A new sliced inverse regression method for multivariate response

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Abstract

A semiparametric regression model of a q-dimensional multivariate response $\mathbf{y}$ on a p-dimensional covariate $\mathbf{x}$ is considered. A new approach is proposed based on sliced inverse regression (SIR) 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. The choice of the dimension of the EDR space is discussed. Moreover, a way to cluster components of $\mathbf{y}$ related to the same EDR space is provided. Thus, the proposed multivariate SIR method can be used properly on each cluster instead of blindly applying it on all components of $\mathbf{y}$. The numerical performances of multivariate SIR are illustrated on a simulation study. Applications to a remote sensing dataset and to the Minneapolis elementary schools data are also provided. Although the proposed methodology relies on SIR, it opens the door for new regression approaches with a multivariate response. They could be built similarly based on other reduction dimension methods.

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 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 $\mathbf{x}$ 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

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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 or smoothing splines approaches for instance.

In this paper, a q-dimensional response variable $\mathbf{y}$ 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 $\mathbf{x}$ without loss of information is to identify linear combinations $\beta_1'\mathbf{x}, \ldots, \beta_K'\mathbf{x}$ such that

$$\mathbf{y} \perp \mathbf{x} | (\beta_1'\mathbf{x}, \ldots, \beta_K'\mathbf{x}), \tag{1}$$

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

$$\mathbf{y} = f(\mathbf{B}'\mathbf{x}, \boldsymbol{\varepsilon}), \tag{2}$$

where $f : \mathbb{R}^{K+r} \to \mathbb{R}^q$ is an arbitrary and unknown link function, $\boldsymbol{\varepsilon}$ is a r-dimensional random error variable independent of $\mathbf{x}$ (with $r \geq 1$). Li et al. (2003) consider a regression model with an additive error term: $\mathbf{y} = g(\mathbf{B}'\mathbf{x}) + \boldsymbol{\varepsilon}$, where g is an unknown link function taking its values in $\mathbb{R}^q$.

In the following, a slightly more restrictive regression model is considered:

$$\begin{cases} y^{(1)} = f_1(\mathbf{B}'\mathbf{x}, \varepsilon^{(1)}), \\ \vdots \\ y^{(q)} = f_q(\mathbf{B}'\mathbf{x}, \varepsilon^{(q)}), \end{cases} \tag{3}$$

where for $j = 1, \ldots, q$, $y^{(j)}$ (resp. $\varepsilon^{(j)}$) stands for the jth component of $\mathbf{y}$ (resp. of $\boldsymbol{\varepsilon}$) and the link function f_j is an unknown real-valued function. For $j = 1, \ldots, q$, $\mathbf{B}^{(j)}$ is defined as a matrix containing a basis of the (marginal) EDR space from the marginal regression of $y^{(j)}$ given $\mathbf{x}$. The

following marginal condition is assumed:

$$\text{(MC)} \quad \forall j \in \{1, \ldots, q\},\ \text{Span}(\mathbf{B}^{(j)}) = \text{Span}(\mathbf{B}).$$

In this paper, we propose an approach to estimate Span($\mathbf{B}$). It is based on combining information from the marginal regression of each component $y^{(j)}$ of $\mathbf{y}$. We shall also discuss the estimation of the EDR space when (MC) does not hold, by considering model (4) presented thereafter.

Remark 1. The information from the marginal regression is sufficient to recover the whole EDR space in model (3). However, this is not always the case when working with model (2). Let us illustrate this point with the following regression model proposed by Zhu et al. (2010b):

$$\begin{pmatrix} y^{(1)} \\ y^{(2)} \end{pmatrix} \sim \mathcal{N}_2 \left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \sin(\mathbf{B}'\mathbf{x}) \\ \sin(\mathbf{B}'\mathbf{x}) & 1 \end{pmatrix} \right).$$

In this example, the information of interest is only in the correlations between the components of the response variables. Consequently, none of the available marginal regression provides useful information about the EDR space while considering the entire $\mathbf{y}$ allows to recover it.

The vectors β_k are not individually identifiable neither in model (2), nor in the more restrictive one (3). Thus, the main objective is to estimate a basis of the K-dimensional EDR space. When $q = 1$, many numerical methods have been introduced to achieve this goal. Let us mention four 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)), sliced average variance estimation (see for details Cook (2000), Prendergast (2007) or Shao et al. (2009)) and minimum average variance estimation (Xia et al. (2002), Cížek and Härdle (2006)). For the sake of simplicity, we shall only focus here on the SIR approach which is based on a property of the first moment of the inverse distribution of $\mathbf{x}$ given $\mathbf{y}$. The methodology presented in this paper can, however, be seen as a framework to construct multivariate versions of the aforementioned sufficient dimension reduction techniques.

To find an estimate of the EDR space, SIR requires the following linearity condition:

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

One can observe that the linearity condition does not involve the response variable $\mathbf{y}$ and only concerns the distribution of the covariate $\mathbf{x}$. Let us mention that when the distribution of $\mathbf{x}$ 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. Hino et al. (2013) recently used an estimator of the

differential entropy of $\mathbf{x}$ to get rid of (LC). Scrucca (2011) relies on SIR to study a parametric model without assuming this condition. To conclude this brief discussion on the linearity condition, using a Bayesian argument of Hall and Li (1993), it can be shown that (LC) approximately holds for many high-dimensional datasets (that is when p is large).

As previously mentioned, the proposed approach to estimate the EDR space relies on combining estimates from the marginal regressions of model (3). Moreover, one can naturally take the information from these regressions into account to detect if a common EDR space really exists for all the components of $\mathbf{y}$ as in model (3). Otherwise, one shall consider the following more general regression model for multivariate response regression:

$$\begin{cases} y^{(1)} &= f_1(\mathbf{B}_1'\mathbf{x}, \varepsilon^{(1)}), \\ \vdots &= \vdots \\ y^{(q_1)} &= f_{q_1}(\mathbf{B}_1'\mathbf{x}, \varepsilon^{(q_1)}), \\ y^{(q_1+1)} &= f_{q_1+1}(\mathbf{B}_2'\mathbf{x}, \varepsilon^{(q_1+1)}), \\ \vdots &= \vdots \\ y^{(q_1+q_2)} &= f_{q_1+q_2}(\mathbf{B}_2'\mathbf{x}, \varepsilon^{(q_1+q_2)}), \\ \vdots &= \vdots \\ y^{(q)} &= f_q(\mathbf{B}_L'\mathbf{x}, \varepsilon^{(q)}), \end{cases} \tag{4}$$

where, for every $l = 1, \ldots, L$, $\mathbf{B}_l$ is a $p \times K$ matrix, K is assumed to be known, $\text{Span}(\mathbf{B}_1) \neq \text{Span}(\mathbf{B}_2) \neq \ldots \neq \text{Span}(\mathbf{B}_L)$ and $\sum_{l=1}^{L} q_l = q$. This means that writing this model as in (3) requires the number of columns of $\mathbf{B}$ to be greater than K. Let us highlight that the resulting model does not satisfy (MC). Although methods exist to estimate $\text{Span}(\mathbf{B})$ without this assumption, estimating $\mathbf{B}_1, \ldots, \mathbf{B}_L$ seems anyway more appropriate than seeking $\mathbf{B}$ when trying to reduce as much as possible the dimension of a model. One then needs to cluster the components of $\mathbf{y}$ associated with the same EDR space. Therefore, for each identified cluster of components, one can use only these components to estimate the corresponding (common) EDR space. In a more general case, one can also assume that the dimension K is specific for each $\mathbf{B}_l$.

The goal of this paper is twofold. First, we introduce a new multivariate SIR approach for estimating the K-dimensional EDR space which is common to the q components of the multivariate response variable in model (3). Then, we propose a way to cluster the components of $\mathbf{y}$ associated with the same EDR space in model (4). This permits to apply properly our multivariate SIR on each cluster instead of blindly applying it on all the components of $\mathbf{y}$.

The paper is organized as follows. Section 2 gives 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. Both these methods rely on a tuning parameter H, called the number of slices. The choice of H and of the dimension K is discussed in Section 3.5. Practical methods to investigate the possible existence of a common EDR space for $\mathbf{y}$ and to detect and identify clusters of components of $\mathbf{y}$ are proposed in Section 3.6. Numerical results based on simulations are exhibited in Section 4 in order to show the good behavior of MSIR and wMSIR approaches and the usefulness of the diagnostic and clustering procedures on the components of $\mathbf{y}$. In Section 5, two real datasets are considered: the first one concerns hyperspectral remote sensing while the second one is the widely studied Minneapolis elementary schools dataset. Finally, concluding remarks are given in Section 6.

2. Brief review of univariate and multivariate SIR approaches

In this section, the regression model (3) is considered. 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

We focus here on a univariate response (i.e. $q = 1$).

