A selective review of sufficient dimension reduction for multivariate response regression

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Abstract

We review sufficient dimension reduction (SDR) estimators with multivariate response in this paper. A wide range of SDR methods are characterized as inverse regression SDR estimators or forward regression SDR estimators. The inverse regression family include pooled marginal estimators, projective resampling estimators, and distance-based estimators. Ordinary least squares, partial least squares, and semiparametric SDR estimators, on the other hand, are discussed as estimators from the forward regression family.

Keywords: Minimum average variance estimation, Partial least squares, Projective resampling, Sliced inverse regression.

1. Introduction

For \( q \)-dimensional response \( Y \) and \( p \)-dimensional predictor \( X \), sufficient dimension reduction (SDR) aims to find \( B \in \mathbb{R}^{p \times d} \) with the smallest possible column space such that

\[
Y \perp X \mid B^\top X,
\]

where \( \perp \) means independence. The column space of \( B \), or \( \text{span}(B) \), is known as the central space, and is denoted as \( S_{Y \mid X} \). The dimension of the central

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space is referred to as the structural dimension. Denote the columns of \( \mathbf{B} \) as \( \mathbf{b}_j, j = 1, \ldots, d \). For a continuous response \( Y \), a regression form of (1) is

\[
Y = g(\mathbf{b}_1^\top \mathbf{X}, \ldots, \mathbf{b}_d^\top \mathbf{X}, \epsilon),
\]

where \( \epsilon \) is \( r \)-dimensional random error independent of \( \mathbf{X} \) (with \( r \geq 1 \)), and \( g : \mathbb{R}^{d+r} \rightarrow \mathbb{R}^q \) is an unknown link function. Given i.i.d. samples \( \{(Y_i, \mathbf{X}_i) : i = 1, \ldots, n\} \) generated from model (2), multivariate response SDR focuses on estimating the indices \( \mathbf{b}_1, \ldots, \mathbf{b}_d \) without necessarily estimating the link function \( g \).

Since the seminal works of Li (1991) and Cook (1998), many SDR methods have been proposed in the literature. Most of these methods focus on the univariate response case with \( q = 1 \). Existing SDR review papers and a recent SDR book follow a similar trend, discussing almost exclusively methods for the univariate response. See, for example, Yin (2010), Ma and Zhu (2013), Li (2018), and Dong (2021). This paper aims to fill in this gap and provides a selective review of SDR with multivariate response. The rest of the paper is organized as follows. In section 2, we review multivariate response SDR methods through inverse regression. Forward regression methods for multivariate response SDR are discussed in section 3. We conclude the paper with some emerging trends in section 4. Without loss of generality, we assume \( \mathbb{E}(\mathbf{X}) = \mathbf{0} \) and \( \mathbb{E}(Y) = \mathbf{0} \) throughout the paper.

2. Multivariate response SDR through inverse regression

2.1. SIR and slicing-based inverse regression methods

Denote \( \text{Var}(\mathbf{X}) = \Sigma_X \) and the standardized predictor as \( \mathbf{Z} = \Sigma_X^{-1/2} \mathbf{X} \). First we review the original SIR with univariate response \( Y \in \mathbb{R} \). Under the following linear conditional mean (LCM) assumption

\[
\mathbb{E}(\mathbf{X} | \mathbf{B}^\top \mathbf{X}) \text{ is linear in } \mathbf{B}^\top \mathbf{X}, \text{ where } \mathbf{B} \text{ is the basis of } \mathcal{S}_{Y|\mathbf{X}}.
\]

Li (1991) showed that \( \mathbb{E}(\mathbf{Z} | Y) \in \mathcal{S}_{Y|\mathbf{Z}} \). Due to an equivariant property of the central space in Theorem 2.2 of Li (2018), we have

\[
\Sigma_X^{-1} \mathbb{E}(\mathbf{X} | Y) = \Sigma_X^{-1/2} \mathbb{E}(\mathbf{Z} | Y) \in \mathcal{S}_{Y|\mathbf{X}}.
\]
Denote \( \xi_h^{(0)} = \Sigma_{X}^{-1} E(X \mid Y \in J_h) \) for \( h = 1, \ldots, H \), where \( J_1, \ldots, J_H \) is a partition of the support of \( Y \). Let

\[
M^{(0)} = \sum_{h=1}^{H} p_h^{(0)} \xi_h^{(0)} \xi_h^{(0)\top},\text{ where } p_h^{(0)} = E(Y \in J_h).
\]

We refer to \( M^{(0)} \) as the SIR kernel matrix. In the case of categorical response, the categories become a natural partition. For continuous response, quantile slicing is used for the partition in the original SIR. In particular, for \( \ell = 1, \ldots, H - 1 \), let \( \tau_{\ell} \) be the \( \ell H^{-1} \)-th population quantile of \( f_Y \), the density function of \( Y \). The partition used in SIR becomes \((-\infty, \tau_1), (\tau_1, \tau_2), \ldots, (\tau_{H-1}, \infty)\). Instead of the continuous response \( Y \), we now have the discretized response \( \tilde{Y} = \sum_{h=1}^{H} I(Y \in J_h) \), where \( I(\cdot) \) denotes the indicator function.

