuentz, Liquet, and Saracco \(2011\)](#) considered the case of a stratified population. In order to avoid the choice of a slicing in SIR, pooled slicing, kernel or spline versions of SIR have been investigated, see for example [Zhu and Fang \(1996\)](#), [Aragon and Saracco \(1997\)](#), [Zhu and Yu \(2007\)](#), [Wu \(2008\)](#), [Kuentz, Liquet, and Saracco \(2010\)](#) or [Azais, Gégout-Petit, and Saracco \(2012\)](#). However, these methods are hard to implement comparing to the basic SIR approach and are often computationally slow. Regularized versions for SIR have been proposed for high-dimensional covariates, see for instance [Zhu, Miao, and Peng \(2006\)](#), [Scrucca \(2007\)](#), [Li and Yin \(2008\)](#), [Bernard-Michel, Gardes, and Girard \(2009\)](#). Sparse SIR has been proposed by [Li and Nachtsheim \(2006\)](#). Hybrid methods of inverse regression-based algorithms have been also studied, see for example [Gannoun and Saracco \(2003\)](#) or [Zhu, Ohtaki, and Li \(2007\)](#).

2.2 Multivariate SIR

In the multivariate framework (that is when $y \in \mathbb{R}^q$ with $q > 1$), [Aragon \(1997\)](#), [Li, Aragon, Shedden, and Agnan \(2003\)](#) considered several estimation methods of the EDR space based on SIR. Note that [Barreda, Gannoun, and Saracco \(2007\)](#) proposed extensions of the following multivariate SIR methods based on SIR_α approach instead of SIR, where SIR_α is a generalization of SIR which combines information from the first two conditional moments of x given $T(y)$.

Complete slicing and marginal slicing approach. In the complete slicing method, the SIR procedure is directly applied on y . To build slices of nearly equal sizes, the following recursive approach is used. The first component of y is sliced. Then, each slice is separately sliced again according to the next component of y , and so on. This extension of univariate SIR to multivariate y

appears straightforward and the theoretical development can be formally carried over. Computation of such estimators suffers from the so-called curse of dimensionality when the dimension q of y is large ($q \geq 4$). Note that [Hsing \(1999\)](#) proposed a version of SIR in which the slices are determined by the nearest neighbors approach and he showed that the EDR directions can be estimated with rate \sqrt{n} under general conditions. Moreover, [Setodji and Cook \(2004\)](#) extended that univariate SIR to multivariate framework by introducing a new way of performing the slicing of y based on k-means method, the corresponding method being called k-means inverse regression.

A natural way to circumvent the curse of dimensionality of complete slicing approach is proposed in the marginal slicing procedure which consists in applying the SIR method on a transformation of y depending on one's interest. For instance, it can be the mean or the median of the $y^{(j)}$'s. One can also take the first few significant components of a principal component analysis of the $y^{(j)}$'s to construct the slices. However, slicing a lower dimensional projection of y may not lead to recover as many EDR directions as slicing the entire y .

For these reasons, these two multivariate approaches (complete slicing and marginal slicing) are not completely satisfactory.

Pooled marginal slicing approach. The idea of the pooled marginal slicing method is to consider the q univariate marginal SIR of each component $y^{(j)}$ of y on x and to combine the corresponding matrices of interest $\Gamma^{(j)} := \mathbb{V}(\mathbb{E}(x|T_j(y^{(j)})))$ matrices in the following pooling:

$$\Gamma_P = \sum_{j=1}^q w_j \Gamma^{(j)}, \quad (3)$$

for positive weights w_j . It has been shown that the eigenvectors associated with the non-null K eigenvalues of $\Sigma^{-1}\Gamma_P$ are EDR directions. [Aragon \(1997\)](#) proposes to use two kinds of weighting for the w_j 's: equal weights or weights proportional to the major eigenvalues found by a preliminary univariate SIR analysis of each component of y . [Saracco \(2005\)](#) obtained the asymptotic normality of the pooled marginal slicing estimator based on SIR_α . [Lue \(2009\)](#) derived the asymptotic weighted chi-squared test for dimension.

Some other multivariate SIR approaches. [Bura and Cook \(2001\)](#) introduced parametric inverse regression that may easily adapt to multivariate response framework. [Yin and Bura \(2006\)](#) proposed a moment-based dimension reduction approach in this context.

Moreover, in order to solve the dimensionality problem in high dimensional space and to rationalize the slicing step, [Li, Aragon, Shedden, and Agnan \(2003\)](#) presented an algorithm based on a duality between SIR variates and MP (most predictable) variates. The term ‘‘variate’’ denotes any

linear combination of either the regressor x or the response variable y . The SIR variates are the variables $b'x$ formed by an EDR direction b found by a SIR analysis. The MP variates $\theta'y$ are defined as those minimizing the ratio $\mathbb{E}[\mathbb{V}(\theta'y|x)]/\mathbb{V}(\theta'y)$, where $\mathbb{V}(\theta'y|x)$ is the associated prediction mean squared error of the best nonlinear prediction $\mathbb{E}[\theta'y|x]$ for the squared error loss. Equivalently, due to ANOVA identity, the MP variates can be found by maximizing the ratio $\mathbb{V}(\mathbb{E}[\theta'y|x])/\mathbb{V}(\theta'y)$, which conducts to the same eigenvalue decomposition as the SIR approach except for the exchanged roles of x and y . This twin relationship between SIR variates and MP variates underlies the development of the alternating SIR algorithm. The idea of the algorithm is to alternate computations of either $\hat{\theta}$ or \hat{b} respectively obtained by the slicing of SIR variates or MP variates constructed at the previous step. [Li, Aragon, Shedden, and Agnan \(2003\)](#) proposed an iterative procedure for the alternating SIR and showed that choosing the canonical directions as an initial projection of the y 's guarantees the convergence of the corresponding algorithm in a finite number of steps (equal to K , the number of EDR directions).

3 A new multivariate SIR approach

The population version of the proposed approach is first described in Subsection 3.1. Then, the corresponding sample version is given in Subsection 3.2 and some asymptotic results are derived in Subsection 3.3.

3.1 Population version

Let us assume that the dimension K of the EDR space is known. For $j = 1, \dots, q$, let $B^{(j)}$ be a $p \times K$ matrix containing a Σ -orthonormal basis of the EDR space from the (univariate) marginal regression model of $y^{(j)}$ given x . Let B be a $p \times K$ matrix such that $B'\Sigma B = I_K$. Let $P_B = BB'\Sigma$ and $P_{B^{(j)}} = B^{(j)}B^{(j)'}\Sigma$ be respectively the Σ -orthogonal projectors on the K -dimensional linear subspaces $\text{Span}(B)$ and $\text{Span}(B^{(j)})$.

Let $Q(B, B^{(1)}, \dots, B^{(q)})$ denote the following proximity measure between $\text{Span}(B)$ and the q marginal EDR spaces $\text{Span}(B^{(1)}), \dots, \text{Span}(B^{(q)})$:

$$Q(B, B^{(1)}, \dots, B^{(q)}) = \frac{1}{Kq} \sum_{j=1}^q \text{Trace}(P_B P_{B^{(j)}}). \quad (4)$$

This measure takes its values in $[0,1]$. Note that $\text{Span}(B) = \text{Span}(B^{(1)}) = \dots = \text{Span}(B^{(q)})$ implies $Q(B, B^{(1)}, \dots, B^{(q)}) = 1$. The closer to one is this measure, the closer to the q marginal EDR spaces is the linear subspace $\text{Span}(B)$.

Let us now consider the following optimization problem:

$$\max_{B \in \mathcal{M}_\Sigma} Q(B, B^{(1)}, \dots, B^{(q)}),$$

where \mathcal{M}_Σ is the set of Σ -orthogonal $p \times K$ matrices. Let us define

$$B^* = \arg \max_{B \in \mathcal{M}_\Sigma} Q(B, B^{(1)}, \dots, B^{(q)}). \quad (5)$$

A solution of (5) is given by the following lemma.