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

Let T denote a monotone (but not necessarily strictly monotone) transformation of y. Assume that $\mathbb{E}((\mathbf{x}'\mathbf{x})^2) < \infty$ and let $\mu = \mathbb{E}(\mathbf{x})$ and $\mathbf{\Sigma} = \mathbb{V}(\mathbf{x})$ supposed to be invertible. Under model (3) and (LC), Li (1991) established the following geometric property: the centered inverse regression curve, $\mathbb{E}(\mathbf{x}|T(y)) - \mu$ as y varies, is contained in the linear subspace of $\mathbb{R}^p$ spanned by $\mathbf{\Sigma B}$. A straightforward consequence is that the covariance matrix,

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

is degenerated in any direction $\mathbf{\Sigma}$-orthogonal to Span($\mathbf{B}$). Therefore, the eigenvectors associated with the non-null eigenvalues of $\mathbf{\Sigma}^{-1}\mathbf{\Gamma}$ 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 $s_1, \ldots, s_h, \ldots, s_H$. With such a transformation T, the subspace recovered through a

slicing (based on the inverse $\mathbf{x}|T(y)$ function) may fall short of the space recovered through y in its entirety (based on the $\mathbf{x}|y$ function). However, the main advantage of the slicing is that the matrix of interest can be rewritten as

$$\mathbf{\Gamma} = \sum_{h=1}^{H} p_h(\mathbf{m}_h - \mu)(\mathbf{m}_h - \mu)',$$

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

Estimation process. In the usual statistical framework, when a sample $\{(\mathbf{x}_i, y_i), i = 1, \ldots, n\}$ is available, it is straightforward to estimate the matrices $\mathbf{\Sigma}$ and $\mathbf{\Gamma}$, 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 some details on this method.

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 et al. (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 et al. (2010) or Azaïs et al. (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

et al. (2006), Scrucca (2007), Li and Yin (2008), Bernard-Michel et al. (2008). Amato et al. (2006) developed an extension of SIR when $\mathbf{x}$ is a sampled function. 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 et al. (2007). Conditional quantiles of y given $\mathbf{x}$ can be estimated by combining SIR with kernel regression, see Gannoun et al. (2004).

2.2. Multivariate SIR

In the multivariate framework (that is when $\mathbf{y} \in \mathbb{R}^q$ with $q > 1$), Aragon (1997), Li et al. (2003) considered several estimation methods of the EDR space based on SIR. Note that Barreda et al. (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 $\mathbf{x}$ given $T(\mathbf{y})$.

Complete slicing and marginal slicing approaches. In the complete slicing method, the SIR procedure is directly applied on $\mathbf{y}$. To build slices of nearly equal sizes, the following recursive approach is used. The first component of $\mathbf{y}$ is sliced. Then, each slice is separately sliced again according to the next component of $\mathbf{y}$, and so on. This extension of univariate SIR to multivariate $\mathbf{y}$ 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 $\mathbf{y}$ 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 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 the multivariate framework by introducing a new slicing of $\mathbf{y}$ based on k-means method. The corresponding method is called k-means inverse regression (KIR).

A natural way to circumvent the curse of dimensionality of the complete slicing approach is proposed in the marginal slicing procedure which consists in applying SIR on a transformation of $\mathbf{y}$ 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 $\mathbf{y}$ may not lead to recover as many EDR directions as slicing the entire $\mathbf{y}$.

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 (PMS) method is to consider the q univariate marginal SIR of each component $y^{(j)}$ of $\mathbf{y}$ on $\mathbf{x}$ and to combine the

corresponding matrices of interest $\mathbf{\Gamma}^{(j)} := \mathbb{V}(\mathbb{E}(\mathbf{x}|T_j(y^{(j)})))$ in the following pooling:

$$\mathbf{\Gamma}_P = \sum_{j=1}^{q} w_j \mathbf{\Gamma}^{(j)}, \tag{5}$$

for positive weights w_j. It has been shown that the eigenvectors associated with the non-null K eigenvalues of $\mathbf{\Sigma}^{-1}\mathbf{\Gamma}_P$ 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 $\mathbf{y}$. 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. For $j = 1, \ldots, q$, rather than constructing $\mathbf{\Gamma}^{(j)}$ from $y^{(j)}$, one can also build it from a linear combination $\tau'\mathbf{y}$ of $\mathbf{y}$. This method which is called projective resampling was introduced by Li et al. (2008). To ensure good performances, the number of linear combinations to handle should be greater than the sample size n.

Some other multivariate SIR approaches. Bura and Cook (2001) introduced the 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 when p is large and to rationalize the slicing step, Li et al. (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 $\mathbf{x}$ or the response variable $\mathbf{y}$. The SIR variates are the variables $b'\mathbf{x}$ formed by an EDR direction b obtained with SIR. The MP variates $\theta'\mathbf{y}$ are defined as those minimizing the ratio $\mathbb{E}[\mathbb{V}(\theta'\mathbf{y}|\mathbf{x})]/\mathbb{V}(\theta'\mathbf{y})$, where $\mathbb{V}(\theta'\mathbf{y}|\mathbf{x})$ is the associated prediction mean squared error of the best nonlinear prediction $\mathbb{E}[\theta'\mathbf{y}|\mathbf{x}]$ for the squared error loss. Equivalently, due to ANOVA identity, the MP variates can be found by maximizing the ratio $\mathbb{V}(\mathbb{E}[\theta'\mathbf{y}|\mathbf{x}])/\mathbb{V}(\theta'\mathbf{y})$, which conducts to the same eigenvalue decomposition as the SIR approach except for the exchanged roles of $\mathbf{x}$ and $\mathbf{y}$. 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 $\widehat{\theta}$ or $\widehat{b}$ respectively obtained by the slicing of SIR variates or MP variates constructed at the previous step. Li et al. (2003) proposed an iterative procedure for the alternating SIR and showed that choosing the canonical directions as an initial projection of the $\mathbf{y}$'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 MSIR approach is first described in Section 3.1. Let us highlight that it does not rely on SIR and can thus be a starting point for the definition of other

multivariate inverse regression methods. Then, the corresponding sample version based on SIR is given in Section 3.2 and some asymptotic results are derived in Section 3.3. We then modify MSIR to handle a weighting in the components of $\mathbf{y}$ in Section 3.4. Methods to choose K and H are discussed in Section 3.5. Finally, procedures to withdraw or cluster components of $\mathbf{y}$ are detailled in Section 3.6.

3.1. Population version

Let us assume that the dimension K of the EDR space is known. Let $P_{\mathbf{M},\mathbf{\Sigma}}$ be the $\mathbf{\Sigma}$-orthogonal projector on the linear subspace spanned by the columns of a $p \times K$ matrix $\mathbf{M}$. A proximity measure between two projectors $P_{\mathbf{M}_1,\mathbf{\Sigma}_1}$ and $P_{\mathbf{M}_2,\mathbf{\Sigma}_2}$ is given by the squared trace correlation:

$$r(\mathbf{M}_1, \mathbf{\Sigma}_1, \mathbf{M}_2, \mathbf{\Sigma}_2) := \frac{1}{K} \text{Trace}\left(P_{\mathbf{M}_1,\mathbf{\Sigma}_1} P_{\mathbf{M}_2,\mathbf{\Sigma}_2}\right),$$

for full column rank matrices $\mathbf{M}_1$ and $\mathbf{M}_2$.

For $j = 1, \ldots, q$, recall that $\mathbf{B}^{(j)}$ is a $p \times K$ matrix spanning the EDR space from the marginal regression of $y^{(j)}$ given $\mathbf{x}$. It is assumed to be $\mathbf{\Sigma}$-orthonormal. Let $\mathbf{D}$ be a $p \times K$ matrix such that $\mathbf{D}'\mathbf{\Sigma}\mathbf{D} = \mathbf{I}_K$, where $\mathbf{I}_K$ is the identity matrix of order K. Let $Q(\mathbf{D}, \mathbf{B}^{(1)}, \ldots, \mathbf{B}^{(q)})$ denote the following proximity measure between Span($\mathbf{D}$) and the q marginal EDR spaces Span($\mathbf{B}^{(1)}$), ..., Span($\mathbf{B}^{(q)}$):

$$Q(\mathbf{D}, \mathbf{B}^{(1)}, \ldots, \mathbf{B}^{(q)}) := \frac{1}{q} \sum_{j=1}^{q} r\left(\mathbf{D}, \mathbf{\Sigma}, \mathbf{B}^{(j)}, \mathbf{\Sigma}\right). \tag{6}$$

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

Let us now consider the following optimization problem:

$$\mathbf{V} := \arg \max_{\mathbf{D} \in \mathcal{M}_{\mathbf{\Sigma}}} Q(\mathbf{D}, \mathbf{B}^{(1)}, \ldots, \mathbf{B}^{(q)}), \tag{7}$$

where $\mathcal{M}_{\mathbf{\Sigma}}$ is the set of $\mathbf{\Sigma}$-orthogonal $p \times K$ matrices. A solution of (7) is given by the following theorem.

Theorem 1. *Under model (3) and assumption (MC), the $p \times K$ matrix $\mathbf{V}$ is formed by the eigenvectors $v_1, \ldots, v_K$ associated with the K non-null eigenvalues of $\mathbb{B}\mathbb{B}'\mathbf{\Sigma}$ where $\mathbb{B}$ is the $p \times (Kq)$ matrix defined as $\mathbb{B} := [\mathbf{B}^{(1)}, \ldots, \mathbf{B}^{(q)}]$. Moreover, we have Span($\mathbf{V}$) = Span($\mathbf{B}$) where Span($\mathbf{B}$) is the EDR space.*

The proof is given in Appendix A.2. From Theorem 1, one can estimate a basis of the EDR space based on estimators of matrices $\mathbb{B}$ and $\mathbf{\Sigma}$. This is the goal of the next subsection where $\mathbb{B}$ is estimated using SIR.

3.2. Sample version

Let $\{(\mathbf{x}_i, \mathbf{y}_i),\ i = 1, \ldots, n\}$ be a sample of independent observations from model (3). Each $\mathbf{y}_i$ is a q-dimensional random variable. Le us assume that the sample size n is larger than the dimension p of each covariate $\mathbf{x}_i$.