According to Theorem 2.3 of Li (2018), it can be shown that

\[
S_{\tilde{Y}\mid X} \subseteq S_{Y\mid X}.
\]  

(5)

Applying (4) to \( \tilde{Y} \), we have

\[
\xi_h^{(0)} \in S_{\tilde{Y}\mid X}.
\]  

(6)

Equations (5) and (6) lead to \( \text{span}(M^{(0)}) \subseteq S_{Y\mid X} \). Denote \( \hat{M}^{(0)} \) as the sample version of \( M^{(0)} \). SIR then uses the eigenvectors corresponding to the \( d \) leading eigenvalues of \( \hat{M}^{(0)} \) to recover the central space \( S_{Y\mid X} \).

Many slicing-based inverse regression methods have been proposed in the literature after the introduction of the original SIR. We discuss the extensions that are relevant for multivariate response methods to be reviewed in later sections. To synthesize the intraslice means across different slices, the original SIR takes an eigenvalue decomposition approach and can be suboptimal in terms of asymptotic efficiency. Cook and Ni (2005) suggested a minimum discrepancy approach and proposed the inverse regression estimator with optimal asymptotic efficiency. Note that \( M^{(0)} \) is directly related to \( \Lambda_I = \text{Var}(E(Z \mid \tilde{Y})) \) through \( M^{(0)} = \Sigma_{X}^{-1/2} \Lambda_I \Sigma_{X}^{-1/2} \). Let

\[
\Lambda_{II} = E \left\{ [\text{Var}(Z \mid \tilde{Y}) - E(\text{Var}(Z \mid \tilde{Y}))]^2 \right\}
\]

Under LCM and an additional constant conditional variance (CCV) assump-
tion that $\text{Var}(X | B^\top X)$ is nonrandom, Li (1991) showed that $\text{span}(A_\Pi) \subseteq S_{Y|Z}$, and this becomes known as the SIR-II method. For $\alpha \in [0, 1]$, SIR-$\alpha$ (Li, 1991) uses $(1 - \alpha)A_1^2 + \alpha A_\Pi$ to recover the central space. While the original SIR only uses information from the intraslice means, SIR-II and SIR-$\alpha$ synthesizes both the intraslice means and the intraslice variances. Other slicing-based inverse regression methods include sliced average variance estimation (SAVE) (Cook and Weisberg, 1991), covariance inverse regression estimator (CIRE) (Cook and Ni, 2006), and directional regression (Li and Wang, 2007).

2.2. Pooled marginal estimators for multivariate response SDR

In the original SIR, we use quantile slicing to partition the support of the univariate response. Direct analogy of this strategy no longer works in the case of multivariate response $Y = (Y_1, \ldots, Y_q)^\top$. For example, if each marginal response is dichotomized through median split, the support of $Y \in \mathbb{R}^q$ is then partitioned into $2^q$ hypercubes. As $q$ increases, the number of observations within each hypercube decreases exponentially, which deteriorates the estimation efficacy. Pooled marginal estimators do not have this limitation, as we demonstrate in this section.

Note that $Y \perp X \mid B^\top X$ in (1) implies $Y_i \perp X \mid B^\top X$, $i = 1, \ldots, q$. From the definition of central space, we have the following observation.

**Proposition 1.** For $i = 1, \ldots, q$, $S_{Y_i|X} \subseteq S_{Y|X}$.

Proposition 1 is the key to pooled marginal slicing estimators and pooled marginal estimators in general. It implies that we can combine univariate response SDR estimators of $S_{Y_i|X}$ to get the multivariate response SDR estimator.