Lemma 1. *The $p \times K$ matrix B^* is formed by the eigenvectors associated with the K non-null eigenvalues of $\Sigma \mathbb{B} \mathbb{B}' \Sigma$ where \mathbb{B} is the $p \times (Kq)$ matrix defined as $\mathbb{B} = [B^{(1)}, \dots, B^{(q)}]$.*

Proof. Recall that, since the bases $B, B^{(1)}, \dots, B^{(q)}$ are assumed to be Σ -orthonormal, we have $P_B = BB' \Sigma$ and $P_{B^{(j)}} = B^{(j)} B^{(j)'} \Sigma$. It follows that

$$\begin{aligned} Kq \times Q(B, B^{(1)}, \dots, B^{(q)}) &= \sum_{j=1}^q \text{Trace}(BB' \Sigma B^{(j)} B^{(j)'} \Sigma) \\ &= \sum_{j=1}^q \text{Trace}(B' \Sigma B^{(j)} B^{(j)'} \Sigma B) \\ &= \text{Trace} \left(B' \Sigma \left\{ \sum_{j=1}^q B^{(j)} B^{(j)'} \right\} \Sigma B \right) \\ &= \text{Trace}(B' \Sigma \mathbb{B} \mathbb{B}' \Sigma B). \end{aligned}$$

Hence, since it is well known that $\arg \max_B \text{Trace}(B' \Sigma \mathbb{B} \mathbb{B}' \Sigma B)$ is given by the $p \times K$ matrix formed by the K non-null eigenvalues of $\Sigma \mathbb{B} \mathbb{B}' \Sigma$, the proof is complete. \square

Lemma 2. *Under model (2) and assumption (LC), we have $\text{Span}(B^*) = \text{Span}(\Sigma \mathcal{B})$.*

Proof. Under assumption (LC) and model (2), for each marginal component $y^{(j)}$, $j = 1, \dots, q$ of y , we have $\text{Span}(B^{(j)}) = \text{Span}(\mathcal{B})$ using univariate SIR theory. Each marginal inverse regression provides the true EDR space $\text{Span}(\mathcal{B})$. From this result, it is straightforward to see that the linear subspace spanned by the $p \times (Kq)$ matrix $\Sigma \mathbb{B}$ is equal to the linear subspace spanned by the $p \times K$ matrix $\Sigma \mathcal{B}$, that is $\text{Span}(\Sigma \mathbb{B}) = \text{Span}(\Sigma \mathcal{B})$. Moreover, we clearly have $\text{Span}(\Sigma \mathbb{B}) = \text{Span}(\Sigma \mathbb{B} \mathbb{B}' \Sigma)$ and thus $\text{Span}(\Sigma \mathbb{B} \mathbb{B}' \Sigma) = \text{Span}(\Sigma \mathcal{B})$. Therefore, this result together with Lemma 1 complete the proof. \square

Theorem 1. *The eigenvectors v_1, \dots, v_K associated with the K non-null eigenvalues of the Σ -symmetric matrix $\mathbb{B} \mathbb{B}' \Sigma$ span the EDR space.*

Proof. From Lemma 2, in order to obtain a basis of the EDR space, that is of $\text{Span}(\mathcal{B})$ instead of the linear subspace $\text{Span}(\Sigma\mathcal{B})$, it is easy to see that we just need to consider the matrix $\mathbb{B}\mathbb{B}'\Sigma$ instead of $\Sigma\mathbb{B}\mathbb{B}'\Sigma$. Since $\mathbb{B}\mathbb{B}'\Sigma$ is a Σ -symmetric matrix of rank K , we can easily obtain a Σ -orthonormal basis of the EDR space formed by the eigenvectors associated to the K non-null eigenvalues of this matrix. \square

From Theorem 1, we can estimate a basis of the EDR space based on estimators of matrices \mathbb{B} and Σ . This is the goal of the next subsection.

3.2 Sample version

Let $\{(x_i, y_i), i = 1, \dots, n\}$ be a sample of independent observations from model (2) with $x_i \in \mathbb{R}^p$ and $y_i \in \mathbb{R}^q$. We assume that the sample size n is larger than the dimension p of the covariate x .

Let $\bar{x} := \frac{1}{n} \sum_{i=1}^n x_i$ and $\widehat{\Sigma} := \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})'$ be the empirical mean and the covariance matrix of the x_i 's.

In order to estimate the matrix \mathbb{B} , we have to estimate each $p \times K$ matrix $B^{(j)}$ with usual univariate SIR from the subsample $\{(x_i, y_i^{(j)}), i = 1, \dots, n\}$ where $y_i^{(j)}$ stands for the j th component of y_i . To this end, let us assume that the support of $y^{(j)}$ is partitioned into a fixed number of slices denoted by $s_1^{(j)}, \dots, s_h^{(j)}, \dots, s_{H^{(j)}}^{(j)}$. Let $p_h^{(j)} := \mathbb{P}(y^{(j)} \in s_h^{(j)})$ and $m_h^{(j)} := \mathbb{E}(x|y^{(j)} \in s_h^{(j)})$. Thus, the matrix $\Gamma^{(j)} := \sum_{h=1}^{H^{(j)}} p_h^{(j)} (m_h^{(j)} - \mu)(m_h^{(j)} - \mu)'$ is estimated by $\widehat{\Gamma}^{(j)} := \sum_{h=1}^{H^{(j)}} \hat{p}_h^{(j)} (\widehat{m}_h^{(j)} - \bar{x})(\widehat{m}_h^{(j)} - \bar{x})'$ with $\hat{p}_h^{(j)} := \frac{1}{n} \sum_{i=1}^n \mathbb{I}[y_i^{(j)} \in s_h^{(j)}]$ and $\widehat{m}_h^{(j)} := \frac{1}{n\hat{p}_h^{(j)}} \sum_{i=1}^n x_i \mathbb{I}[y_i^{(j)} \in s_h^{(j)}]$ where $\mathbb{I}[\cdot]$ is the indicator function. Then, the matrix $B^{(j)}$ is estimated by

$$\widehat{B}^{(j)} = \left[\hat{b}_1^{(j)}, \dots, \hat{b}_K^{(j)} \right],$$

where the vectors $\hat{b}_k^{(j)}$, $k = 1, \dots, K$ are the $\widehat{\Sigma}$ -orthonormal eigenvectors associated with the K largest eigenvalues of the matrix $\widehat{\Sigma}^{-1}\widehat{\Gamma}^{(j)}$. It follows that the matrix \mathbb{B} is directly estimated by

$$\widehat{\mathbb{B}} = \left[\widehat{B}^{(1)}, \dots, \widehat{B}^{(q)} \right].$$

Finally, a $\widehat{\Sigma}$ -orthonormal estimated basis of the EDR space is given by the vectors $\hat{v}_1, \dots, \hat{v}_K$ defined as the eigenvectors associated with the K largest eigenvalues of the matrix $\widehat{\mathbb{B}}\widehat{\mathbb{B}}'\widehat{\Sigma}$.

3.3 An asymptotic result

The following assumptions are necessary to state our asymptotic result. Let $n_h^{(j)} := n\hat{p}_h^{(j)}$ be the number of observations in the slice $s_h^{(j)}$.

- (A1) Observations $\{(x_i, y_i), i = 1, \dots, n\}$ are independently drawn from regression model (2).

- (A2) For each component $y^{(j)}$ of y , the support is partitioned into a fixed number $H^{(j)}$ of slices such that $p_h^{(j)} > 0$ for $h = 1, \dots, H^{(j)}$.
- (A3) For $j = 1, \dots, q$ and $h = 1, \dots, H^{(j)}$, $n_h^{(j)} \rightarrow \infty$ as $n \rightarrow \infty$.

Theorem 2. *Under linearity condition (LC) and (A1)-(A3), we have, for $k = 1, \dots, K$,*

$$\hat{v}_k = v_k + O_p(n^{-1/2}),$$

that is, the estimated EDR space $\text{Span}(\hat{v}_1, \dots, \hat{v}_K)$ converges in probability to the EDR space.