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

In order to estimate the matrix $\mathbb{B}$, we have to estimate each $p \times K$ matrix $\mathbf{B}^{(j)}$ with usual univariate SIR from the subsample $\{(\mathbf{x}_i, y_i^{(j)}),\ i = 1, \ldots, n\}$ where $y_i^{(j)}$ stands for the jth component of $\mathbf{y}_i$. To this end, let us assume that the support of $y^{(j)}$ is partitioned into a fixed number of slices denoted by $s_1^{(j)}, \ldots, s_h^{(j)}, \ldots, s_{H^{(j)}}^{(j)}$. Let $p_h^{(j)} := \mathbb{P}\left(y^{(j)} \in s_h^{(j)}\right)$ and $\mathbf{m}_h^{(j)} := \mathbb{E}\left(\mathbf{x} | y^{(j)} \in s_h^{(j)}\right)$. Thus, the matrix $\mathbf{\Gamma}^{(j)} := \sum_{h=1}^{H^{(j)}} p_h^{(j)}(\mathbf{m}_h^{(j)} - \mu)(\mathbf{m}_h^{(j)} - \mu)'$ is estimated by $\widehat{\mathbf{\Gamma}}^{(j)} := \sum_{h=1}^{H^{(j)}} \hat{p}_h^{(j)}(\widehat{\mathbf{m}}_h^{(j)} - \bar{\mathbf{x}})(\widehat{\mathbf{m}}_h^{(j)} - \bar{\mathbf{x}})'$ with $\hat{p}_h^{(j)} := \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}[y_i^{(j)} \in s_h^{(j)}]$ and $\widehat{\mathbf{m}}_h^{(j)} := \frac{1}{n\hat{p}_h^{(j)}}\sum_{i=1}^{n} \mathbf{x}_i \mathbb{I}[y_i^{(j)} \in s_h^{(j)}]$ where $\mathbb{I}[.]$ is the indicator function. Assuming that $\mathbf{\Gamma}^{(j)}$ has K non-null eigenvalues, we build the $\mathbf{\Sigma}$-orthonormal basis $\mathbf{B}^{(j)}$ of the marginal EDR space by binding the K eigenvectors of $\mathbf{\Sigma}^{-1}\mathbf{M}$ corresponding to its K largest eigenvalues. Then, $\mathbf{B}^{(j)}$ is estimated by

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

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

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

Finally, a $\widehat{\mathbf{\Sigma}}$-orthonormal estimated basis of the EDR space is given by the vectors $\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_K$ defined as the eigenvectors associated with the K largest eigenvalues of the matrix $\widehat{\mathbb{B}}\widehat{\mathbb{B}}'\widehat{\mathbf{\Sigma}}$ and we write $\widehat{\mathbf{V}} := [\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_K]$.

Remark 2. Similarly to the pooled marginal slicing (PMS) presented in Section 2.2, MSIR relies on the univariate version of SIR, applied to each component of $\mathbf{y}$. While both methods need estimates of $\mathbf{\Gamma}^{(1)}, \ldots, \mathbf{\Gamma}^{(q)}$, estimates of $\mathbf{B}^{(1)}, \ldots, \mathbf{B}^{(q)}$ are only required by MSIR. Computing such estimates is useful to explore the relations between components of $\mathbf{y}$ as explained in Section 3.6.

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 $\{(\mathbf{x}_i, \mathbf{y}_i),\ i = 1, \ldots, n\}$ are independently drawn from a given regression model.

- (A2) For each component $y^{(j)}$ of $\mathbf{y}$, the support is partitioned into a fixed number $H^{(j)}$ of slices such that $p_h^{(j)} > 0$ for $h = 1, \ldots, H^{(j)}$.

- (A3) For $j = 1, \ldots, q$ and $h = 1, \ldots, H^{(j)}$, $n_h^{(j)} \to \infty$ as $n \to \infty$.

Theorem 2. *Under model (3) and assumptions (MC), (LC) and (A1)-(A3), if for $j = 1, \ldots, q$, $\mathbf{\Gamma}^{(j)}$ has K non-null eigenvalues, we have, for $k = 1, \ldots, K$,*

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

that is, the estimated EDR space Span($\widehat{\mathbf{V}}$) converges in probability to the EDR space.

The poof is given in Appendix A.3.

Remark 3. Using Delta-method and asymptotic results of Tyler (1981) and Saracco (1997), it is possible to obtain the asymptotic normality of

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

where vec($\mathbf{M}$) stands for the "vec" operator applied to matrix $\mathbf{M}$. More precisely, this operator rearranges the p^2 elements of $\mathbf{M}$ in the form of a p^2-dimensional column vector by stacking the p columns of $\mathbf{M}$ 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 $\hat{\mathbf{v}}_k$, associated with eigenvalues assumed to be different (that is $\lambda_1 > \cdots > \lambda_K > 0$).

3.4. A weighted version of MSIR

Following the idea used in pooled marginal slicing approach in which the matrix of interest $\mathbf{\Gamma}_P$ is a weighted average of the marginal matrices $\mathbf{\Gamma}^{(j)}$, 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 $\mathbf{y}$).

More precisely, for $j = 1, \ldots, q$, let $\lambda_k^{(j)}, k = 1, \ldots, p$ be the eigenvalues of the eigendecomposition $\mathbf{\Sigma}^{-1}\mathbf{\Gamma}^{(j)}v_k^{(j)} = \lambda_k^{(j)}v_k^{(j)}$ where $\lambda_1^{(j)} \geq \lambda_2^{(j)} \geq \cdots \geq \lambda_p^{(j)}$. Let us define, for each component $y^{(j)}$ of $\mathbf{y}$, 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, the following $qK \times qK$ matrix of weights is introduced:

$$\mathbb{W} = \text{diag}(\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(j)}, \ldots, \mathbf{W}^{(q)}),$$

with $\mathbf{W}^{(j)} = \frac{\pi^{(j)}}{\pi_\star}\mathbf{I}_K$ for $j = 1, \ldots, q$. Note that, from a theoretical point of view, under model (3) and (LC), the matrix of weights is given by $\mathbb{W} = \frac{1}{q}\mathbf{I}_{qK}$ since $\lambda_k^{(j)} = 0$ for $j = 1, \ldots, q$ and $k = K+1, \ldots, p$.

The population version of wMSIR consists in noticing that the eigenvectors $\tilde{v}_1, \ldots, \tilde{v}_K$ associated with the K largest eigenvalues of the $\mathbf{\Sigma}$-symmetric matrix $\mathbb{B}\mathbb{W}\mathbb{B}'\mathbf{\Sigma}$ span the EDR space. We write $\widetilde{\mathbf{V}} := [\tilde{v}_1, \ldots, \tilde{v}_K]$. To show this result, one can proceed analogously to the proof of Theorem 1.

Let $\hat{\lambda}_k^{(j)}$ be the kth eigenvalue of $\widehat{\mathbf{\Sigma}}^{-1}\widehat{\mathbf{\Gamma}}^{(j)}$. The sample version of wMSIR is obtained by substituting the empirical matrices $\widehat{\mathbb{B}}$, $\widehat{\mathbb{W}}$ and $\widehat{\mathbf{\Sigma}}$ for their theoretical counterparts $\mathbb{B}$, $\mathbb{W}$ and $\mathbf{\Sigma}$, where $\widehat{\mathbb{W}} = \text{diag}(\widehat{\mathbf{W}}^{(1)}, \ldots, \widehat{\mathbf{W}}^{(q)})$ with, for $j = 1, \ldots, q$, $\widehat{\mathbf{W}}^{(j)} = \frac{\hat{\pi}^{(j)}}{\hat{\pi}_\star}\mathbf{I}_K$, $\hat{\pi}^{(j)} = \frac{\sum_{k=1}^K \hat{\lambda}_k^{(j)}}{\sum_{k=1}^p \hat{\lambda}_k^{(j)}}$ and $\hat{\pi}_\star = \sum_{j=1}^q \hat{\pi}^{(j)}$. Therefore, one can get the corresponding estimated EDR directions $\widehat{\widehat{\mathbf{V}}} := \left[\widehat{\widehat{\mathbf{v}}}_1, \ldots, \widehat{\widehat{\mathbf{v}}}_K\right]$.

Theorem 3. *Under model (3) and assumptions (MC), (LC) and (A1)-(A3), if for $j = 1, \ldots, q$, $\mathbf{\Gamma}^{(j)}$ has K non-null eigenvalues, we have, for $k = 1, \ldots, K$,*

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

that is, the estimated EDR space Span($\widehat{\widehat{\mathbf{V}}}$) converges in probability to the EDR space.

The proof is given in Appendix A.4.

3.5. Discussion on the choice of K and H

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 $\beta_k'\mathbf{x}$ in model (1) is a priori unknown and hence must be determined from the data. In addition, the number of slices H in MSIR has to be chosen.

Several approaches to determine K 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), Barrios and Velilla (2007) or 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 $\widehat{\mathbb{B}}\widehat{\mathbb{B}}'\widehat{\mathbf{\Sigma}}$: the idea is to determine the number of the significantly non-null eigenvalues.

