Statistica Sinica Preprint No: SS-2020-0398

Title	Metric Learning via Cross-Validation
Manuscript ID	SS-2020-0398
URL	http://www.stat.sinica.edu.tw/statistica/
DOI	10.5705/ss.202020.0398
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Notice: Accepted version subject to English editing.	

Statistica Sinica

Metric Learning via Cross-Validation

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Abstract: In this paper, we propose a *cross-validation metric learning* approach to learn a distance metric for dimension reduction in the multiple-index model. We minimize a leave-one-out cross-validation-type loss function, where the unknown link function is approximated by a metric-based kernel-smoothing function. To the best of the authors' knowledge, we are the first to reduce the dimensionality for multiple-index models in a framework of metric learning. The resulting metric contains crucial information on both the central mean subspace and the optimal kernel-smoothing bandwidth. Under weak assumptions on the design of predictors, asymptotic theories are established for the consistency and convergence rate of estimated directions as well as the optimal rate of bandwidth. Furthermore, a novel estimation procedure is developed for determining the structural dimension of the central mean subspace. It is relatively easy-to-implement numerically by employing fast gradient-based algorithms. Various empirical studies illustrate its advantages over other existing methods.

Key words and phrases: Multiple-index model, Sufficient dimension reduction; Nonparamet-

ric regression.

1. Introduction

The performance of many successful machine learning algorithms, such as k-nearest neighbors (Cover and Hart, 1967) (KNN) and support vector machine (Cortes and Vapnik, 1995), heavily rely on a notion of metric or distance between pairs of inputs. The Euclidean distance is a commonly-used distance metric which, however, ignores how samples distribute in the feature space, especially in high dimensional settings. A great deal of effort has been devoted to learning a proper pseudometric or Mahalanobis distance in various circumstances, for example, classification, regression, and clustering etc. A comprehensive discussion may be found in Bellet et al. (2013). It is known that learning a Mahalanobis metric is equivalent to identifying a linear transformation of the feature vectors (or predictors) and applying the standard Euclidean metric to the transformed data (Xing et al., 2003). When the linear projection is of lower-rank, it is particularly important for data visualization, dimension reduction and algorithm efficiency. Specifically, for two entries $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^p$, the Mahalanobis metric

$$d_{\mathbf{M}}(\mathbf{x}, \mathbf{x}') \equiv \sqrt{(\mathbf{x} - \mathbf{x}')^\top \mathbf{M} (\mathbf{x} - \mathbf{x}')} = \|\mathbf{A}^\top (\mathbf{x} - \mathbf{x}')\|,$$

for a $p \times p$ positive semi-definite matrix $\mathbf{M}$, where the second equality is due to the decomposition that $\mathbf{M} = \mathbf{A}\mathbf{A}^\top$ for some $\mathbf{A}$ with $\text{rank}(\mathbf{A}) \le p$. Goldberger et al.

(2005) presented a neighborhood components analysis by maximizing a variant of the leave-one-out KNN score via gradient-based algorithms, which is conceptually appealing and effective for a low-rank $\mathbf{A}$. Nevertheless, its theoretical justifications are generally quite challenging. The large margin nearest neighbors algorithm (LMNN) by Weinberger et al. (2006); Weinberger and Saul (2009) directly learned a metric $\mathbf{M}$ to determine the "target neighbors" in KNN classification based on certain local pairs or triples conditions. For regression problems, Weinberger and Tesauro (2007) constructed a novel metric learning algorithm for kernel regression without any theoretical justification for the resulting metric; Noh et al. (2017) investigated an effective approach for reducing the bias and mean square error in kernel regression under Gaussian models. Though both works studied metric-learning for kernel regression, they did not consider the problems for multiple-index models, which have received much attention and were investigated intensively in many scientific fields.

In this paper, we focus on dimension reduction for the multiple-index model in a framework of metric learning. To be precise, for a response $Y \in \mathbb{R}$ and a vector of predictors $\mathbf{X} \in \mathbb{R}^p$, we concentrate on reducing the dimensionality of the mean function $f(\mathbf{X}) = E(Y|\mathbf{X})$, leaving the rest of $Y|\mathbf{X}$ as "nuisance parameters". A reduced-rank structure of the regressors $f(\mathbf{x})$ leads to the popular multiple-index model

$$Y = g(\mathbf{L}_0^\top \mathbf{X}) + \epsilon, \tag{1.1}$$

where $g : \mathbb{R}^{r_0} \to \mathbb{R}$ is an unknown link function ($r_0 \leq p$), $\mathbf{L}_0$ is a $p \times r_0$ column orthogonal matrix and the noise ϵ satisfies $E(\epsilon|\mathbf{X}) = 0$ almost surely. The subspace spanned by the column vectors of $\mathbf{L}_0$ is referred to as the *central mean subspace* (CMS) introduced by Cook and Li (2002), which is of major concern in the literature. It is well defined and is unique under mild conditions. We refer r_0 as the structural dimension of the CMS and the column vectors of $\mathbf{L}_0$ as the directions in CMS.