Before we state the pooled marginal slicing method, we need the modified LCM assumption

$$E(X \mid B^\top X) \text{ is linear in } B^\top X, \text{ where } B \text{ is the basis of } S_{Y|X}. \quad (7)$$

Compared to (3), note that (7) accounts for multivariate response. Unless specified otherwise, LCM refers to (7) hereafter. We also state the modified CCV assumption as

$$\text{Var}(X \mid B^\top X) \text{ is nonrandom, where } B \text{ is the basis of } S_{Y|X}. \quad (8)$$
For $i = 1, \ldots, q$, let $J_{i,1}, \ldots, J_{i,H}$ be a partition of the support of $Y_i$. Denote

$$\xi_{i,h} = \Sigma_X^{-1}E(X \mid Y_i \in J_{i,h}), p_{i,h} = E(Y_i \in J_{i,h}),$$

and $M_i = \sum_{h=1}^{H} p_{i,h} \xi_{i,h} \xi_{i,h}^\top$.

Under LCM, we have $\text{span}(M_i) \subseteq S_{Y_i|X} \subseteq S_{Y|X}$. The pooled marginal slicing (PMS) (Aragon, 1997) defines the weighted sum of $M_i$ as

$$M_{\text{PMS}} = \sum_{i=1}^{q} w_i M_i.$$}

Then we have $\text{span}(M_{\text{PMS}}) \subseteq S_{Y|X}$. The eigenvectors corresponding to the $d$ leading eigenvalues of $M_{\text{PMS}}$, the sample version of $M_{\text{PMS}}$, can be used to recover $S_{Y|X}$. Aragon (1997) suggested to choose $w_i$ either as equal weights or proportional to the leading eigenvalues of $M_i$. Pooled marginal slicing avoids partitioning of the overall support of the multivariate response and the “curse of dimensionality”, as only marginal response slicing is involved. Lue (2009) studied the asymptotic properties of the sample PMS estimator, and extended the sequential test approach in Li (1991) to decide the structural dimension of $S_{Y|X}$. Note that $M_{\text{PMS}}$ is based on combining $q$ original SIR kernel matrices $M_i \in \mathbb{R}^{p \times p}$. Pooled marginal slicing that combines $q$ kernel matrices of SIR-$\alpha$ is studied in Saracco (2005) and Barreda et al. (2007). SAVE with pooled marginal slicing is discussed in Yoo et al. (2010). Coudret et al. (2014) proposed a new marginal slicing method that combines the leading eigenvectors of $M_i$ instead of $M_i$ itself.

For univariate response SDR methods that do not require slicing such as principal Hessian directions (PHD) (Li, 1992) and central K-th moment space estimation (CKMS) (Yin and Cook, 2002), Proposition 1 can be applied directly to get the pooled marginal estimators of $S_{Y|X}$. Extensions of CKMS to multivariate response SDR are studied in Cook and Setodji (2003) and Yin and Bura (2006), and PHD with multivariate response is discussed in Lue (2010). Following the minimum discrepancy approach in Cook and Ni (2005), Yoo and Cook (2007) combined marginal CKMS estimators optimally to achieve asymptotic efficiency.

Similar to their univariate response counterparts, multivariate response SDR methods that are related to SIR and SIR-$\alpha$ require the LCM assumption \[\text{7}\], while multivariate response methods that are based on SAVE and PHD
require both the LCM assumption \[7\] and the CCV assumption \[8\].

2.3. Projective resampling for multivariate response SDR

Consider the following two statements: (i) \(Y \perp X \mid B\top X\); (ii) for any fixed vector \(v \in \mathbb{R}^q\), \(v^\top Y \perp X \mid B\top X\). It can be shown that the two statements imply each other. This observation is the basis of the projective resampling (PR) method proposed in Li et al. (2008). The next result is adapted from Theorem 3.1 of Li et al. (2008).

**Proposition 2.** Suppose \(V\) is a random vector uniformly distributed on unit sphere \(S^q\). For each realization \(v \in \mathbb{R}^q\), let \(M(v) \in \mathbb{R}^{p \times p}\) be a positive semi-definite matrix such that \(\text{span}[M(v)] = S_{v^\top Y \mid X}\). Then \(\text{span}\{E[M(V)]\} = S_{Y \mid X}\).

In Proposition 1, the conclusion implies that the pooled marginal estimators are unbiased and may only recover a proper subset of the full central space. Proposition 2, on the other hand, states that the projective resampling estimators can exhaustively recover the central space \(S_{Y \mid X}\) as long as the estimation of \(S_{v^\top Y \mid X}\) is exhaustive for any fixed \(v\).