In the univariate response model, Liquet and Saracco (2012) proposed to consider a risk function which can be replaced in this multivariate context by:

$$R_{h,k} := \mathbb{E}\left(r(\mathbf{V}_k, \mathbf{\Sigma}, \widehat{\mathbf{V}}_k, \widehat{\mathbf{\Sigma}})\right), \tag{8}$$

where $\mathbf{V}_k := [v_1, \ldots, v_k]$, $\widehat{\mathbf{V}}_k := [\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_k]$ and h is the number of slices used to obtain $\mathbf{V}_k$ and $\widehat{\mathbf{V}}_k$. 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.

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 $k = 1, \ldots, p$ 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 $\widehat{K} << p$ 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 investigate the stability of the corresponding k-dimensional linear subspace. Although boxplots of $\widehat{R}_{h,k}$ are also useful to determine the optimal number of slices $\widehat{H}$, wMSIR is not really sensitive to this parameter as shown in Section 4.

3.6. Analyzing components of $\mathbf{y}$ *through MSIR*

Recall that the estimate $\widehat{\mathbf{V}}$ (resp. $\widehat{\widetilde{\mathbf{V}}}$) of MSIR (resp. wMSIR) is computed from the estimated EDR directions $\widehat{\mathbf{B}}^{(j)}$ associated with each component of $\mathbf{y}$. From these estimates, it is straightforward to calculate the proximity measure $\hat{r}_j := r(\widehat{\mathbf{B}}^{(j)}, \widehat{\mathbf{\Sigma}}, \widehat{\mathbf{V}}, \widehat{\mathbf{\Sigma}})$ (resp. $\hat{\tilde{r}}_j := r(\widehat{\mathbf{B}}^{(j)}, \widehat{\mathbf{\Sigma}}, \widehat{\widetilde{\mathbf{V}}}, \widehat{\mathbf{\Sigma}})$) between each estimated marginal EDR space and the estimated common one, for $j = 1, \ldots, q$. Then it is easy to sort these measures in descending order and to draw the associated scree plot. For $j = 1, \ldots, q$, assuming model (3) and observing a low value of $\hat{r}_j$ or $\hat{\tilde{r}}_j$ could indicate an unprecise estimate of $\mathbf{B}^{(j)}$ since $\hat{r}_j$ and $\hat{\tilde{r}}_j$ tends to 1 in probability as n goes to ∞. One can then withdraw the component $y^{(j)}$ of $\mathbf{y}$ to improve the accuracy of $\widehat{\mathbf{V}}$ or $\widehat{\widetilde{\mathbf{V}}}$.

In addition, assuming model (3) with a low dimensional common EDR space for the whole components of $\mathbf{y}$ does not always seem realistic in real data analysis. Therefore, applying any multivariate SIR method on $\mathbf{y}$ should not provide a suitable dimension reduction. However, it makes sense to assume that only groups of components of $\mathbf{y}$ rely on model (3) with small values of K, as in model (4). For this model, a methodology is introduced to identify the variables $y^{(j)}$ which share the same EDR space. Thus, we obtain clusters of components on which applying a multivariate SIR approach is sensible. Note that performing marginal univariate SIR on each component $y^{(j)}$ of $\mathbf{y}$ leads to consistent estimates of each K-dimensional EDR space, since for $l = 1, \ldots, L$, it is assumed that the rank of $\mathbf{B}_l$ is equal to K. Recalling notations of Section 3.2, we obtain q_1 estimates $\text{Span}(\widehat{\mathbf{B}}^{(1)})$, $\ldots$, $\text{Span}(\widehat{\mathbf{B}}^{(q_1)})$ of $\text{Span}(\mathbf{B}_1)$, q_2 estimates $\text{Span}(\widehat{\mathbf{B}}^{(q_1+1)})$, $\ldots$, $\text{Span}(\widehat{\mathbf{B}}^{(q_1+q_2)})$ of $\text{Span}(\mathbf{B}_2)$, and so on, but values of $q_1, \ldots, q_L$ are unknown, as well as the number L of clusters.

For $(j, j^\star) \in \{1, \ldots, q\}^2$, we define $\hat{r}_{j,j^\star} := r(\widehat{\mathbf{B}}^{(j)}, \widehat{\mathbf{\Sigma}}, \widehat{\mathbf{B}}^{(j^\star)}, \widehat{\mathbf{\Sigma}})$. Without any loss of generality, assume that $L = 2$. Let us define $(j_1, j_2, j_3, j_4) \in \{1, \ldots, q_1\}^2 \times \{q_1 + 1, \ldots, q_1 + q_2\}^2$. We thus have the following Lemma.

Lemma 1. *Under model (4) and assumptions (LC) and (A1)-(A3), $\hat{r}_{j_1,j_2}$ and $\hat{r}_{j_3,j_4}$ tend to 1 in probability.*

The proof of this Lemma is given in Appendix A.1. Let us remark that, however, $\hat{r}_{j_1,j_3}$ does not converge to 1 in probability since $r(\mathbf{B}_1, \mathbf{\Sigma}, \mathbf{B}_2, \mathbf{\Sigma}) < 1$. This leads to the following criterion to cluster components of $\mathbf{y}$: for $(j, j^\star) \in \{2, \ldots, q\} \times \{1, \ldots, j-1\}$, components $y^{(j)}$ and $y^{(j^\star)}$ are classified in the same cluster if $\hat{r}_{j,j^\star}$ is close to 1. To do so, we can perform, for instance, a hierarchical ascending classification on the $q \times q$ (symmetrtic) matrix of the proximity measures $\hat{r}_{j,j^\star}$ (with $\hat{r}_{j,j} = 1$ for $j = 1, \ldots, q$). Other clustering procedures can be applied on this matrix, such as a multidimensional scaling together with the k-means method. In Sections 4-5, we give illustrations of a clustering step for simulated and real datasets, which clearly improves the estimation of the corresponding EDR spaces.

Remark 4. Computing the common estimated EDR space for each obtained cluster is not time consuming since $\widehat{\mathbf{B}}^{(1)}, \ldots, \widehat{\mathbf{B}}^{(q)}$ have already been computed. This is not the case for the k-means inverse regression (KIR) which requires new computations. In addition, applying PMS instead of MSIR or wMSIR on a cluster of $\mathbf{y}$ requires to store the $p \times p$ matrices $\widehat{\mathbf{\Gamma}}^{(1)}, \ldots, \widehat{\mathbf{\Gamma}}^{(q)}$ and summing some of them, which represent more computational time and more memory space than required by MSIR or wMSIR method, especially when p is large.

4. A simulation study

This section illustrates the ability of the proposed MSIR and wMSIR approaches, together with the diagnostic procedures on the components of $\mathbf{y}$, to properly estimate EDR spaces. The two following subsections respectively correspond to models (3) and (4).

4.1. Single EDR space model

Two simulation models are considered here. For a given sample size n and a dimension p, 100 replications of the covariate $\mathbf{x}$ are generated from the p-dimensional normal distribution $\mathcal{N}_p(\boldsymbol{\mu}, \mathbf{\Sigma})$ with the same pair $(\boldsymbol{\mu}, \mathbf{\Sigma})$. Here, $\boldsymbol{\mu}$ is randomly generated from the $\mathcal{N}_p(0, \mathbf{I}_p)$ distribution and $\mathbf{\Sigma} = \mathbf{L}\mathbf{L}' + 0.1\mathbf{I}_p$ where $\mathbf{L}$ 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 (3) with $K = 1$. Secondly, MSIR and wMSIR are evaluated with a multiple indices model ($K = 2$).

Single index model. Consider the following single index model:

$$\begin{cases} y^{(1)} &= \mathbf{x}'\beta_1 + \varepsilon^{(1)}, \\ y^{(2)} &= (\mathbf{x}'\beta_1)^3 + 3\varepsilon^{(2)}, \\ y^{(3)} &= \mathbf{x}'\beta_1(1 + \varepsilon^{(3)}), \end{cases} \tag{9}$$

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

Samples of size $n = 100$ are generated from (9), with $p = 20$. Then, the EDR direction is estimated using the following methods, with $H = 10$ slices:

- univariate SIR for each component of $\mathbf{y}$ which produces estimates $\widehat{\mathbf{B}}^{(1)}$, $\widehat{\mathbf{B}}^{(2)}$ and $\widehat{\mathbf{B}}^{(3)}$,
- MSIR which gives the estimate $\widehat{\mathbf{V}}$,
- wMSIR that leads to the estimate $\widehat{\widetilde{\mathbf{V}}}$,
- k-means inverse regression which provides the estimate $\widehat{\mathbf{V}}_{\mathrm{KIR}}$,
- pooled marginal slicing, leading to the estimate $\widehat{\mathbf{V}}_{\mathrm{PMS}}$.

For each estimator $\widehat{\mathbf{B}} \in \left\{\widehat{\mathbf{B}}^{(1)}, \widehat{\mathbf{B}}^{(2)}, \widehat{\mathbf{B}}^{(3)}, \widehat{\mathbf{V}}, \widehat{\widetilde{\mathbf{V}}}, \widehat{\mathbf{V}}_{\mathrm{KIR}}, \widehat{\mathbf{V}}_{\mathrm{PMS}}\right\}$, the squared trace correlation $r(\widehat{\mathbf{B}}) := r(\widehat{\mathbf{B}}, \mathbf{\Sigma}, \mathbf{B}, \mathbf{\Sigma})$ between the estimated EDR space and the true EDR space is computed. The closer to one is $r(\widehat{\mathbf{B}})$, the better is the estimate. Note that for $K = 1$, the criterion $r(\widehat{\mathbf{B}})$ corresponds to the squared cosine of the angle between $\widehat{\mathbf{B}}$ and β_1.