Proof. For each component $y^{(j)}$ of y and under the assumptions (LC), (A1)-(A3), from univariate SIR theory of Li (1991), each estimated EDR space $\hat{B}^{(j)}$ converges to $B^{(j)}$ at root n rate: that is, for $j = 1, \dots, q$, $\hat{B}^{(j)} = B^{(j)} + O_p(n^{-1/2})$. It follows that $\hat{\mathbb{B}} = \mathbb{B} + O_p(n^{-1/2})$. Since $\hat{\Sigma} = \Sigma + O_p(n^{-1/2})$, we get $\hat{\mathbb{B}}\hat{\mathbb{B}}'\hat{\Sigma} = \mathbb{B}\mathbb{B}'\Sigma + O_p(n^{-1/2})$. Therefore, the eigenvectors associated with the largest K eigenvalues of $\hat{\mathbb{B}}\hat{\mathbb{B}}'\hat{\Sigma}$ converge to the corresponding ones of $\mathbb{B}\mathbb{B}'\Sigma$ at the same rate: $\hat{v}_k = v_k + O_p(n^{-1/2})$ for $k = 1, \dots, K$. Consequently, the estimated EDR space $\text{Span}(\hat{v}_1, \dots, \hat{v}_K)$ converges to $\text{Span}(v_1, \dots, v_K)$ at root n rate. Since $\text{Span}(v_1, \dots, v_K) = \text{Span}(\mathcal{B})$, the estimated EDR space converges to the true one in probability. \square

Remark on asymptotic normality. Using Delta-method, asymptotic results of Tyler (1981) and Saracco (1997), it is possible to obtain the asymptotic normality of

$$\sqrt{n} \left(\text{vec}(\hat{\mathbb{B}}\hat{\mathbb{B}}'\hat{\Sigma}) - \text{vec}(\mathbb{B}\mathbb{B}'\Sigma) \right),$$

where $\text{vec}(M)$ stands for the “vec” operator applied to matrix M . More precisely, this operator rearranges the p^2 elements of M in the form of a p^2 -dimensional column vector by stacking the p columns of M one under the other. Then, the asymptotic normality of the eigenprojector onto the estimated EDR space can be derived, as well as the asymptotic distribution of the estimated EDR directions \hat{v}_k , associated with eigenvalues assumed to be different (that is $\lambda_1 > \dots > \lambda_K > 0$).

3.4 A weighted version of MSIR

Following the idea used in pooled marginal slicing approach in which the matrix of interest Γ_P is a weighted average of the marginal matrices $\Gamma^{(j)}$, we can consider a weighted version of the multivariate SIR method introduced in this paper, named wMSIR hereafter. As it has already been proposed by Aragon (1997) or Lue (2009), we shall use weights based on the proportion of eigenvalues corresponding to significant eigenvectors (which are EDR directions) in each marginal SIR (i.e. univariate SIR on each marginal component of y).

More precisely, for $j = 1, \dots, q$, let $\lambda_k^{(j)}, k = 1, \dots, p$ be the eigenvalues of the eigendecomposition $\Sigma^{-1}\Gamma^{(j)}v_k^{(j)} = \lambda_k^{(j)}v_k^{(j)}$ where $\lambda_1^{(j)} \geq \lambda_2^{(j)} \geq \dots \geq \lambda_p^{(j)}$. Let us define, for each component $y^{(j)}$ of y , the proportion of eigenvalues corresponding to significant eigenvectors: $\pi^{(j)} = \frac{\sum_{k=1}^K \lambda_k^{(j)}}{\sum_{k=1}^p \lambda_k^{(j)}}$. Let us also define $\pi_\star = \sum_{j=1}^q \pi^{(j)}$. Then, we can introduce the following $qK \times qK$ matrix of weights

$$\mathbb{D} = \text{diag}(D^{(1)}, \dots, D^{(j)}, \dots, D^{(q)})$$

with $D^{(j)} = \frac{\pi^{(j)}}{\pi_\star} I_K$ for $j = 1, \dots, q$ where I_K is the identity matrix of order K . Note that, from a theoretical point of view, under model (2) and (LC), the matrix of weights is such that $\mathbb{D} = \frac{1}{q} I_{qK}$ since $\lambda_k^{(j)} = 0$ for $j = 1, \dots, q$ and $k = K + 1, \dots, p$.

The population version of wMSIR consists in noticing that the eigenvectors $\tilde{v}_1, \dots, \tilde{v}_K$ associated with the K largest eigenvalues of the Σ -symmetric matrix $\mathbb{B}\mathbb{D}\mathbb{B}'\Sigma$ span the EDR space. To show this result, one can proceed analogously to the proofs of Lemma 2 and Theorem 1.

Let $\hat{\lambda}_k^{(j)}$ be the k th eigenvalue of $\hat{\Sigma}^{-1}\hat{\Gamma}^{(j)}$. The sample version of wMSIR is obtained by substituting the empirical matrices $\hat{\mathbb{B}}, \hat{\mathbb{D}}$ and $\hat{\Sigma}$ for their theoretical counterparts \mathbb{B}, \mathbb{D} and Σ , where $\hat{\mathbb{D}} = \text{diag}(\hat{D}^{(1)}, \dots, \hat{D}^{(q)})$ with, for $j = 1, \dots, q$, $\hat{D}^{(j)} = \frac{\hat{\pi}^{(j)}}{\hat{\pi}_\star} I_K$, $\hat{\pi}^{(j)} = \frac{\sum_{k=1}^K \hat{\lambda}_k^{(j)}}{\sum_{k=1}^p \hat{\lambda}_k^{(j)}}$ and $\hat{\pi}_\star = \sum_{j=1}^q \hat{\pi}^{(j)}$. Therefore, one can get the corresponding estimated EDR directions $\hat{v}_1, \dots, \hat{v}_K$.

Theorem 3. *Under linearity condition (LC) and (A1)-(A3), we have, for $k = 1, \dots, K$,*

$$\hat{v}_k = \tilde{v}_k + O_p(n^{-1/2}),$$

that is, the estimated EDR space $\text{Span}(\hat{v}_1, \dots, \hat{v}_K)$ converges in probability to the EDR space.

Proof. We can proceed analogously to the proof of Theorem 2. It is sufficient to show that $\hat{\mathbb{D}} = \mathbb{D} + O_p(n^{-1/2})$. Since, for each component $y^{(j)}$ of y and under assumptions (LC) and (A1)-(A3), from univariate SIR theory of Li (1991), each estimated eigenvalue $\hat{\lambda}_k^{(j)}$ converges to $\lambda_k^{(j)}$ at root n rate, we have $\hat{\pi}^{(j)} = \pi^{(j)} + O_p(n^{-1/2})$ and $\hat{\pi}_\star = \pi_\star + O_p(n^{-1/2})$. We thus get $\hat{D}^{(j)} = D^{(j)} + O_p(n^{-1/2})$ and $\hat{\mathbb{D}} = \mathbb{D} + O_p(n^{-1/2})$.

Consequently, $\hat{\mathbb{B}}\hat{\mathbb{D}}\hat{\mathbb{B}}'\hat{\Sigma} = \mathbb{B}\mathbb{D}\mathbb{B}'\Sigma + O_p(n^{-1/2})$ and the eigenvectors associated with the largest K eigenvalues of $\hat{\mathbb{B}}\hat{\mathbb{D}}\hat{\mathbb{B}}'\hat{\Sigma}$ converge to the corresponding ones of $\mathbb{B}\mathbb{D}\mathbb{B}'\Sigma$ at the same rate: $\hat{v}_k = \tilde{v}_k + O_p(n^{-1/2})$ for $k = 1, \dots, K$. Therefore, the estimated EDR space $\text{Span}(\hat{v}_1, \dots, \hat{v}_K)$ converges to $\text{Span}(\tilde{v}_1, \dots, \tilde{v}_K)$ at root n rate. Since $\text{Span}(\tilde{v}_1, \dots, \tilde{v}_K) = \text{Span}(\mathcal{B})$, the estimated EDR space converges to the true one in probability. \square

3.5 Discussion on the choice of dimension K

Up to now, the dimension K of the EDR space was assumed to be known. However, in most applications based on real datasets, the number K of indices $\beta'_k x$ in model (1) is a priori unknown

and hence must be determined from the data.