We notice that there is a vast literature in statistics on dimension reduction of the model (1.1) and its variants. One of the most fundamental and powerful methods is the seminal sliced inverse regression (SIR) invented by Li (1991). It can be used to find vectors outside the CMS but inside the central subspace, the smallest subspace capturing the complete dependence of Y on $\mathbf{X}$ (Cook and Li, 2002). Li (1991) also developed a sequential testing procedure to determine the dimension of CMS when r_0 is unknown. Since then, many state-of-the-art inverse regression-based approaches have been developed, such as the sliced average variance estimation (SAVE) (Shao et al., 2007); see Bura and Cook (2001a); Bura (2003); Cook and Li (2004); Cook and Ni (2005); Yin and Cook (2006), among many others. These methods are computationally simple and thus widely applied in data mining. But it is known that the inverse regression based methods usually need strong assumptions on the design of $\mathbf{X}$, such as the elliptical symmetry condition, similar to the requirement in the principal Hessian directions method (pHd) (Li, 1992; Cook, 1998). As an important alternative, Xia et al. (2002) invented a novel minimum average variance estimation method (MAVE) based on the local linear smoothing. Based on MAVE, they also proposed a consistent estimate for the dimension of the CMS. Other related approaches including the average derivative estimation (Härdle and Stoker, 1989), the structure adaptive approach (SA) (Hristache et al., 2001) and the outer products of gradients (OPG) (Samarov, 1993), are designed to estimate the derivative of the regressor $g(\mathbf{L}_0^\top \mathbf{x})$ pertaining to the CMS. More advancements can be found in Xia (2008); Wang and Xia (2008); Dalalyan et al. (2008); Chen et al. (2011); Alquier and Biau (2013); Akritas (2016) etc. Overall, compared with the inverse regression, direct regression methods are easy-to-implement and are superior in finite sample performance (Hristache et al., 2001; Xia et al., 2002; Xia, 2007). With the bandwidth carefully chosen, direct regression methods reported elegant results. Ma and Zhu (2012) provided a novel semiparametric approach to estimate CMS through solving estimating equations and studied its efficiency issues in Ma and Zhu (2014). Recently, an important discussion paper (Cannings and Samworth, 2017) introduced a general classifier for high dimensional data using random projections.

In this paper, we propose the *cross-validation metric learning* (CVML) approach for learning a distance metric that contains crucial information on the CMS and the nonparametric link function in model (1.1). For any fixed dimension r, such that $1 \leq r \leq p$, the CVML procedure is proposed to minimize a leave-one-out cross-validation-type sum of squared errors over matrix $\mathbf{A} \in \mathbb{R}^{p\times r}$, in which the link function is approximated by the Nadaraya-Waston kernel estimator. One can thus estimate the directions of the CMS and the bandwidth of the link function simultaneously by the singular value decomposition $\hat{\mathbf{M}} = \hat{\mathbf{A}}\hat{\mathbf{A}}^\top = \hat{\mathbf{L}}_1\hat{\mathbf{H}}^{-2}\hat{\mathbf{L}}_1^\top$. When $r = r_0$, the CVML estimate for the directions of the CMS is shown to be consistent at a certain convergence rate. Further, a sequential procedure is developed to determine the dimension r_0 of the CMS when it is unknown. The results of simulation studies show that the proposal outperforms other alternatives in terms of estimating the directions and dimension of the CMS. The CVML procedure is model-free in the sense that its validity does not rely on any specific functional relation between the response variable and predictors, thus makes it practically appealing. Furthermore, unlike many other metric learning algorithms, such as methods developed in Xing et al. (2003); Weinberger et al. (2006); Weinberger and Saul (2009), the loss function of the proposed CVML is differentiable and free of local constraints. As a result, computation of the proposal is straightforward with the help of gradient-based algorithms.

The rest of the paper is organized as follows. Section 2 describes the proposed CVML procedure for estimating the directions and the dimension of the CMS and presents the related theoretical results of consistency, asymptotic expansion and convergence rate. Results of simulations and real data applications are given in Sections 3–4. Assumptions and remarks are summarized in Appendix. Technical proofs are provided in the supplementary material.