Boxplots of this criterion are drawn on Figure 1(a). It appears that $\widehat{\mathbf{B}}^{(3)}$ exhibits low squared trace correlation. This phenomenon can be explained by the heteroscedasticity in the third marginal model of (9). Even if $\widehat{\mathbf{B}}^{(3)}$ is necessary to compute $\widehat{\mathbf{V}}$ and $\widehat{\widetilde{\mathbf{V}}}$, the poor estimates of $\mathbf{B}^{(3)}$ do not imply a significant loss in the squared trace correlations related to $\widehat{\mathbf{V}}$ and to $\widehat{\widetilde{\mathbf{V}}}$. One can also observe that the weighting in wMSIR seems to improve the estimation of the EDR space since values of $r(\widehat{\widetilde{\mathbf{V}}})$ are globally greater than those of $r(\widehat{\mathbf{V}})$. This trend is confirmed in Figure 1(b) where the values of $r(\widehat{\mathbf{V}})$ are plotted versus those of $r(\widehat{\widetilde{\mathbf{V}}})$. It appears that wMSIR seems to be uniformly better than MSIR in this simulation. In addition, Figure 1(a) shows that the pooled marginal slicing produces slightly better estimates than wMSIR in this example and that wMSIR outperforms the k-means inverse regression.

The poor quality of the estimate $\widehat{\mathbf{B}}^{(3)}$ can be observed directly from the simulated data. Figure 2(a) provides boxplots of values of $\hat{\tilde{r}}_j$ for $j = 1, 2, 3$. Considering that the first quartile of the third boxplot is equal to 0.84 and that the minimum value of the first and the second ones are respectively equal to 0.94 and 0.95, it makes sense to withdraw the third component of $\mathbf{y}$ from the analysis for at least a forth of the datasets. Let $\widehat{\widetilde{\mathbf{V}}}^{\star}$ be the wMSIR estimate built only from $y^{(1)}$ and $y^{(2)}$. Quality measures for $\widehat{\widetilde{\mathbf{V}}}^{\star}$ and for the PMS estimate are compared in Figure 2(b). One can observe that the selection based on the $\hat{\tilde{r}}_j$'s improves performances of the wMSIR method, so that it produces better quality measures than the PMS without this selection step.

To study the sensitivity of wMSIR with respect to n and p, several samples are generated for various values of these parameters. In Figure 3(a), boxplots of 100 values of $r(\widehat{\widetilde{\mathbf{V}}})$ are drawn for

(a) Boxplots of quality measures $r(\widehat{\mathbf{B}})$ for various estimators $\widehat{\mathbf{B}}$

(b) Plot of $r(\widehat{\mathbf{V}})$ versus $r(\widehat{\widehat{\mathbf{V}}})$

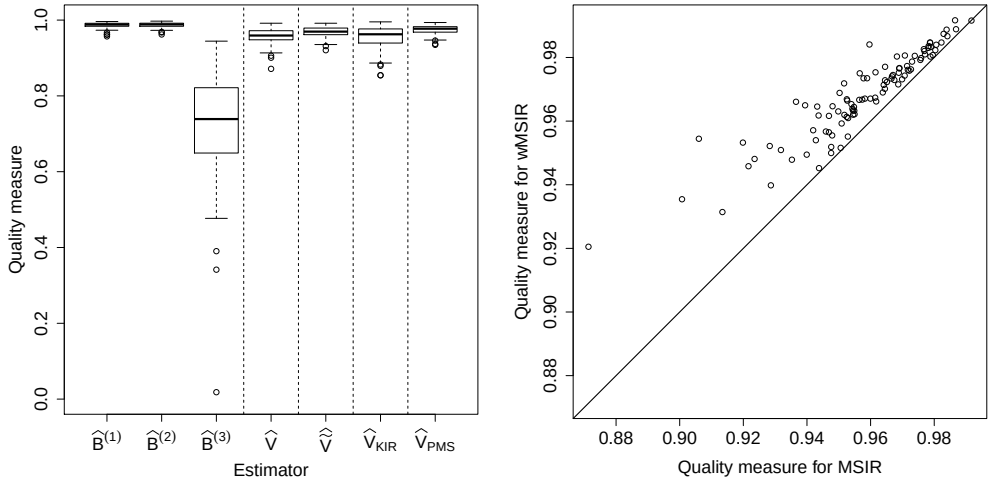


Figure 1: Comparison of estimators of $\mathbf{B}$ on 100 samples from model (9) with $n = 100$ and $p = 20$. The line in (b) corresponds to the first bisecting line.

(a) Values of $\hat{\tilde{r}}_j$ for each component $y^{(j)}$ of $\mathbf{y}$

(b) Plot of $r(\widehat{\widehat{\mathbf{V}}}^{\star})$ versus $r(\widehat{\mathbf{V}}_{\mathrm{PMS}})$

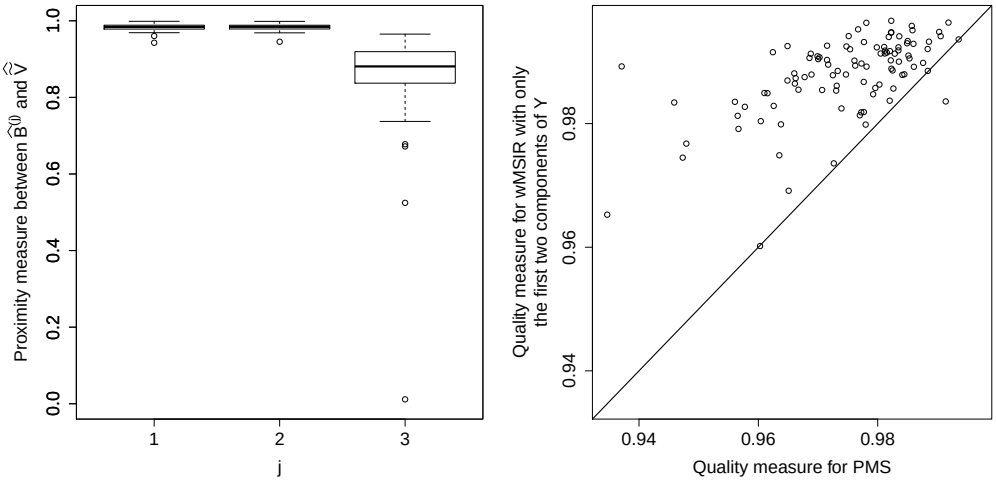


Figure 2: Study of the contribution of $y^{(3)}$ to $\widehat{\widehat{\mathbf{V}}}$ for 100 samples generated from model (9) with $n = 100$ and $p = 20$.

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. Notice that for every value of (n, p) in Figure 3(a), estimates are very precise since most of the values of $r(\widehat{\widetilde{\mathbf{V}}})$ are greater than 0.85.

In the previous analyses, the number of slices H was set to 10 to have enough slices to study the functions that link $\mathbf{x}'\beta_1$ to each component of $\mathbf{y}$ and enough points in each slice. In Figure 4(a), we observe that for wMSIR, one can arbitrarily choose a number of slices between 10 and 20 and obtain an estimate of the EDR space which is as reliable as the one computed with $H = 10$.

Multiple indices model. Consider now a more complex model than model (9). It is defined by:

$$\begin{cases} y^{(1)} &= \exp(\mathbf{x}'\beta_1) \times (\mathbf{x}'\beta_2) + \varepsilon^{(1)}, \\ y^{(2)} &= (\mathbf{x}'\beta_1) \times \exp(\mathbf{x}'\beta_2) + \varepsilon^{(2)}, \end{cases} \tag{10}$$

where $\beta_1 = [\beta_{1,1}, \ldots, \beta_{1,p}]'$, $\beta_2 = [\beta_{2,1}, \ldots, \beta_{2,p}]'$, 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 (10), we clearly have $K = 2$.

Samples are generated from model (10) for various n and p. Then, these samples are used to estimate the corresponding EDR space with wMSIR with $H = 10$ slices. This leads to boxplots of $r(\widehat{\widetilde{\mathbf{V}}})$ displayed in Figure 3(b). We observe lower and more scattered values of $r(\widehat{\widetilde{\mathbf{V}}})$ than in Figure 3(a). The complexity of the link function between $\mathbf{y}$ and $\mathbf{x}$ and the greater dimension K are believable reasons for this phenomenon. Apart from this feature, Figure 3(b) provides identical evolutions of $r(\widehat{\widetilde{\mathbf{V}}})$ with n and p to those observed for the single index model in Figure 3(a). Note that for both model (9) and model (10), the behavior of MSIR and wMSIR when n and p vary are similar. That is why only results concerning wMSIR are drawn in Figure 3.

Examining Figure 4(b), it seems that the quality of wMSIR estimates is less connected to the chosen number of slices for model (9) than for model (10). For the latter, performances of wMSIR are nevertheless similar for values of H from 4 to 10.