Several approaches have been proposed in the literature for univariate SIR. Some of them are based on hypothesis tests on the nullity of the last $(p - K)$ eigenvalues, see for instance [Li \(1991\)](#), [Schott \(1994\)](#), [Bai and He \(2004\)](#) or [Barrios and Velilla \(2007\)](#), [Nkiet \(2008\)](#). In the multivariate response framework, [Lue \(2009\)](#) derived an asymptotic weighted chi-squared test for dimension adapted to the pooled marginal slicing estimator. In our case, a crude choice of the dimension can be also made by a visual inspection of the eigenvalues scree plot of the matrix $\widehat{\mathbb{B}}\widehat{\mathbb{B}}'\widehat{\Sigma}$: the idea is to determine the number of the significantly non-null largest eigenvalues.

Other approaches relying on a quality measure based on the squared trace correlation between the true EDR space $\text{Span}(\mathcal{B})$ and its estimate have been proposed in the univariate response model, see for instance [Ferré \(1998\)](#) or [Liquet and Saracco \(2008, 2012\)](#). The graphical bootstrap-based procedure of [Liquet and Saracco \(2012\)](#) can be easily adapted to the multivariate response framework by fixing the same number H of slices for each marginal SIR. Let $P_{M,\Sigma}$ be the Σ -orthogonal projector on the linear subspace spanned by the columns of the matrix M . As mentioned before, the criterion used to study the closeness between two k -dimensional linear subspaces is the squared trace correlation defined as

$$r(V_k, \Sigma, \widehat{V}_k, \widehat{\Sigma}) := \frac{1}{k} \text{Trace} \left(P_{V_k, \Sigma} \widehat{P}_{\widehat{V}_k, \widehat{\Sigma}} \right),$$

where $V_k := [v_1, \dots, v_k]$ and $\widehat{V}_k := [\widehat{v}_1, \dots, \widehat{v}_k]$. The corresponding risk function is

$$R_{h,k} = \mathbb{E} \left(r(V_k, \Sigma, \widehat{V}_k, \widehat{\Sigma}) \right), \quad (6)$$

where h is the number of slices used to obtain V_k and \widehat{V}_k . This risk function only makes sense for any dimension k lower than or equal to the true dimension K of the EDR space. For the true dimension K , $R_{h,K}$ converges to one as n tends to infinity. In our dimension reduction context, a value of $R_{h,k}$ close to one indicates that the set of the k estimated indices is close to the ideal set. So in terms of dimensionality, k is a feasible solution. On the other hand, a value of $R_{h,k}$ sufficiently different from 1 means that this estimated set is slightly different from the ideal one. Thus, for a fixed n , a reasonable way to assess whether an EDR direction is available is to graphically evaluate how much $R_{h,k}$ departs from one. From a computational point of view, consistent estimates of $R_{h,k}$ are required. [Liquet and Saracco \(2012\)](#) use a bootstrap estimator $\widehat{R}_{h,k}$ of this criterion in order to determine the pair (H, K) of parameters. The proposed graphical method consists in evaluating the $\widehat{R}_{h,k}$ values for all $k = 1, \dots, p$ and some reasonable values of h , and in observing how much the criterion departs from one. The best choice will be the pair $(\widehat{H}, \widehat{K})$ which gives a value of $\widehat{R}_{h,k}$ close to one, such that $\widehat{K} \ll p$ in order to get an effective dimension reduction. In

practice, there is no objective criterion to find a trade-off between a large value of the criterion $\widehat{R}_{h,k}$ and a small value of the dimension K . Then, a visual expertise of the 3D-plot of the $\widehat{R}_{h,k}$ versus (h, k) allows the selection of the best value. It is also useful to provide, for each (h, k) , the boxplots of the bootstrap replication of the squared trace correlation to have a look on how much the corresponding k -dimensional linear subspace is stable.

4 A simulation study

This section illustrates the ability of the proposed MSIR and wMSIR approaches to properly estimate EDR spaces. Two simulation models are considered. For given sample size n and dimension p , 100 replications of the covariate x are generated from the p -dimensional normal distribution $\mathcal{N}_p(\mu, \Sigma)$ with the same pair (μ, Σ) . Here, μ is randomly generated from the $\mathcal{N}_p(0, I_p)$ distribution and $\Sigma = VV' + 0.1I_p$ where V is a $p \times p$ matrix made of entries independently generated from the standard normal distribution $\mathcal{N}_1(0, 1)$. For every model, for all $j \geq 1$, it is assumed that $\varepsilon^{(j)} \sim \mathcal{N}_1(0, 1)$. The dimension K is also assumed to be known in this section. We first study a special case of model (2) with $K = 1$. Secondly, MSIR and wMSIR are evaluated with a multiple indices model.

4.1 Single index model

Consider the following single index model:

$$\begin{cases} y^{(1)} &= x' \beta_1 + \varepsilon^{(1)}, \\ y^{(2)} &= (x' \beta_1)^3 + 3\varepsilon^{(2)}, \\ y^{(3)} &= x' \beta_1(1 + \varepsilon^{(3)}), \end{cases} \quad (7)$$

with $\beta_1 = [\beta_{1,1}, \dots, \beta_{1,p}]'$. We choose for all $i = 1, \dots, p$, $\beta_{1,i} = i \mathbb{I}(i \leq 5) + \mathbb{I}(i > 5)$.

We generate samples of size $n = 100$ from (7), with $p = 20$. Then, the EDR direction is estimated using the following methods, with $H = 10$ slices:

- univariate SIR for each component of y which produces estimates $\widehat{B}^{(1)}$, $\widehat{B}^{(2)}$ and $\widehat{B}^{(3)}$,
- MSIR which gives the estimate $\widehat{V} := \widehat{V}_K = [\widehat{v}_1]$,
- wMSIR that leads to the estimate $\widehat{V} := [\widehat{v}_1]$.

For each estimator $\widehat{B} \in \left\{ \widehat{B}^{(1)}, \widehat{B}^{(2)}, \widehat{B}^{(3)}, \widehat{V}, \widehat{V} \right\}$, we compute the squared trace correlation $r(\widehat{B}) := r(\widehat{B}, \Sigma, \mathcal{B}, \Sigma)$ between the estimated EDR space and the true EDR space. The closer to one is $r(\widehat{B})$,

the better is the estimate. Note that for $K = 1$, the criterion $r(\widehat{B})$ corresponds to the squared cosine of the angle between \widehat{B} and β_1 .

Boxplots of this criterion are drawn on Figure 1(a). It appears that $\widehat{B}^{(3)}$ exhibits low squared trace correlation. This phenomenon can be explained by the heteroscedasticity in the third marginal model of (7). Even if $\widehat{B}^{(3)}$ is necessary to compute \widehat{V} and $\widehat{\widetilde{V}}$, the poor estimates of $B^{(3)}$ do not imply a significant loss in the squared trace correlations related to \widehat{V} and to $\widehat{\widetilde{V}}$. One can also observe that the weighting in wMSIR seems to improve the estimation of the EDR space since values of $r(\widehat{\widetilde{V}})$ are globally greater than those of $r(\widehat{V})$. This trend is confirmed in Figure 1(b) where the values of $r(\widehat{V})$ are plotted versus those of $r(\widehat{\widetilde{V}})$. It appears that wMSIR seems to be uniformly better than MSIR in this simulation.