2. Cross-validation metric learning method

Suppose that $\{(Y_i, \mathbf{X}_i), i = 1, \ldots, n\}$ are independent random copies of $(Y, \mathbf{X})$ taking values in $\mathbb{R} \times \mathbb{R}^p$ and ϵ_i are random errors such that

$$Y_i = g(\mathbf{L}_0^\top \mathbf{X}_i) + \epsilon_i, \quad i = 1, \ldots, n, \tag{2.1}$$

where $\mathbf{X}_i$ is supported by a bounded set Ω.

Note that model (1.1) is not uniquely defined. This is because for any orthonormal transformation $\mathbf{Q} \in \mathbb{R}^{r_0 \times r_0}$,

$$f(\mathbf{x}) = g(\mathbf{L}_0^\top \mathbf{x}) = g(\mathbf{Q}^\top \mathbf{Q} \mathbf{L}_0^\top \mathbf{x}) \equiv g_1(\mathbf{L}_0^{*\top} \mathbf{x}),$$

where $g_1(\mathbf{u}) = g(\mathbf{Q}^\top \mathbf{u})$ and $\mathbf{L}_0^* = \mathbf{L}_0 \mathbf{Q}^\top$. Although $\mathbf{L}_0$ is not unique, the subspace spanned by the column vectors of $\mathbf{L}_0$, denoted by $\mathcal{S}(\mathbf{L}_0)$, is unique with the projection matrix $\mathbf{L}_0 \mathbf{L}_0^\top$. In this paper, $\mathcal{S}(\mathbf{L}_0)$ is referred to as the CMS.

2.1. Estimating the directions in CMS

Given the true projection matrix $\mathbf{L}_0$, the regression function can be written as

$$f(\mathbf{x}) = E(Y | \mathbf{X} - \mathbf{x} \in \mathbf{L}_0^\perp),$$

where $\mathbf{L}_0^\perp$ denotes the space spanned by vectors perpendicular to $\mathcal{S}(\mathbf{L}_0)$. We estimate $f(\cdot)$ by means of the kernel smoothing method as follows.

For any fixed $1 \le r \le p$, set $\mathbf{M} = \mathbf{L}_1 \mathbf{H}^{-2} \mathbf{L}_1^\top$, where $\mathbf{L}_1$ is of size $p \times r$ satisfying $\mathbf{L}_1^\top \mathbf{L}_1 = \mathbf{I}_r$ and $\mathbf{H} = \text{diag}(h_1, \ldots, h_r)$ is the bandwidth matrix with $h_1 > 0, \ldots, h_r >$

0. Hence, the matrix $\mathbf{M}$ is positive semi-definite and can be viewed as a distance metric between two samples. The kernel function based on the distance metric $\mathbf{M}$ is defined as

$$K_{\mathbf{M}}(\mathbf{t}) = \frac{1}{h_1 \cdots h_r} K(\mathbf{t}^\top \mathbf{M} \mathbf{t}) = \frac{1}{h_1 \cdots h_r} K(\mathbf{t}^\top \mathbf{L}_1 \mathbf{H}^{-2} \mathbf{L}_1^\top \mathbf{t}), \ \mathbf{t} \in \mathbb{R}^p,$$

where $K(\cdot)$ is a univariate kernel function defined on $[0, \infty)$ with a bounded support satisfying $\int_{\mathbf{s} \in \mathbb{R}^r} K(\|\mathbf{s}\|^2) d\mathbf{s} = 1$.

Heuristically, the Nadaraya-Waston kernel-smoothing estimator of $f(\mathbf{x})$ is

$$\hat{f}_n(\mathbf{x}) = \frac{\sum_{i=1}^n Y_i K_{\mathbf{M}}(\mathbf{X}_i - \mathbf{x})}{\sum_{i=1}^n K_{\mathbf{M}}(\mathbf{X}_i - \mathbf{x})}, \text{ for any } \ \mathbf{x} \in \mathbb{R}^p,$$

where $\mathbf{M}$ is unknown and to be estimated. Thus, we define

$$K_{j,i}^* = \frac{K_{\mathbf{M}}(\mathbf{X}_j - \mathbf{X}_i)}{\sum_{l \neq i} K_{\mathbf{M}}(\mathbf{X}_l - \mathbf{X}_i)}, \text{ for } \ j \neq i,$$