In practice, we take an i.i.d. sample \(v^{(1)}, \ldots, v^{(m_n)}\) from a uniform distribution on \(S^p\). For example, we can take \(v^{(j)} = G^{(j)}/\|G^{(j)}\|\). Here \(\| \cdot \|\) denotes the Euclidean norm and \(G^{(1)}, \ldots, G^{(m_n)}\) are i.i.d. \(N(0, I_p)\). Let \(J^{(j),1}, \ldots, J^{(j),H}\) be a partition of the support of \(v^{(j)}\). For \(j = 1, \ldots, m_n\), denote

\[
\xi^{(j),h} = \Sigma X^{-1} E(X \mid v^{(j)} \top Y \in J^{(j),h}),
\]

\[
p^{(j),h} = E(v^{(j)} \top Y \in J^{(j),h}),
\]

\[
M^{(j)} = \sum_{h=1}^H p^{(j),h} \xi^{(j),h} \xi^{(j),h}\top.
\]

The projective resampling SIR kernel matrix becomes

\[
M_{PR} = \frac{1}{m_n} \sum_{j=1}^{m_n} M^{(j)}
\]

At the sample level, the estimator of \(M_{PR}\) is denoted as \(\hat{M}_{PR}\). PR-SIR then uses eigenvectors corresponding to the \(d\) leading eigenvalues of \(\hat{M}_{PR}\) to recover the central space. Under some regularity assumptions, Theorem 3.2 of Li et al. (2002) states that \(\hat{M}_{PR}\) is a \(\sqrt{n}\) consistent estimator of \(E[M(V)]\)
as long as \( n = O(m_n) \). In addition to SIR, projective resampling can be combined with other univariate SDR methods. Li et al. (2002) discussed PR-SAVE. Distance covariance (DCOV) (Székely et al., 2007) for SDR with univariate response is studied in Sheng and Yin (2013, 2016), and PR-DCOV is proposed for multivariate response SDR in Chen et al. (2019).

2.4. Distance-based methods for multivariate response SDR

Contour regression (Li et al., 2005) is originally proposed for univariate response SDR, and it can be easily adapted for multivariate response. Let \((\tilde{X}, \tilde{Y})\) be an independent copy of \((X, Y)\). Denote \( Z = \Sigma_X^{-1/2} X, \tilde{Z} = \Sigma_X^{-1/2} \tilde{X} \), and \( A(\varepsilon) = E[(Z - \tilde{Z})(Z - \tilde{Z})^\top \mid ||Y - \tilde{Y}|| < \varepsilon] \). Let \( A_{CR} = (2I_p - A(\varepsilon))^2 \). Under LCM (7) and CCV (8), it can be shown that \( \text{span}(A_{CR}) \subseteq S_{Y|Z} \). See, for example, Theorem 6.1 in Li (2018). Denote \( M_{CR} = \Sigma_X^{-1/2} A_{CR} \Sigma_X^{-1/2} \).

The equivariant property of the central space leads to \( \text{span}(M_{CR}) \subseteq S_{Y|X} \).

At the sample level, let \( \{(Y_i, X_i) : i = 1, \ldots, n\} \) be an i.i.d. sample. Denote \( \hat{\Sigma}_X \) as the sample variance of \( X \), \( \hat{\mu}_X \) as the sample mean of \( X \), and \( \hat{Z}_i = \Sigma_X^{-1/2} (X_i - \hat{\mu}_X) \). For a given \( \varepsilon > 0 \), compute the index set

\[
G(\varepsilon) = \{(i, j) : 1 \leq i < j \leq n, \|Y_i - Y_j\| < \varepsilon\}. \tag{9}
\]

Let \( |G(\varepsilon)| \) be the cardinality of \( G(\varepsilon) \). Then \( A(\varepsilon) \) can be estimated by

\[
\hat{A}(\varepsilon) = |G(\varepsilon)|^{-1} \sum_{(i,j) \in G(\varepsilon)} (\hat{Z}_i - \hat{Z}_j)(\hat{Z}_i - \hat{Z}_j)^\top,
\]

and \( M_{CR} \) is estimated by

\[
\hat{M}_{CR} = \hat{\Sigma}_X^{-1/2} (2I_p - \hat{A}(\varepsilon))^2 \hat{\Sigma}_X^{-1/2}.
\]

The eigenvectors corresponding to the \( d \) leading eigenvalues of \( \hat{M}_{CR} \) are the final contour regression estimator.