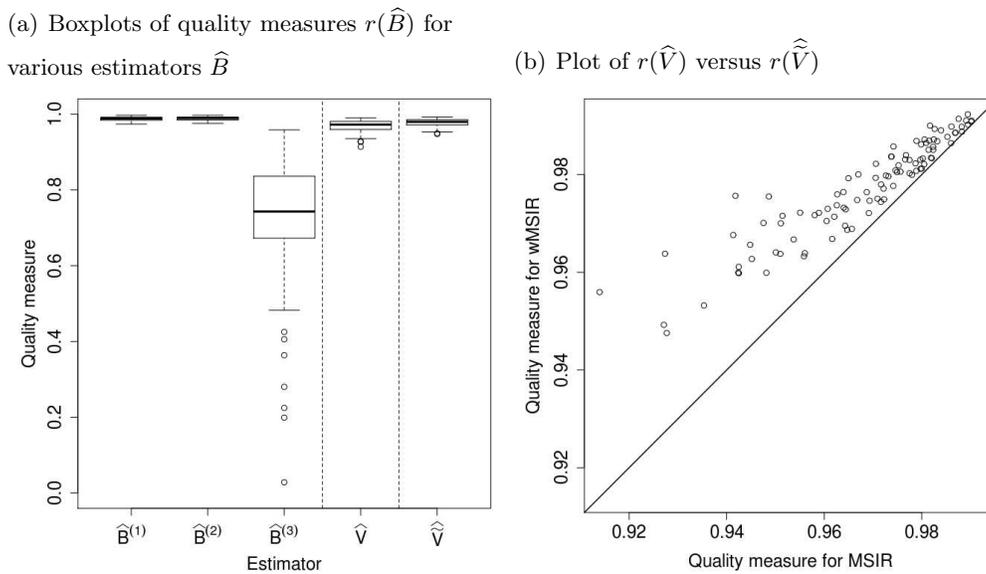
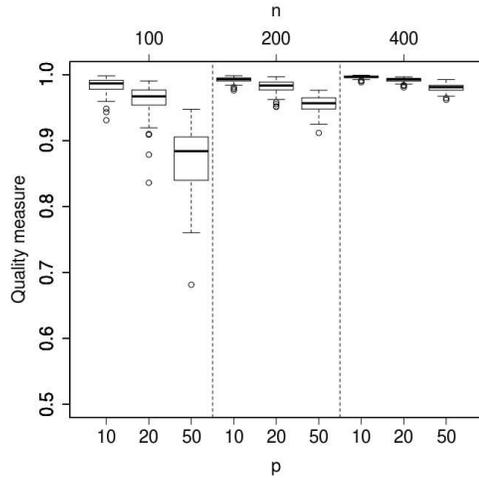


Figure 1: Comparison of estimators of \mathcal{B} on 100 samples from model (7) with $n = 100$ and $p = 20$. The line in (b) corresponds to the first bisecting line.

To study the sensitivity of MSIR with respect to n and p , several samples are generated for various values of these parameters. In Figures 2(a) and 2(b), we respectively draw boxplots of 100 values of $r(\widehat{V})$ and $r(\widehat{\widetilde{V}})$ for each pair (n, p) . Not surprisingly, estimated EDR spaces become closer to the true one when n increases. Moreover, one can also observe that estimates of the EDR space are more precise when p is small. This phenomenon can be explained by the fact that $p \times p$ matrices have to be estimated in both MSIR and wMSIR methods. Notice that for every value of (n, p) in Figure 2, estimates are very precise since there is no value of $r(\widehat{V})$ or $r(\widehat{\widetilde{V}})$ less than 0.65. Moreover, comparing Figure 2(a) with Figure 2(b), one can also observe that wMSIR seems to outperform MSIR.

(a) MSIR



(b) wMSIR

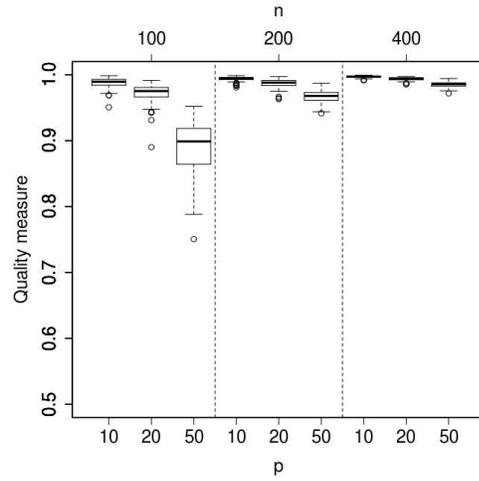
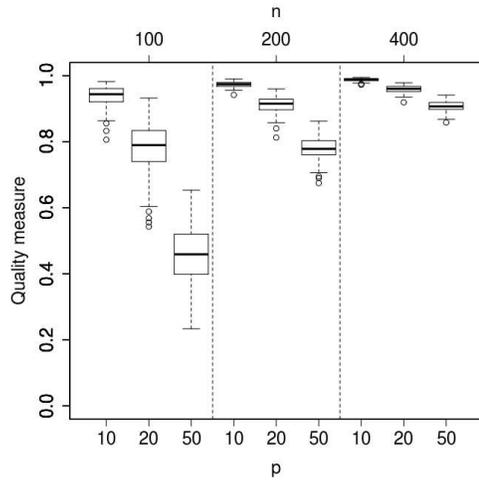


Figure 2: Boxplots of quality measure for MSIR method (a) and for wMSIR method (b), for 100 samples generated from model (7) for various values of n and p .

(a) MSIR



(b) wMSIR

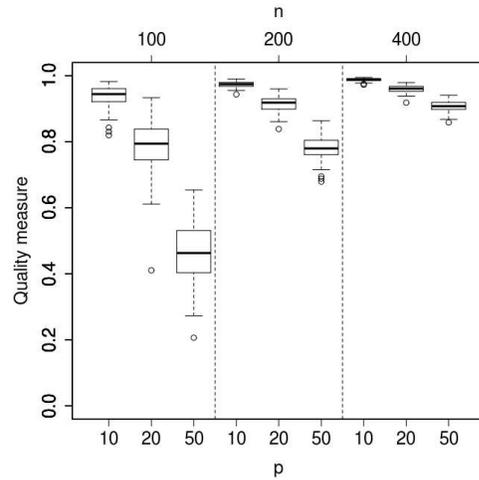


Figure 3: Boxplots of quality measure for MSIR method (a) and for wMSIR method (b), for 100 samples generated from model (8) for various values of n and p .

4.2 Multiple indices model

Consider now a more complex model than model (7). It is defined by:

$$\begin{cases} y^{(1)} &= \exp(x'\beta_1) \times x'\beta_2 + \varepsilon^{(1)}, \\ y^{(2)} &= (x'\beta_1) \times \exp(x'\beta_2) + \varepsilon^{(2)}, \end{cases} \quad (8)$$

where $\beta_1 = [\beta_{1,1}, \dots, \beta_{1,p}]'$, $\beta_2 = [\beta_{2,1}, \dots, \beta_{2,p}]'$, with $\beta_{1,i} = i \mathbb{I}(i \leq 5) + \mathbb{I}(i > 5)$ and $\beta_{2,i} = (-1)^{i-1}(1 + \mathbb{I}(i \in \{3, 4\}))$. Note that, in model (8), we clearly have $K = 2$.

Samples are generated from model (8) for various n and p . Then, these samples are used to estimate the corresponding EDR space with MSIR and wMSIR with $H = 10$ slices. This leads to boxplots of $r(\widehat{V})$ and $r(\widehat{\widehat{V}})$ displayed in Figure 3. We observe lower and more scattered values of $r(\widehat{V})$ and $r(\widehat{\widehat{V}})$ than in Figure 2. The complexity of the link function between y and x and the greater dimension K are believable reasons for this phenomenon. Differences between MSIR and wMSIR estimates are less significant in Figure 3 than in Figure 2. Apart from these features, Figure 3 provides identical evolutions of $r(\widehat{V})$ and $r(\widehat{\widehat{V}})$ with n and p to those observed for the single index model in Figure 2.