4.2. Multiple EDR spaces model

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

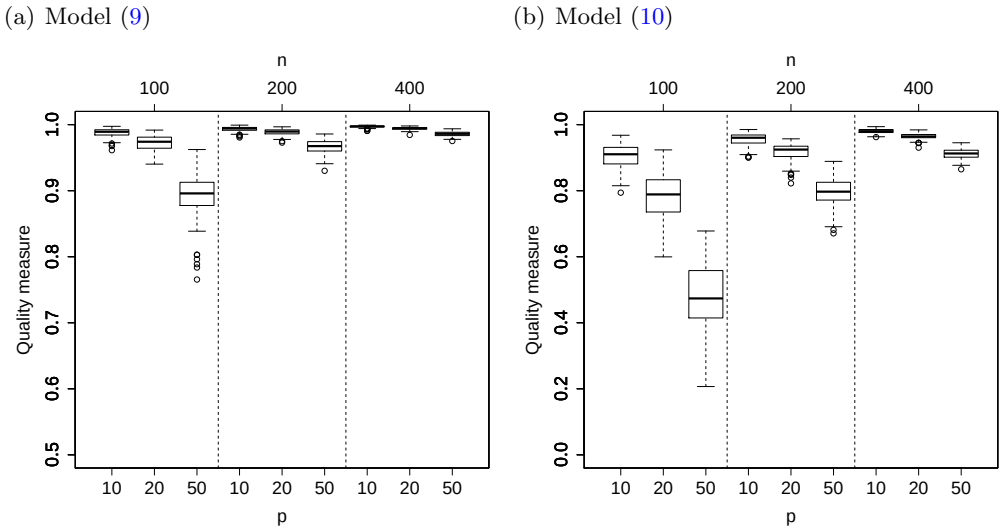


Figure 3: Boxplots of quality measure for the wMSIR method, for 100 samples generated from (a) model (9) or from (b) model (10) with various values of n and p.

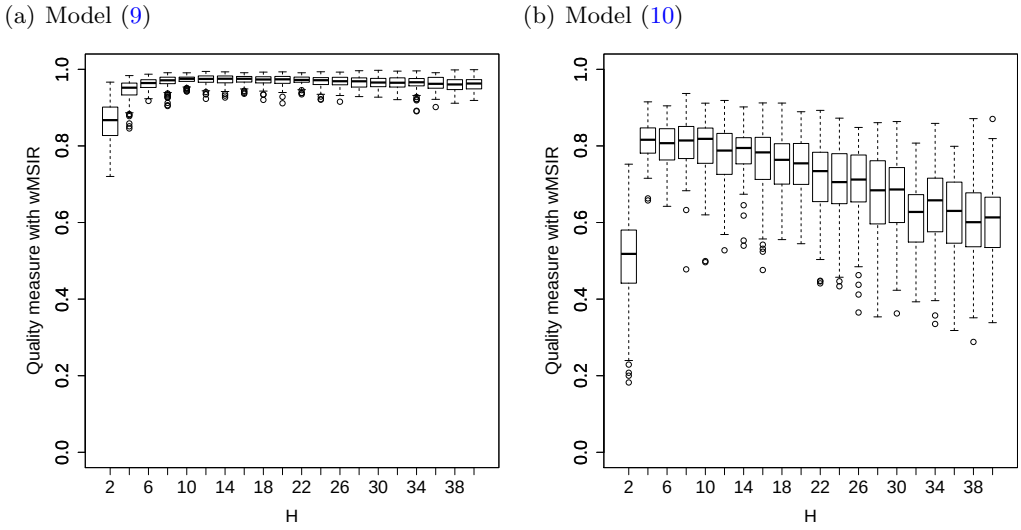


Figure 4: Boxplots of quality measure for the wMSIR method for 100 samples generated (a) from the model (9) and (b) from the model (10), with $n = 100$, $p = 20$ and various values of H.

$$\begin{cases} y^{(1)} &= \mathbf{x}'\beta_1 + \varepsilon^{(1)}, \\ y^{(2)} &= (\mathbf{x}'\beta_1)^3 + 3\varepsilon^{(2)}, \\ y^{(3)} &= \mathbf{x}'\beta_1(1+\varepsilon^{(3)}), \\ y^{(4)} &= \mathbf{x}'((1-\theta_1)\beta_1 + \theta_1\beta_2) + \varepsilon^{(4)}, \\ y^{(5)} &= (\mathbf{x}'((1-\theta_1)\beta_1 + \theta_1\beta_2))^3 + 3\varepsilon^{(5)}, \\ y^{(6)} &= \mathbf{x}'((1-\theta_1)\beta_1 + \theta_1\beta_2)(1+\varepsilon^{(6)}), \\ y^{(7)} &= \mathbf{x}'((1-\theta_2)\beta_1 + \theta_2\beta_3) + \varepsilon^{(7)}, \\ y^{(8)} &= (\mathbf{x}'((1-\theta_2)\beta_1 + \theta_2\beta_3))^3 + 3\varepsilon^{(8)}, \\ y^{(9)} &= \mathbf{x}'((1-\theta_2)\beta_1 + \theta_2\beta_3)(1+\varepsilon^{(9)}), \\ y^{(10)} &= \varepsilon^{(10)}, \\ y^{(11)} &= \varepsilon^{(11)}, \\ y^{(12)} &= \varepsilon^{(12)}, \end{cases} \tag{11}$$

based on model (9), where $(\theta_1, \theta_2) \in [0,1]^2$ and for $j = 1, \ldots, 12$, $\varepsilon^{(j)} \sim \mathcal{N}_1(0,1)$.

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

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

Figure 5 presents values of $\hat{r}_{j,j^\star}$ for $(j, j^\star) \in \{2, \ldots, q\} \times \{1, \ldots, j-1\}$, computed from a sample of size $n = 1000$. Darker squares correspond to values of $\hat{r}_{j,j^\star}$ close to 1. Thus, focusing only on the nine darkest squares of Figure 5 leads to cluster components $y^{(1)}$, $y^{(2)}$ and $y^{(3)}$ together as well as components $y^{(4)}$, $y^{(5)}$ and $y^{(6)}$, and to make a group which contains components $y^{(7)}$, $y^{(8)}$ and $y^{(9)}$. Note also that for $j \in \{1,2,3\}$, we have $\hat{r}_{3j,3j-1} < \hat{r}_{3j-2,3j-1}$ and $\hat{r}_{3j,3j-2} < \hat{r}_{3j-2,3j-1}$. Recalling that for the considered values of j, $y^{(3j)}$ is the third component of each model (9) embedded in model (11), these inequalities can be explained by the heteroscedasticity in this component which leads to imprecise estimates of the relevant EDR direction as pointed out on Figure 1(a).

In this example, the interpretation of Figure 5 can easily be done because components of $\mathbf{y}$ 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 $\mathbf{y}$ 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 an agglomerative hierarchical clustering algorithm based on the dissimilarity $1 - \hat{r}_{j,j^\star}$ between $\widehat{\mathbf{B}}^{(j)}$ and $\widehat{\mathbf{B}}^{(j^\star)}$.

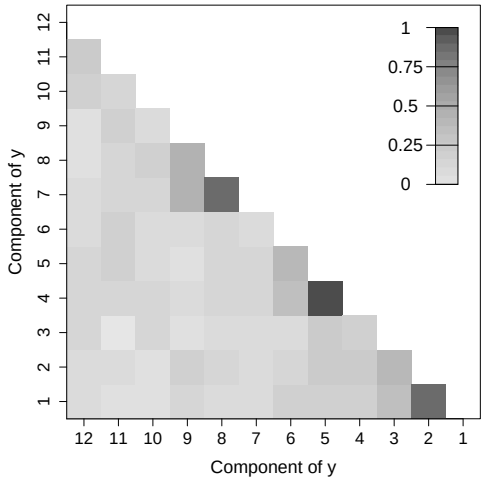


Figure 5: Values of $\hat{r}_{j,j^\star}$ in various shades of grays for $(j, j^\star) \in \{2, \ldots, q\} \times \{1, \ldots, j-1\}$ and for a sample of size $n = 1000$ generated from model (11) with $\theta_1 = \theta_2 = 1$ and $p = 20$.

A model with 5 clusters. A new sample of size $n = 1000$ is generated from model (11) with $\theta_1 = 1$ and $\theta_2 = 0$ which leads to $l = 5$ clusters:

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

The hierarchical clustering algorithm applied to the estimates $\widehat{\mathbf{B}}^{(j)}$ for $j = 1, \ldots, q$ and produces the dendrogram of Figure 6(a). A classification directly based on this procedure would not be really accurate. For instance, in model (11), $y^{(11)}$ and $y^{(12)}$ belong to two different clusters. On Figure 6(a), to divide $y^{(11)}$ and $y^{(12)}$ into two groups, the tree can be cut at a level of 0.70. 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 6(a) allows to order components of $\mathbf{y}$ in such a way that those which are linked by high squared trace correlation are close from each other. Thus, in Figure 6(b), we displayed values of $\hat{r}_{j,j^\star}$ for $j^\star \prec j$ where $\prec$ denotes the ordering in Figure 6(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 6(b). Not surprisingly, one can observe again that the squared trace correlations between components $y^{(3)}$, $y^{(6)}$, $y^{(9)}$ and the components corresponding to their group are quite low. Finally, components $y^{(12)}$, $y^{(11)}$ and $y^{(10)}$ appears to form three distinct clusters.