An important step in the sample version estimation of contour regression is to get index set \( G(\varepsilon) \) in (9), which directly depends on the pairwise Euclidean distance between two responses \( Y_i \) and \( Y_j \). Nearest neighbor inverse regression (NNIR) (Hsing, 1999) is another method that uses distances between responses. In particular, for a fixed index \( i \), let \( i^* \) be the response
index that corresponds to the nearest neighbor of $Y_i$ such that
\[ \|Y_i^* - Y_i\| = \min_{1 \leq j \leq n, j \neq i} \|Y_j - Y_i\|. \]

The sample level kernel matrix for NNIR is then defined as
\[ \hat{M}_{NN} = \hat{\Sigma}^{-1/2} X \hat{\Lambda}_{NN} \hat{\Sigma}^{-1/2} X, \]
where \( \hat{\Lambda}_{NN} = \frac{1}{2n} \sum_{i=1}^{n} (\hat{Z}_i \hat{Z}_i^\top + \hat{Z}_i^\top \hat{Z}_i). \)

The corresponding population level kernel matrix is
\[ M_{NN} = \Sigma^{-1/2} \Lambda_{NN} \Sigma^{-1/2}, \]
where \( \Lambda_{NN} = \text{Var}(E(Z | Y)). \)

From Theorem 3 and Lemma 5 of Hsing (1999), we know that \( \hat{M}_{NN} \) is a \( \sqrt{n} \) consistent estimator of \( M_{NN}. \) Under the LCM assumption (7), it is easy to see that \( \text{span}(M_{NN}) \subseteq S_{Y|X}. \)

Ying and Yu (2020) proposed Fréchet SDR with metric-spaced valued response, and their weighted inverse regression ensemble (WIRE) estimator can be directly adapted for multivariate response SDR. In particular, the kernel matrix for the WIRE is
\[ M_{WIRE} = \Sigma^{-1/2} \Lambda_{WIRE} \Sigma^{-1/2}, \]
where \( \Lambda_{WIRE} = -E(E(Z | Y) E^\top(\tilde{Z} | \tilde{Y})\|Y - \tilde{Y}\|). \)

Note that \( \Lambda_{WIRE} \) can be reexpressed as
\[ \Lambda_{WIRE} = -E(E(Z | Y) E^\top(\tilde{Z} | \tilde{Y})\|Y - \tilde{Y}\|), \]
which is a distance-weighted average of \( E(Z | Y) E^\top(\tilde{Z} | \tilde{Y})\|Y - \tilde{Y}\|). \) Under the LCM assumption (7), we can easily show that \( \text{span}(M_{WIRE}) \subseteq S_{Y|X}. \)

2.5. Other inverse regression methods for multivariate response SDR

Following similar arguments for equation (11), we have \( \Sigma^{-1} X E(X | Y) \in S_{Y|X} \) under the LCM assumption (7). Instead of slicing the response to estimate \( E(X | Y) \), Bura and Cook (2001) imposed a parametric model between response \( X \) and predictor \( f(Y) \), where \( f: \mathbb{R}^q \rightarrow \mathbb{R}^m \) is a known function, and model \( E(X | Y) \) as a linear function of \( f(Y) \).

In classical SIR, quantile slicing is used to partition the support of the response. K-means inverse regression (KMIR) (Setodji and Cook, 2004) extends this idea and sets the sample level observations into \( K \) groups through
K-means clustering (Hartigan, 1975) of the $n$ responses. In particular, denote $C_k$ as the $k$th response cluster and $n_k$ as the cluster size for $k = 1, \ldots, K$. Then $\bar{Z}_k = n_k^{-1} \sum_{Y_i \in C_k} \bar{Z}_i$ becomes the intra-cluster mean of the standardized predictor, and the kernel matrix of sample level KMIR is

$$\hat{M}_{\text{KMIR}} = \hat{\Sigma}_X^{-1/2} \hat{\Lambda}_{\text{KMIR}} \hat{\Sigma}_X^{-1/2}$$

where $\hat{\Lambda}_{\text{KMIR}} = \frac{1}{n} \sum_{k=1}^{K} n_k \bar{Z}_k \bar{Z}_k^\top$.

KMIR is based on SIR, and can be easily extended to other slicing-based inverse regression methods. For example, Wen et al. (2009) combined CIRE with K-means clustering, and SAVE with K-means clustering is discussed in Yoo et al. (2010).

Denote $m(y) = \mathbb{E}(Z \mid Y = y)$ and let $f_Y(y)$ be the density function of $Y$. For $\omega \in \mathbb{R}^q$, the Fourier transformation of $m(y)f_Y(y)$ becomes

$$\psi(\omega) = \int e^{i\omega^\top y} m(y)f_Y(y)dy = a(\omega) + b(\omega)i.$$ 

Here $i^2 = -1$ is the imaginary unit, $a(\omega)$ and $b(\omega)$ are the real part and the imaginary part of $\psi(\omega)$, respectively. Under LCM, it can be shown that $\text{span}\{a(\omega), b(\omega)\} \subseteq S_{Y \mid X}$. It turns out that $\psi(\omega)$ can be simplified as $\mathbb{E}(e^{i\omega^\top Y Z})$, which can be estimated easily at the sample level. Fourier transformation for univariate response SDR is first discussed in Zhu and Zeng (2006), and its multivariate response extensions include Zhu et al. (2010), Weng and Yin (2018), and Wang et al. (2021).