5 Clustering components of the response variable

In real data analysis, assuming model (2) with a common EDR space for all q components of y does not always seem realistic. Therefore, applying MSIR on y should not provide accurate results. However, it makes sense to assume that groups of components of y rely on model (2) but for different EDR spaces. The goal of this section is to propose a methodology in order to identify variables $y^{(j)}$ which share the same EDR space. Thus, we obtain clusters of components on which applying MSIR is sensible.

5.1 A multiple EDR spaces model

To detail this procedure, consider the following general model for multivariate response regression:

$$\left\{ \begin{array}{l} y^{(1)} = f_1(\mathcal{B}'_1 x, \varepsilon^{(1)}), \\ \vdots = \vdots \\ y^{(q_1)} = f_{q_1}(\mathcal{B}'_1 x, \varepsilon^{(q_1)}), \\ y^{(q_1+1)} = f_{q_1+1}(\mathcal{B}'_2 x, \varepsilon^{(q_1+1)}), \\ \vdots = \vdots \\ y^{(q_1+q_2)} = f_{q_1+q_2}(\mathcal{B}'_2 x, \varepsilon^{(q_1+q_2)}), \\ \vdots = \vdots \\ y^{(q)} = f_q(\mathcal{B}'_l x, \varepsilon^{(q)}), \end{array} \right. \quad (9)$$

where for every $i = 1, \dots, l$, \mathcal{B}_i is a $p \times K$ matrix, K is assumed to be known, $\text{Span}(\mathcal{B}_1) \neq \text{Span}(\mathcal{B}_2) \neq \dots \neq \text{Span}(\mathcal{B}_l)$ and $\sum_{i=1}^l q_i = q$. This means that writing this model as in (2) requires the number of columns of \mathcal{B} to be greater than K . However, performing marginal univariate SIR on each component $y^{(j)}$ of y leads to consistent estimates of each K -dimensional EDR space, since for $i = 1, \dots, l$, \mathcal{B}_i has K columns. Recalling notations of Section 3.2, we obtain q_1 estimates $\text{Span}(\hat{B}^{(1)}), \dots, \text{Span}(\hat{B}^{(q_1)})$ of $\text{Span}(\mathcal{B}_1)$, q_2 estimates $\text{Span}(\hat{B}^{(q_1+1)}), \dots, \text{Span}(\hat{B}^{(q_1+q_2)})$ of $\text{Span}(\mathcal{B}_2)$, and so on.

Without any loss of generality, assume that $l = 2$. Let us define $(j_1, j_2, j_3, j_4) \in \{1, \dots, q_1\}^2 \times \{q_1 + 1, \dots, q_1 + q_2\}^2$. For $j = 1, \dots, q$, recall that $P_{\hat{B}^{(j)}, \hat{\Sigma}}$ is the $\hat{\Sigma}$ -orthogonal projector onto $\text{Span}(\hat{B}^{(j)})$. According to Theorem 4 of Saracco (1997), we have that $P_{\hat{B}^{(j)}, \hat{\Sigma}} = P_{\mathcal{B}_1, \Sigma} + O_P(n^{-1/2})$, for $j \in \{j_1, j_2\}$ and $P_{\hat{B}^{(j)}, \hat{\Sigma}} = P_{\mathcal{B}_2, \Sigma} + O_P(n^{-1/2})$, for $j \in \{j_3, j_4\}$. Thus, $r(\hat{B}^{(j_1)}, \hat{\Sigma}, \hat{B}^{(j_2)}, \hat{\Sigma})$ tends to 1 in probability. Indeed, we have

$$\begin{aligned} r(\hat{B}^{(j_1)}, \hat{\Sigma}, \hat{B}^{(j_2)}, \hat{\Sigma}) &= \frac{1}{K} \text{Trace}(P_{\hat{B}^{(j_1)}, \hat{\Sigma}} P_{\hat{B}^{(j_2)}, \hat{\Sigma}}) \\ &= \frac{1}{K} \text{Trace}((P_{\mathcal{B}_1, \Sigma} + O_P(n^{-1/2}))(P_{\mathcal{B}_1, \Sigma} + O_P(n^{-1/2}))) \\ &= \frac{1}{K} \text{Trace}(P_{\mathcal{B}_1, \Sigma}) + O_P(n^{-1/2}) \\ &= 1 + O_P(n^{-1/2}). \end{aligned}$$

Similarly, $r(\hat{B}^{(j_3)}, \hat{\Sigma}, \hat{B}^{(j_4)}, \hat{\Sigma})$ tends to 1 in probability. This is not the case for $r(\hat{B}^{(j_1)}, \hat{\Sigma}, \hat{B}^{(j_3)}, \hat{\Sigma})$ because $\frac{1}{K} \text{Trace}(P_{\mathcal{B}_1, \Sigma} P_{\mathcal{B}_2, \Sigma}) < 1$.

This leads to the following criterion to cluster components of y : for $(j, j^*) \in \{2, \dots, q\} \times \{1, \dots, j-1\}$, components $y^{(j)}$ and $y^{(j^*)}$ are put in the same cluster if $r(\hat{B}^{(j)}, \hat{\Sigma}, \hat{B}^{(j^*)}, \hat{\Sigma})$ is close to 1. Afterwards, computing \hat{V} or \hat{V} for each obtained cluster is not time consuming since for $j = 1, \dots, q$, $\hat{B}^{(j)}$ have already been computed.

5.2 Illustration on simulated data

Consider model (9) with $q = 12$, $p = 20$ and $K = 1$. Define for $i = 1, \dots, p$, the i th component of respectively β_1 , β_2 and β_3 as $\beta_{1,i} := i \mathbb{I}(i \leq 5) + \mathbb{I}(i > 5)$, $\beta_{2,i} := 6 - i + 5 \lfloor \frac{i}{5} \rfloor$ and $\beta_{3,i} := (-1)^{i-1}(1 + \mathbb{I}(i \in \{3, 4\}))$. The random variable y is drawn from the following model:

$$\left\{ \begin{array}{l} y^{(1)} = x' \beta_1 + \varepsilon^{(1)}, \\ y^{(2)} = (x' \beta_1)^3 + 3\varepsilon^{(2)}, \\ y^{(3)} = x' \beta_1 (1 + \varepsilon^{(3)}), \\ y^{(4)} = x' ((1 - \theta_1) \beta_1 + \theta_1 \beta_2) + \varepsilon^{(4)}, \\ y^{(5)} = (x' ((1 - \theta_1) \beta_1 + \theta_1 \beta_2))^3 + 3\varepsilon^{(5)}, \\ y^{(6)} = x' ((1 - \theta_1) \beta_1 + \theta_1 \beta_2) (1 + \varepsilon^{(6)}), \\ y^{(7)} = x' ((1 - \theta_2) \beta_1 + \theta_2 \beta_3) + \varepsilon^{(7)}, \\ y^{(8)} = (x' ((1 - \theta_2) \beta_1 + \theta_2 \beta_3))^3 + 3\varepsilon^{(8)}, \\ y^{(9)} = x' ((1 - \theta_2) \beta_1 + \theta_2 \beta_3) (1 + \varepsilon^{(9)}), \\ y^{(10)} = \varepsilon^{(10)}, \\ y^{(11)} = \varepsilon^{(11)}, \\ y^{(12)} = \varepsilon^{(12)}, \end{array} \right. \quad (10)$$

based on model (7), where $(\theta_1, \theta_2) \in [0, 1]$ and for $j = 1, \dots, 12$, $\varepsilon^{(j)} \sim \mathcal{N}_1(0, 1)$.