(a) Dendrogram of components of $\mathbf{y}$

(b) Values of $\hat{r}_{j,j^\star}$ in various shades of grays for $j^\star \prec j$

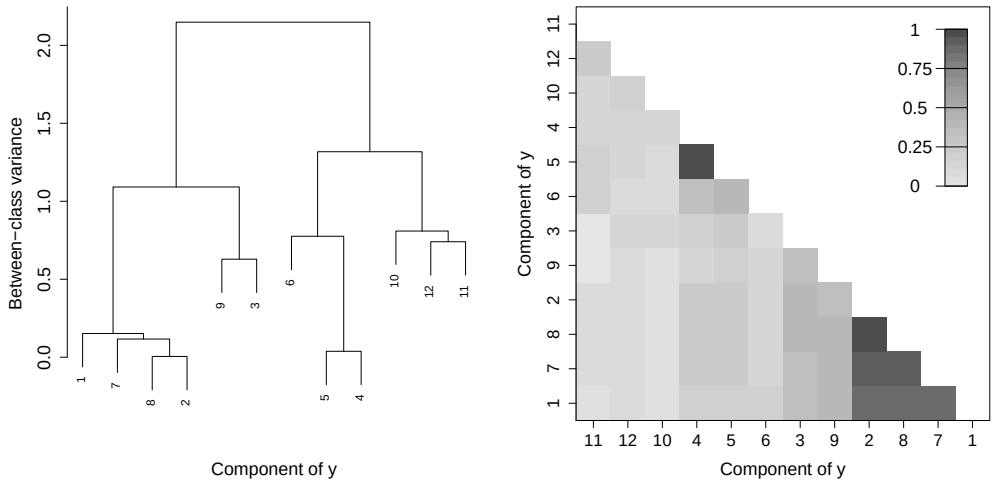


Figure 6: Clustering analysis for a sample of size $n = 1000$ generated from model (11) with $\theta_1 = 1$, $\theta_2 = 0$ and $p = 20$.

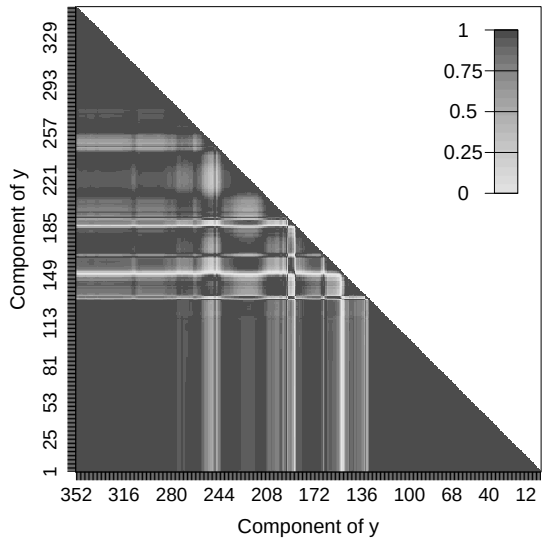
5. Real data illustrations

5.1. Remote sensing data

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 $\mathbf{x}$ and observed spectra $\mathbf{y}$. The reader may refer to Bernard-Michel et al. (2009a) 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 $\mathbf{y} = g(\mathbf{x})$. The $p = 3$ 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 $\mathbf{y}$ is made of $q = 352$ 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 $\{(\mathbf{x}_i, \mathbf{y}_i), i = 1, \ldots, n\}$ 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 7. Two clusters of wavelengths have been identified, corresponding to two different orientations of $\widehat{\mathbf{v}}_1$. It appears on Figure 8(a) that, in the first cluster, only the proportion of dust $x^{(2)}$ has an important contribution to the EDR

(a) Values for $(j, j^\star) \in \{2, \ldots, q\} \times \{1, \ldots, j-1\}$



(b) Values for $j^\star \prec j$ where $\prec$ denotes an ordering produced by a hierarchical clustering algorithm

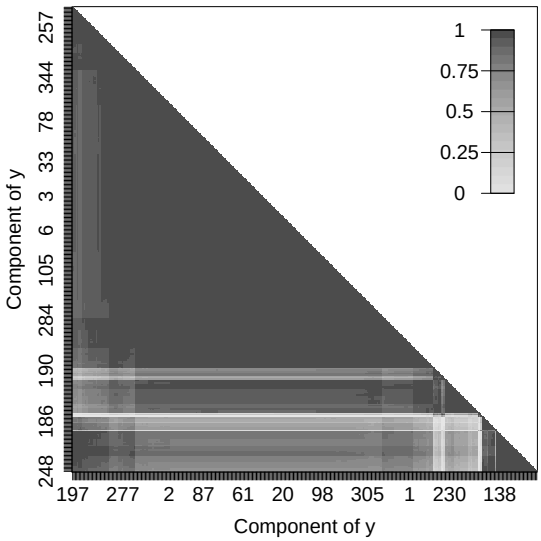


Figure 7: Values of $\hat{r}_{j,j^\star}$ in various shades of grays for hyperspectral data.

direction. In the second cluster, the estimated EDR direction is close to $(1, 1, 0)$. This corresponds to the index $x^{(1)} + x^{(2)}$ which is equal 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 8(b) permits one to visualize the clustering of the wavelengths: it reveals which wavelengths are more sensitive to the presence of water ice or dust.

5.2. Minneapolis elementary schools data

Another dataset which is widely studied in the dimension reduction context with a multivariate response is related to test results of students in Minneapolis elementary schools. These data are for example presented in Cook (2009); Cook and Setodji (2003); Yin and Bura (2006). The response variable $\mathbf{y}$ is made of $q = 4$ components. The first (resp. third) component is the proportion of pupils scoring below the average on a fourth (resp. sixth) grade test. The second (resp. fourth) one is the proportion of marks above the average. Following Yin and Bura (2006), our goal is to explain $\mathbf{y}$ with a 8-dimensional variable $\mathbf{x}$. The seven first components $\mathbf{x}$ are called $x^{(1)}, \ldots, x^{(7)}$ and are respectively the squared root of the percentages of children receiving an aid called AFDC, children who do not live with both parents, people in the area of a school who completed high school, people who suffer from poverty, minority, mobility and pupils who attend school regularly. The last component of $\mathbf{x}$, named $x^{(8)}$, is the mean number of pupils for each teacher. Note that Yoo (2009) analyzed the variables $x^{(1)}$, $x^{(2)}$ and $x^{(3)}$ while Cook (2009) focused on some increasing functions of these variables and Cook and Setodji (2003) considered $x^{(1)}$, $x^{(2)}$, $x^{(3)}$, $x^{(4)}$ and $x^{(8)}$.

(a) Values of $\widehat{\tilde{v}}_{1,1}$ (circles), $\widehat{\tilde{v}}_{1,2}$ (triangles) and $\widehat{\tilde{v}}_{1,3}$ (crosses) for each cluster

(b) Clustering of the wavelengths

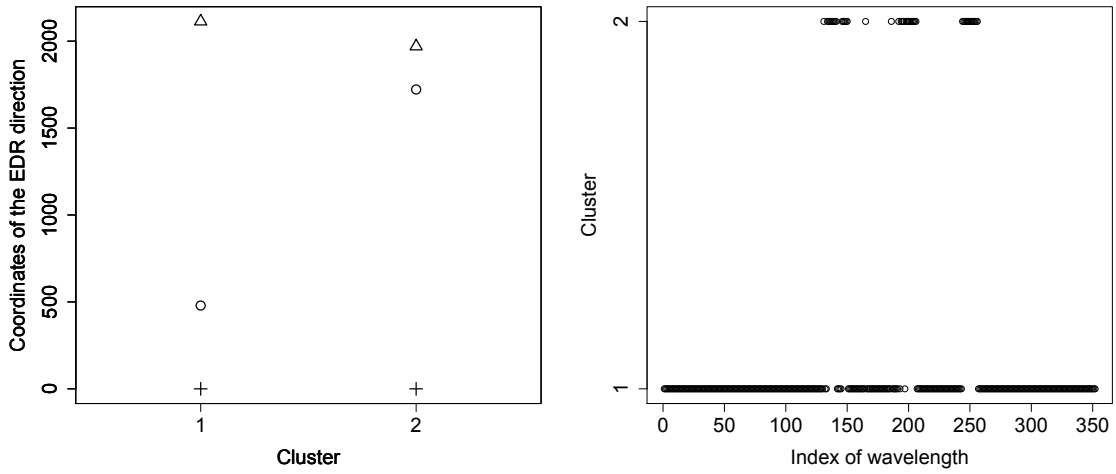


Figure 8: Clustering of the components of $\mathbf{y}$ and estimates $\widehat{\tilde{\mathbf{v}}}_1 = [\widehat{\tilde{v}}_{1,1}, \widehat{\tilde{v}}_{1,2}, \widehat{\tilde{v}}_{1,3}]'$ of the EDR direction for each cluster.

We first compute $\widehat{\widetilde{\mathbf{V}}}$ with $p = 8$ components of $\mathbf{x}$. A stepwise algorithm is then used with the AIC to perform a linear regression of $\mathbf{x}'\widehat{\widetilde{\mathbf{V}}}$ on $\mathbf{x}$ and sort the components of $\mathbf{x}$ with respect to how much they explain $\mathbf{x}'\widehat{\widetilde{\mathbf{V}}}$. The first three sorted variables are $x^{(1)}$, $x^{(2)}$, and $x^{(3)}$. Besides, regressing $\mathbf{x}'\widehat{\widetilde{\mathbf{V}}}$ on $\{x^{(1)}, x^{(2)}, x^{(3)}\}$ produces an adjusted coefficient of determination of 95.42%. This encourages us to take $\mathbf{x} = (x^{(1)}, x^{(2)}, x^{(3)})'$.