3. Multivariate response SDR through forward regression

3.1. Multivariate response regression under link violation

Li and Duan (1989) made an interesting discovery about univariate response regression under link violation. In particular, consider a special case of model (2) as $Y = g(b^\top X, \epsilon)$, where $Y$ is univariate response, $g(\cdot)$ is an unknown bivariate link function, and $\epsilon$ is independent of $X$. Li and Duan (1989) suggested that we can assume the unknown link function is linear, and proceed with ordinary least squares estimation to get $b_{\text{OLS}} = \Sigma_X^{-1} \mathbb{E}(XY)$. Then under the LCM assumption that $\mathbb{E}(X \mid b^\top X)$ is linear in $b^\top X$, we have $b_{\text{OLS}} = cb$ for some $c \in \mathbb{R}$. Using the terminology of SDR, this is to say $b_{\text{OLS}} \in S_{Y \mid X}$.
For \( Y \in \mathbb{R}^q, X \in \mathbb{R}^p, B \in \mathbb{R}^{p \times q}, \) and \( \epsilon \in \mathbb{R}^q \) independent of \( X \), the classical multivariate response linear regression model is

\[
Y = B^\top X + \epsilon. \tag{10}
\]

The corresponding least squares estimation aims to minimize \( \mathbb{E}(\epsilon^\top \epsilon) \) over \( B \), which leads to \( B_{\text{OLS}} = \Sigma_X^{-1} \Sigma_{XY} \) with \( \Sigma_{XY} = \mathbb{E}(XY^\top) \). Under model (10), it is easy to see that \( B_{\text{OLS}} = B \). On the other hand, suppose the true model is (1) or (2). Following similar arguments in Li and Duan (1989) or Theorem 8.3 in Li (2018), we still have \( \text{span}(B_{\text{OLS}}) \subseteq S_Y|X \) under the LCM assumption (7).

### 3.2. Reduced rank regression, envelopes, and partial least squares

Let \( A \in \mathbb{R}^{q \times m}, D \in \mathbb{R}^{m \times p}, \) and \( m < \min(p, q) \). The reduced rank regression model (Izenman, 1975) considers

\[
Y = B^\top X + \epsilon, \quad \text{where} \quad B^\top = AD \quad \text{and} \quad \text{rank}(A) = \text{rank}(D) = m. \tag{11}
\]

An important difference between (10) and (11) is that \( B \) has full rank in (10) and reduced rank \( \text{rank}(B) = m \) in (11). For a positive definite matrix \( \Gamma \in \mathbb{R}^{q \times q} \), we may minimize \( \mathbb{E}(\epsilon^\top \Gamma \epsilon) \) over \( A \in \mathbb{R}^{q \times m} \) and \( D \in \mathbb{R}^{m \times p} \) under the constraint that \( \text{rank}(A) = \text{rank}(D) = m \). From Theorem 1 of Izenman (1975), we know the solution of this minimization problem leads to

\[
B_{\text{RR}} = \Sigma_X^{-1} \Sigma_{XY} \Gamma^{1/2} \left( \sum_{j=1}^{m} u_j u_j^\top \right) \Gamma^{-1/2},
\]

where \( u_j \) is the eigenvector corresponding to the \( j \)th leading eigenvalue of \( \Gamma^{1/2} \Sigma_X^\top \Sigma_X^{-1} \Sigma_{XY} \Gamma^{1/2} \). If we choose \( \Gamma = \{\text{Var}(Y)\}^{-1} \), Theorem 2 of Izenman (1975) states that \( B_{\text{RR}} \) is directly related to the canonical correlation analysis (CCA) (Hotelling, 1936). CCA for univariate response SDR and model-free variable selection are studied in Zhou and He (2008) and Alothman et al. (2018), respectively. It is easy to see that

\[
\text{span}(B_{\text{RR}}) \subseteq \text{span}(\Sigma_X^{-1} \Sigma_{XY}) = \text{span}(B_{\text{OLS}}).
\]