A model with 6 clusters. We first choose $\theta_1 = \theta_2 = 1$ which produces the $l = 6$ following clusters:

$$\left\{ y^{(1)}, y^{(2)}, y^{(3)} \right\}, \left\{ y^{(4)}, y^{(5)}, y^{(6)} \right\}, \left\{ y^{(7)}, y^{(8)}, y^{(9)} \right\}, \left\{ y^{(10)} \right\}, \left\{ y^{(11)} \right\}, \left\{ y^{(12)} \right\}.$$

We plot, in Figure 4, values of $r(\hat{B}^{(j)}, \hat{\Sigma}, \hat{B}^{(j^*)}, \hat{\Sigma})$ for $(j, j^*) \in \{2, \dots, q\} \times \{1, \dots, j-1\}$, computed from a sample of size $n = 1000$. Darker squares correspond to values of $r(\hat{B}^{(j)}, \hat{\Sigma}, \hat{B}^{(j^*)}, \hat{\Sigma})$ close to 1. Thus, Figure 4 leads to cluster components $y^{(1)}$ and $y^{(2)}$ together as well as components $y^{(4)}$, $y^{(5)}$ and $y^{(6)}$. Components $y^{(7)}$ and $y^{(8)}$ can also be grouped together. It is tempting to put $y^{(3)}$ with $y^{(1)}$ and $y^{(2)}$ and to group $y^{(9)}$ with $y^{(8)}$ and $y^{(7)}$ because the related squared trace correlations are high but $r(\hat{B}^{(3)}, \hat{\Sigma}, \hat{B}^{(9)}, \hat{\Sigma})$ is approximately as high as them. Note also that for $j \in \{1, 2, 3\}$, we have $r(\hat{B}^{(3j)}, \hat{\Sigma}, \hat{B}^{(3j-1)}, \hat{\Sigma}) < r(\hat{B}^{(3j-2)}, \hat{\Sigma}, \hat{B}^{(3j-1)}, \hat{\Sigma})$ and $r(\hat{B}^{(3j)}, \hat{\Sigma}, \hat{B}^{(3j-2)}, \hat{\Sigma}) < r(\hat{B}^{(3j-2)}, \hat{\Sigma}, \hat{B}^{(3j-1)}, \hat{\Sigma})$. Recalling that for the considered values of j , $y^{(3j)}$ is the third component of each model (7) embedded in model (10), these inequalities can be explained by the heteroscedasticity in this component which leads to imprecise estimates of the relevant EDR direction as pointed

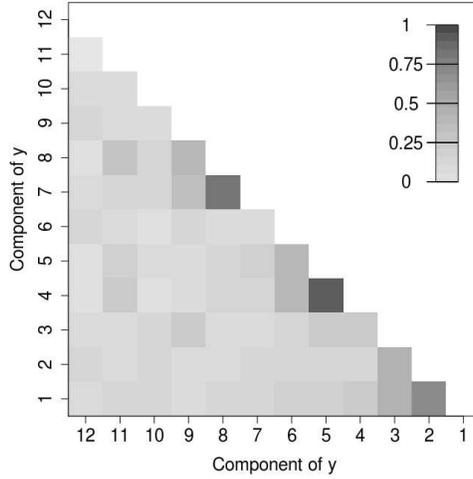


Figure 4: Values of $r(\hat{B}^{(j)}, \hat{\Sigma}, \hat{B}^{(j^*)}, \hat{\Sigma})$ in various shades of grays for $(j, j^*) \in \{2, \dots, q\} \times \{1, \dots, j-1\}$ and for a sample of size $n = 1000$ generated from model (10) with $\theta_1 = \theta_2 = 1$.

out on Figure 1(a). In addition, on Figure 4, component $y^{(11)}$ could be unexpectedly grouped with $y^{(4)}$ and $y^{(5)}$ or with $y^{(8)}$.

In this example, the interpretation of Figure 4 can easily be done because components of y are already clustered in the definition of the model. In other words, every component between two others that are related to the same EDR space belongs to a marginal model based on this EDR space. In practical cases, the components of y may not be ordered that way which means that the corresponding representation of the squared trace correlations may be cluttered. To tackle this problem, we use a agglomerative hierarchical clustering algorithm based on the dissimilarity $1 - r(\hat{B}^{(j)}, \hat{\Sigma}, \hat{B}^{(j^*)}, \hat{\Sigma})$ between $\hat{B}^{(j)}$ and $\hat{B}^{(j^*)}$.

A model with 5 clusters. We generate a new sample of size $n = 1000$ from model (10) with $\theta_1 = 1$ and $\theta_2 = 0$ which leads to $l = 5$ clusters:

$$\left\{ y^{(1)}, y^{(2)}, y^{(3)}, y^{(7)}, y^{(8)}, y^{(9)} \right\}, \left\{ y^{(4)}, y^{(5)}, y^{(6)} \right\}, \left\{ y^{(10)} \right\}, \left\{ y^{(11)} \right\}, \left\{ y^{(12)} \right\}.$$

The hierarchical clustering algorithm applied to the estimates $\hat{B}^{(j)}$ for $j = 1, \dots, q$ and produces the dendrogram of Figure 5(a). A classification directly based on this procedure would not be really accurate. For instance, in model (10), $y^{(11)}$ and $y^{(10)}$ belong to two different clusters. On Figure 5(a), to divide $y^{(11)}$ and $y^{(10)}$ into two groups, the tree has to be cut at a level around 0.75. This implies grouping $y^{(1)}, y^{(7)}, y^{(2)}$ and $y^{(8)}$ together and putting $y^{(3)}$ and $y^{(9)}$ in another group while components of both groups are actually related with the same EDR space. However, the dendrogram of Figure 5(a) allows to order components of y in such a way that those which

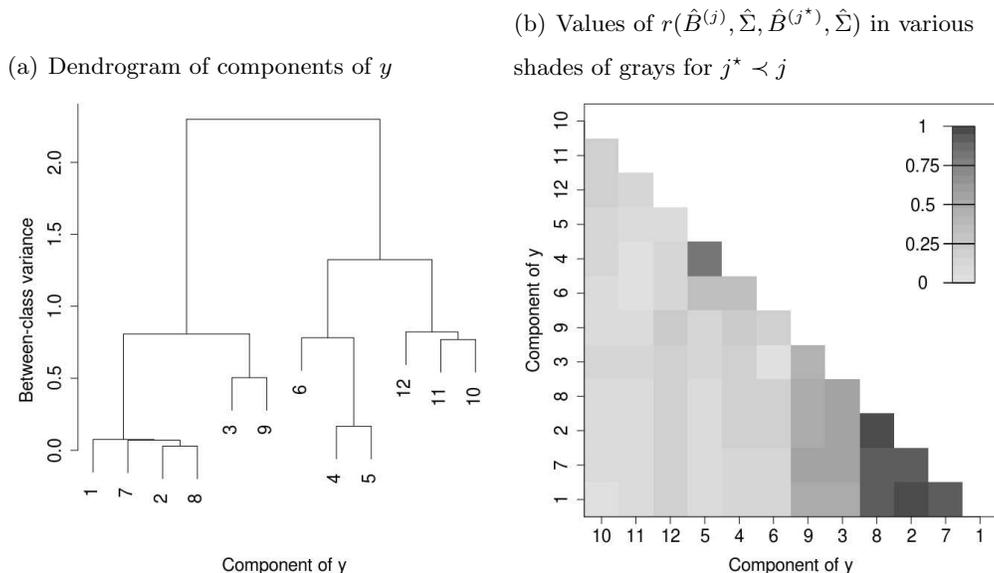


Figure 5: Clustering analysis for a sample of size $n = 1000$ generated from model (10) with $\theta_1 = 1$ and $\theta_2 = 0$.

are linked by high squared trace correlation are close from each other. Thus, in Figure 5(b), we displayed values of $r(\hat{B}^{(j)}, \hat{\Sigma}, \hat{B}^{(j^*)}, \hat{\Sigma})$ for $j^* \prec j$ where \prec denotes the ordering in Figure 5(a). It becomes clear, then, that components $y^{(1)}, y^{(7)}, y^{(2)}, y^{(8)}, y^{(3)}$ and $y^{(9)}$ should be clustered in the same group. Note that another cluster containing $y^{(6)}, y^{(4)}$ and $y^{(5)}$ can be made from Figure 5(b). Not surprisingly, we observe again that the squared trace correlation between components $y^{(3)}, y^{(6)}, y^{(9)}$ and the components that correspond to the group they respectively belong to is quite low. Finally, components $y^{(12)}, y^{(11)}$ and $y^{(10)}$ appears to form three distinct clusters.