Working with this 3-dimensional covariate and with $H = 8$, $\widehat{\mathbf{B}}^{(j)}$ is computed for $j = 1, \ldots, 4$, with $K = 1$, which is the size of the dimension chosen in Cook (2009), Cook and Setodji (2003) and Yin and Bura (2006). We then construct the matrix $\widehat{\mathbb{B}}\widehat{\mathbb{B}}'\widehat{\mathbf{\Sigma}}$. Its eigenvalues are 0.96, 0.04 and 0.01 which confirms the choice of $K = 1$. We can not build several groups of components of $\mathbf{y}$ since the least value of $\hat{r}(j, j^\star)$ for $(j, j^\star) \in \{1, \ldots, 4\}$ is equal to 0.75, neither we can withdraw a component from $\mathbf{y}$ since the least value of $\hat{\tilde{r}}_j$ for $j \in \{1, \ldots, 4\}$ is equal to 0.92. In addition, we find $\widehat{\widetilde{\mathbf{V}}} = (0.673, -0.406, -0.528)'$.

Letting $\widehat{\mathbf{V}}_Y$ the EDR direction found by Yoo (2009), it appear that $r(\widehat{\widetilde{\mathbf{V}}}, \widehat{\mathbf{\Sigma}}, \widehat{\mathbf{V}}_Y, \widehat{\mathbf{\Sigma}}) = 0.97$. The signs of the elements of $\widehat{\widetilde{\mathbf{V}}}$ make also sense compared to results from Cook (2009) and Cook and Setodji (2003).

6. Concluding remarks

In this paper, we proposed the new multivariate SIR approaches MSIR and wMSIR for estimating the EDR space. The idea consists in performing first several marginal SIR analyzes. A common EDR space is then deduced from the marginal ones by maximizing the proximity criterion defined in (6). This optimization problem benefits from a closed-form solution.

MSIR and wMSIR 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, our approach allows to deal with datasets that come from a model including several different EDR spaces. It is then possible to estimate each of them from clusters of components of the response variable rather than blindly apply a multivariate SIR procedure on the whole variable. In addition, 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.

Let us highlight that a similar two-step approach can be created from any variant of the SIR method or any sufficient dimension reduction technique. For instance, it is straightforward to build multivariate regularized SIR approaches from Bernard-Michel et al. (2009b), multivariate SIR$_\alpha$ approaches from Gannoun and Saracco (2003) or multivariate kernel SIR methods from Wu (2008) and to obtain the associated clustering step. To avoid the choice of the number H of slices, one may also consider building a multivariate version of the CUME procedure from Zhu et al. (2010a).

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Appendix A. Proofs

Appendix A.1. Proof of Lemma 1

For $j = 1, \ldots, q$, recall that $P_{\widehat{\mathbf{B}}^{(j)},\widehat{\mathbf{\Sigma}}}$ is the $\widehat{\mathbf{\Sigma}}$-orthogonal projector onto Span$(\widehat{\mathbf{B}}^{(j)})$. According to Theorem 4 of Saracco (1997), we have that $P_{\widehat{\mathbf{B}}^{(j)},\widehat{\mathbf{\Sigma}}} = P_{\mathbf{B}_1,\mathbf{\Sigma}} + O_P(n^{-1/2})$, for $j \in \{j_1, j_2\}$ and $P_{\widehat{\mathbf{B}}^{(j)},\widehat{\mathbf{\Sigma}}} = P_{\mathbf{B}_2,\mathbf{\Sigma}} + O_P(n^{-1/2})$, for $j \in \{j_3, j_4\}$. It follows that

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

Similarly, $r(\widehat{\mathbf{B}}^{(j_3)}, \widehat{\mathbf{\Sigma}}, \widehat{\mathbf{B}}^{(j_4)}, \widehat{\mathbf{\Sigma}})$ tends to 1 in probability. □

Appendix A.2. Proof of Theorem 1

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

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

Hence, it is well known that the matrix $\mathbf{V}$ which maximizes $\text{Trace}(\mathbf{D}'\mathbf{\Sigma}\mathbb{B}\mathbb{B}'\mathbf{\Sigma}\mathbf{D})$ over the set of matrices $\mathbf{D}$ such that $\mathbf{D}'\mathbf{\Sigma}\mathbf{D} = \mathbf{I}_K$ is made of the K generalized eigenvectors of $\mathbf{\Sigma}\mathbb{B}\mathbb{B}'\mathbf{\Sigma}$ and $\mathbf{\Sigma}$ associated with K non-null eigenvalues. Thus, $\mathbf{V}$ contains the K eigenvectors of $\mathbf{\Sigma}^{-1}(\mathbf{\Sigma}\mathbb{B}\mathbb{B}'\mathbf{\Sigma}) = \mathbb{B}\mathbb{B}'\mathbf{\Sigma}$ which are associated with K non-null eigenvalues.

In addition, it is clear that $\text{Span}(\mathbf{\Sigma}\mathbb{B}\mathbb{B}'\mathbf{\Sigma}) = \text{Span}(\mathbf{\Sigma}\mathbb{B})$ because $\text{Span}(\mathbf{\Sigma}\mathbb{B}\mathbb{B}'\mathbf{\Sigma}) \subset \text{Span}(\mathbf{\Sigma}\mathbb{B})$ and $\dim(\text{Span}(\mathbf{\Sigma}\mathbb{B}\mathbb{B}'\mathbf{\Sigma})) = K$. Since $\mathbf{\Sigma}$ is invertible, this implies that $\text{Span}(\mathbb{B}\mathbb{B}'\mathbf{\Sigma}) = \text{Span}(\mathbb{B})$. Finally, we have under model (3) and assumption (MC) that for all $j \in \{1, \ldots, q\}$, $\text{Span}(\mathbf{B}) = \text{Span}(\mathbf{B}^{(j)})$. It follows that $\text{Span}(\mathbb{B}) = \text{Span}(\mathbf{B})$ and then $\text{Span}(\mathbf{V}) = \text{Span}(\mathbf{B})$.

Appendix A.3. Proof of Theorem 2

From univariate SIR theory of Li (1991), under the assumptions of Theorem 2, each estimated EDR space $\widehat{\mathbf{B}}^{(j)}$ converges to $\mathbf{B}^{(j)}$ at root n rate: that is, for $j = 1, \ldots, q$, $\widehat{\mathbf{B}}^{(j)} = \mathbf{B}^{(j)} + O_p(n^{-1/2})$. It follows that $\widehat{\mathbb{B}} = \mathbb{B} + O_p(n^{-1/2})$. Since $\widehat{\mathbf{\Sigma}} = \mathbf{\Sigma} + O_p(n^{-1/2})$, we get $\widehat{\mathbb{B}}\widehat{\mathbb{B}}'\widehat{\mathbf{\Sigma}} = \mathbb{B}\mathbb{B}'\mathbf{\Sigma} + O_p(n^{-1/2})$. Therefore, the eigenvectors associated with the largest K eigenvalues of $\widehat{\mathbb{B}}\widehat{\mathbb{B}}'\widehat{\mathbf{\Sigma}}$ converge to the corresponding ones of $\mathbb{B}\mathbb{B}'\mathbf{\Sigma}$ at the same rate: $\hat{\mathbf{v}}_k = v_k + O_p(n^{-1/2})$ for $k = 1, \ldots, K$. Consequently, the estimated EDR space $\text{Span}(\widehat{\mathbf{V}})$ converges to $\text{Span}(\mathbf{V})$ at root n rate. Since under model (3) and assumption (MC) $\text{Span}(\mathbf{V}) = \text{Span}(\mathbf{B})$, the estimated EDR space converges to the true one in probability.

Appendix A.4. Proof of Theorem 3

One can proceed analogously to the proof of Theorem 2. It is sufficient to show that $\widehat{\mathbb{W}} = \mathbb{W} + O_p(n^{-1/2})$. From the univariate SIR theory of Li (1991), for each component $y^{(j)}$ of $\mathbf{y}$, each estimated eigenvalue $\hat{\lambda}_k^{(j)}$ converges to $\lambda_k^{(j)}$ at root n rate under the assumptions of Theorem 3. We then have $\hat{\pi}^{(j)} = \pi^{(j)} + O_p(n^{-1/2})$ and $\hat{\pi}_\star = \pi_\star + O_p(n^{-1/2})$. It follows that $\widehat{\mathbf{W}}^{(j)} = \mathbf{W}^{(j)} + O_p(n^{-1/2})$ and $\widehat{\mathbb{W}} = \mathbb{W} + O_p(n^{-1/2})$.

Consequently, $\widehat{\mathbb{B}}\widehat{\mathbb{W}}\widehat{\mathbb{B}}'\widehat{\mathbf{\Sigma}} = \mathbb{B}\mathbb{W}\mathbb{B}'\mathbf{\Sigma} + O_p(n^{-1/2})$ and the eigenvectors associated with the largest K eigenvalues of $\widehat{\mathbb{B}}\widehat{\mathbb{W}}\widehat{\mathbb{B}}'\widehat{\mathbf{\Sigma}}$ converge to the corresponding ones of $\mathbb{B}\mathbb{W}\mathbb{B}'\mathbf{\Sigma}$ at the same rate: $\widehat{\tilde{\mathbf{v}}}_k = \tilde{v}_k + O_p(n^{-1/2})$ for $k = 1, \ldots, K$. Therefore, the estimated EDR space $\text{Span}(\widehat{\widetilde{\mathbf{V}}})$ converges to $\text{Span}(\widetilde{\mathbf{V}})$ at root n rate. Since, from Theorem 2, $\text{Span}(\widetilde{\mathbf{V}}) = \text{Span}(\mathbf{B})$, the estimated EDR space converges to the true one in probability.

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