If we replace model (11) with model (1), then we still have \( \text{span}(B_{\text{RR}}) \subseteq S_Y|X \) under the LCM assumption.
Denote $\mathcal{S}$ as a subspace of $\mathbb{R}^p$ and let $\mathcal{S}^\perp$ be its orthogonal complement in $\mathbb{R}^p$. Cook et al. (2013) considered the envelope regression model

$$Y = B^\top X + \epsilon,$$

where $\text{span}(B) \subseteq \mathcal{S}$, $\Sigma_X \mathcal{S} \subseteq \mathcal{S}$ and $\Sigma_X \mathcal{S}^\perp \subseteq \mathcal{S}^\perp$. \hfill (12)

Model (12) is known as the predictor envelope model, which is an important extension of the original response envelope regression model in Cook et al. (2010). For an excellent review of response envelope regression and its various extensions, please refer to Cook (2018). Model (12) implies that $\mathcal{S}$ is a reducing subspace of $\Sigma_X$ that contains $\text{span}(B)$. The intersection of all such reducing subspaces is known as the $\Sigma_X$-envelope of $\text{span}(B)$, and is denoted by $\mathcal{E}_{\Sigma_X}(B)$.

Under model (12), we have $B_{\text{OLS}} = \Sigma_X^{-1} \Sigma_{XY} = B$. Together with Proposition 2.4 of Cook et al. (2010), we have

$$\mathcal{E}_{\Sigma_X}(B) = \mathcal{E}_{\Sigma_X}(B_{\text{OLS}}) = \mathcal{E}_{\Sigma_X}(\Sigma_{XY}).$$

Let $C \in \mathbb{R}^{p \times m}$ be a semi-orthogonal basis of $\mathcal{E}_{\Sigma_X}(\Sigma_{XY})$, and we define

$$B_{\text{ENV}} = C(C^\top \Sigma_X C)^{-1} C^\top \Sigma_{XY}. \hfill (13)$$

Following similar argument from Proposition 5 of Cook et al. (2013), we have $B_{\text{ENV}} = B$ under model (12). Furthermore, we still have $B_{\text{ENV}} = B_{\text{OLS}}$ if we replace model (12) with model (1). It follows that $\text{span}(B_{\text{ENV}}) \subseteq \mathcal{S}_{Y|X}$ under the LCM assumption.

Envelope model (12) is closely related to partial least squares (PLS) (Holland, 1988). For integer $a$, define the multivariate Krylov matrix as

$$K_a = (\Sigma_{XY}, \Sigma_X \Sigma_{XY}, \Sigma_X^2 \Sigma_{XY}, \ldots, \Sigma_X^{a-1} \Sigma_{XY}) \in \mathbb{R}^{p \times aq},$$

and denote $\mathcal{K}_a = \text{span}(K_a)$. Cook et al. (2013) showed that there exists an integer $b$ such that $\mathcal{K}_a$ is strictly increasing in $a$ until $a = b$, $\mathcal{K}_a$ becomes a constant for all $a \geq b$, and the constant is $\mathcal{E}_{\Sigma_X}(\Sigma_{XY})$, the $\Sigma_X$-envelope of $\text{span}(\Sigma_{XY})$. Similar to (13), we define

$$B_{\text{PLS}} = K_a(K_a^\top \Sigma_X K_a)^{-1} K_a^\top \Sigma_{XY}. \hfill (14)$$

It follows that $B_{\text{PLS}} = B_{\text{ENV}}$ for large enough $a$, and $\text{span}(B_{\text{PLS}}) \subseteq \mathcal{S}_{Y|X}$ under LCM. Note that the PLS estimator in (14) is exactly parallel to the
univariate response PLS estimation for dimension reduction in Naik and Tsai (2000). The popular SIMPLS algorithm for PLS (de Jong, 1993) is closely related to $B_{\text{PLS}}$, and is demonstrated to be still applicable without assuming linear link functions between $Y$ and $X$ (Cook and Forzani, 2021).

### 3.3. Multiresponse SDR through semiparametric regression

In the case of univariate response, Xia et al. (2002) considered a non-parametric model $Y = m(B^\top X) + \epsilon$ for some $B \in \mathbb{R}^{p \times d}$ and unknown link function $m : \mathbb{R}^d \mapsto \mathbb{R}$. Clearly we have $S_{Y|X} = \text{span}(B)$ under this model. At the sample level, for $i = 1, \ldots, n$, $m(B^\top X_i)$ is approximated by

$$
\hat{m}(B^\top X_i) = m(B^\top X_j) + \hat{m}^\top(B^\top X_j)B^\top(X_i - X_j) = a_j + d_j^\top B^\top(X_i - X_j),
$$

where $\hat{m}(c) = \partial m(c)/\partial c \in \mathbb{R}^d$, $a_j = m(B^\top X_j)$, and $d_j = \hat{m}(B^\top X_j)$. Then we define objective function