6 A real data illustration

As an illustration, we consider a nonlinear inverse problem in remote sensing. The goal is to estimate the physical properties of surface materials on the planet Mars from hyperspectral data. The method is based on the estimation of the functional relationship between some physical parameters x and observed spectra y . We refer to Bernard-Michel, Douté, Fauvel, Gardes, and Girard (2009) for further details. We focus on an observation of the south pole of Mars at the end of summer 2003, collected by the French imaging spectrometer OMEGA on board the Mars Express Mission. A detailed analysis of this image (Douté, Schmitt, Langevin, Bibring, Altieri, Bellucci, Gondet, and Poulet (2007)) revealed that this portion of Mars mainly contains water ice, carbon dioxide and dust. This led to the physical modeling of individual spectra with a surface reflectance model

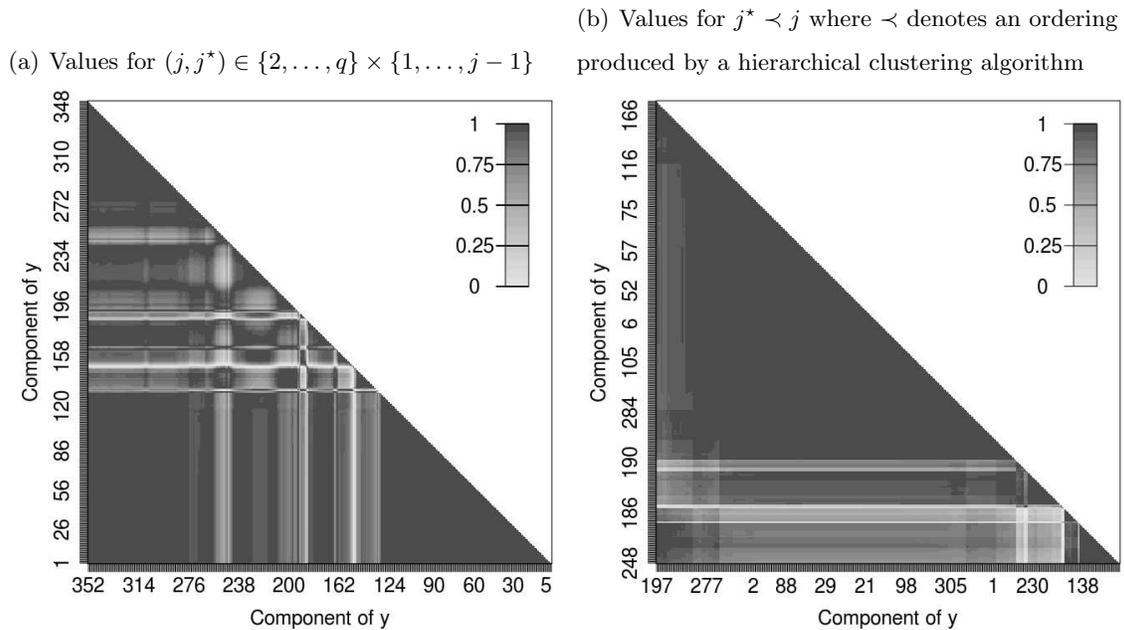


Figure 6: Values of $r(\hat{B}^{(j)}, \hat{\Sigma}, \hat{B}^{(j^*)}, \hat{\Sigma})$ in various shades of grays for hyperspectral data.

$y = g(x)$. The $q = 3$ parameters $x^{(1)}$, $x^{(2)}$ and $x^{(3)}$ are respectively the proportion of carbon dioxide, the proportion of dust, and the grain size of water ice. Let us note that the proportion of water is equal to $1 - x^{(1)} - x^{(2)}$. Each spectra y is made of $p = 352$ wavelengths. The link function g has no close-form expression, but it can be computed thanks to a dedicated software. This yields the simulation of a sample $\{(x_i, y_i), i = 1, \dots, n\}$ of size $n = 6400$.

We ran the clustering procedure described in the above section associated to wMSIR with $H = 10$ slices. The clustering results are depicted on Figure 6(b). Two clusters of wavelengths have been identified, corresponding to two different orientations of \hat{v}_1 . It appears on Figure 7(a) that, in the first cluster, only the proportion of dust $x^{(2)}$ has an important contribution to the EDR direction. In the second cluster, the EDR direction is determined by $x^{(1)} + x^{(2)}$ which corresponds to one minus the proportion of water. Let us note that the grain size of water ice $x^{(3)}$ does not appear in the EDR directions. Figure 7(b) permits to visualize the clustering of the wavelengths: It reveals which wavelengths are more sensible to the presence of water ice or dust.

7 Concluding remarks

In this paper, we proposed a new multivariate SIR approach for estimating the EDR space. The idea consists in performing first several independent univariate SIR analyzes. A common EDR space is then deduced from the marginal ones by maximizing the proximity criterion defined in (4).

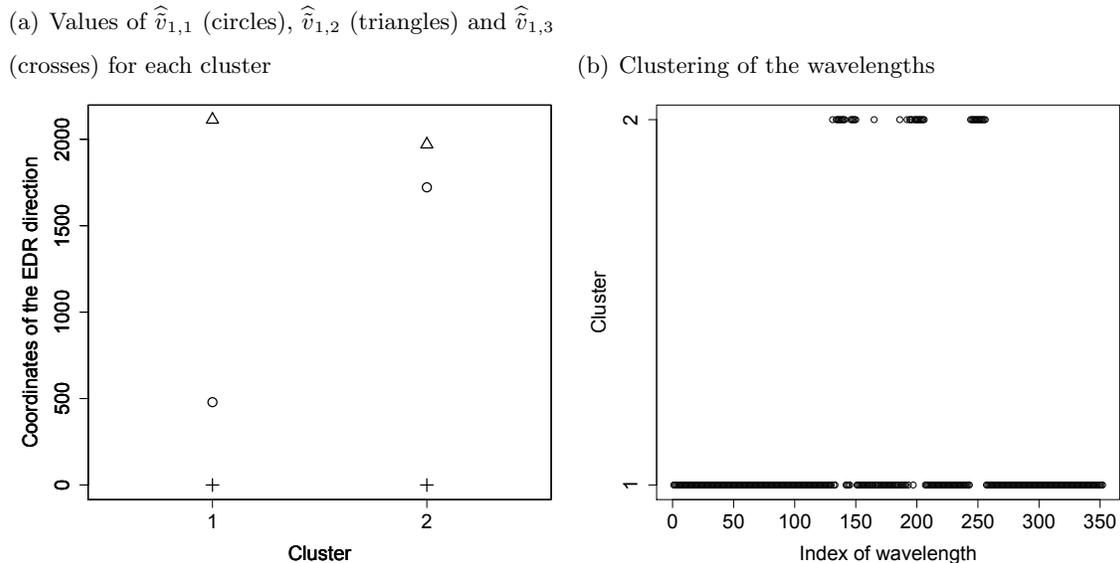


Figure 7: Clustering of the components of y and estimates $\hat{v}_1 = [\hat{v}_{1,1}, \hat{v}_{1,2}, \hat{v}_{1,3}]'$ of the EDR direction for each cluster.

This optimization problem benefits from a closed-form solution.

Let us highlight that this two-step approach can be applied to any variant of the SIR method. For instance, it permits to build multivariate regularized SIR approaches from [Bernard-Michel, Gardes, and Girard \(2009\)](#), multivariate SIR_α approaches from [Gannoun and Saracco \(2003\)](#) or multivariate kernel SIR methods from [Wu \(2008\)](#).

This method can also be run with a graphical procedure that cluster components of the response variable depending on the EDR space they are related with. Therefore, the approach we described allows to deal with datasets that come from a model that includes several different EDR spaces. In addition, we noticed that estimating the EDR space does not cost a significant amount of computational time when it is done in the context of this clustering procedure. R codes are available on request from the authors.

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