$$
\sum_{j=1}^n \sum_{i=1}^n \{Y_i - a_j - d_j^\top B^\top(X_i - X_j)\}^2 w_{ij}, \tag{15}
$$

where $w_{ij} = K_h(X_i - X_j)/\sum_{\ell=1}^n K_h(X_\ell - X_j)$ satisfies $\sum_{i=1}^n w_{ij} = 1$ and $K_h$ denotes a kernel function with bandwidth $h$. MAVE then proceeds to estimate $B$ by minimizing the objective function in (15) over $\{a_j, d_j\}_{j=1}^n$ and $B$ under the constraint $B^\top B = I_d$.

For multivariate response, Yin and Li (2011) studied $f_T(Y)$ as a family of transformations such that $T$ is a random vector and $f_T(Y) = f_T(Y, 1) + t f_T(Y, 1)$. To fix the idea, we may take $f_T(Y) = e^{t^\top T Y}$ as the characteristic function. Let $T_1, \ldots, T_r$ be i.i.d. copies of $T$. The ensemble MAVE then minimizes

$$
\sum_{\ell=1}^2 \sum_{k=1}^r \sum_{j=1}^n \{f_{T_\ell}(Y_i, \ell) - a_{jk}(\ell) - d_{jk}(\ell)B^\top(X_i - X_j)\}^2 w_{ij} \rho_j
$$

to recover the central space. Here $\rho_j$ is a trimming function that excludes some unreliable observations, and we omit its detailed form here.

For $Y \in \mathbb{R}^q$ and $B \in \mathbb{R}^{p \times d}$, Zhang (2021) considered $Y = m(B^\top X) + \epsilon$, where $m(\cdot) = (m_1(\cdot), \ldots, m_q(\cdot))^\top$. Let $a_j = m(B^\top X_j) \in \mathbb{R}^q$ and $D_j = (\hat{m}_1(B^\top X_j), \ldots, \hat{m}_q(B^\top X_j)) \in \mathbb{R}^{d \times q}$. Then $m(B^\top X_i)$ can be approximated
by \( a_j + D_j^\top B^\top (X_i - X_j) \), and multiresponse MAVE proceeds to minimize

\[
\sum_{j=1}^{n} \sum_{i=1}^{n} \{ Y_i - a_j - D_j^\top B^\top (X_i - X_j) \}^\top W \{ Y_i - a_j - D_j^\top B^\top (X_i - X_j) \} w_{ij} \rho_j.
\]

A natural choice of the weight matrix \( W \in \mathbb{R}^{q \times q} \) is the inverse of \( E(\epsilon \epsilon^\top) \), which can be estimated by its sample counterpart. Zhu and Zhong (2015) proposed a similar approach, where \( m(B^\top X_i) \) is estimated by leave-one-out kernel regression and \( B \) is reparameterized such that its first \( d \) rows form an identity matrix. An efficient semiparametric estimator under this model is provided in Zhang et al. (2017), and we omit the details here. The advantage of the semiparametric estimators in this section is that they no longer require the LCM or the CCV assumption, but these estimators are computationally more expensive than the inverse regression estimators and the forward regression estimators that bypass the estimation of the unknown link function \( m(\cdot) \).

4. Conclusions

The dimension reduction methods reviewed in this paper date back to as early as Hotelling (1936), and yet they remain relevant in modern multivariate analysis. For example, in the recent Jubilee volume celebrating the 50th anniversary of *Journal of Multivariate Analysis*, two articles are directly related to SDR. Girard et al. (2022) reviewed extensions of sliced inverse regression, and one such extension is pooled marginal sliced inverse regression. Among many multivariate methods, Cook (2022) discussed the conceptual connections between SDR, partial least squares, and envelopes. In the presence of increasingly complex data, the SDR assumption of dependence of multivariate response variable with respect to only a few linear combinations of the predictors can help data visualization and facilitate data analysis. In this paper, SDR methods with multivariate response are summarized in the inverse regression family and the forward regression family.

There are some emerging trends in the SDR literature with regards to multivariate response regression. Ghosh (2022) cast SDR under the information-theoretic framework, and argued that the central space can be viewed as an information bottleneck. An existing multivariate response SDR method that falls into this framework is Xue et al. (2018). In applications such as missing data analysis, causal inference, and graphical models, a natural assumption
is that response variables interact with each other only through the predictors. Luo (2022) further assumed that the interactions between the response variables only depend on a few linear combinations of the predictors. We expect to see further development of multivariate response SDR along these directions.

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