and $K_{i,i}^* = 0$. Note that $\sum_{j=1}^n K_{j,i}^* = 1$ and $K_{j,i}^* \neq K_{i,j}^*$, for any $i \neq j$. Let $\mathbb{S}_+^p$ be the cone of symmetric positive semi-definite $p \times p$ real-valued matrices. The proposed estimator of $\mathbf{M}$ is the minimizer of

$$\text{CM}_n(\mathbf{M}) = \frac{1}{n} \sum_{i=1}^n \{\hat{f}^{(-i)}(\mathbf{X}_i) - Y_i\}^2 w(\mathbf{X}_i), \tag{2.2}$$

over all $\mathbf{M} \in \mathbb{S}_+^p$, denoted by $\hat{\mathbf{M}}$, where

$$\hat{f}^{(-i)}(\mathbf{X}_i) = \sum_{j=1}^n Y_j K_{j,i}^* = \frac{\sum_{j \neq i} Y_j K_{\mathbf{M}}(\mathbf{X}_j - \mathbf{X}_i)}{\sum_{j \neq i} K_{\mathbf{M}}(\mathbf{X}_j - \mathbf{X}_i)} \tag{2.3}$$

and $w(\cdot)$ is a bounded and positive weight function with support Ω° strictly inside Ω. The objective function (2.2) is essentially a leave-one-out cross-validation based on the squared errors, and thus the proposed procedure is called *cross-validation metric learning*. The weight function $w(\cdot)$ is introduced to handle the boundary effect by letting $w(\mathbf{x}) = 0$ if $\inf_{\mathbf{y}\in\partial\Omega} \|\mathbf{x} - \mathbf{y}\| < c$ for some constant $c > 0$, where $\partial\Omega$ is the boundary of Ω.

In real application, to obtain $\hat{\mathbf{M}}$, we remove the constraint $\mathbf{M} \in \mathbb{S}_+^p$ by the decomposition $\mathbf{M} = \mathbf{A}\mathbf{A}^\top$, for all $\mathbf{A} \in \mathbb{R}^{p\times r}$. Let $\text{vec}(\mathbf{A})$ denote the vectorization of a matrix $\mathbf{A}$ by its column vectors and $\mathbf{A}_1 \otimes \mathbf{A}_2$ denote the Kronecker product of $\mathbf{A}_1$ and $\mathbf{A}_2$. Then, (2.3) can be written as

$$\hat{f}^{(-i)}(\mathbf{X}_i) = \sum_{j=1}^{n} Y_j K^*_{j,i} = \frac{\sum_{j\neq i} Y_j K(\|(\mathbf{I}_r \otimes \mathbf{X}_{ij}^\top)\text{vec}(\mathbf{A})\|^2)}{\sum_{j\neq i} K(\|(\mathbf{I}_r \otimes \mathbf{X}_{ij}^\top)\text{vec}(\mathbf{A})\|^2)},$$

where $\mathbf{X}_{ij} \equiv \mathbf{X}_j - \mathbf{X}_i$. Taking derivative of (2.2) with respect to $\text{vec}(\mathbf{A})$ yields a gradient rule:

$$\frac{\partial \text{CM}_n(\mathbf{M})}{\partial \text{vec}(\mathbf{A})} = -\frac{2}{n}\sum_{i=1}^{n} \frac{\partial \hat{f}^{(-i)}(\mathbf{X}_i)}{\partial \text{vec}(\mathbf{A})}\{Y_i - \hat{f}^{(-i)}(\mathbf{X}_i)\}w(\mathbf{X}_i), \tag{2.4}$$

where

$$\frac{\partial \hat{f}^{(-i)}(\mathbf{X}_i)}{\partial \text{vec}(\mathbf{A})} = \frac{2\sum_{j\neq i} \dot{K}(\|\mathbf{A}^\top\mathbf{X}_{ij}\|^2)\{Y_j - \hat{f}^{(-i)}(\mathbf{X}_i)\}(\mathbf{I}_r \otimes \mathbf{X}_{ij}\mathbf{X}_{ij}^\top)\text{vec}(\mathbf{A})}{\sum_{j\neq i} K(\|\mathbf{A}^\top\mathbf{X}_{ij}\|^2)}.$$

Here, $\dot{K}(\cdot)$ denotes the first derivative of the kernel function $K(\cdot)$. Therefore, the numerical computation of the proposed CVML can be carried out by employing gradient-based algorithms, such as conjugate gradient or gradient descent. In particular, when $r \ll p$, the computation would be rather efficient. To further improve the computational efficiency, one may also consider using algorithms such as stochastic gradient decent. Once $\hat{\mathbf{M}}$ is obtained, the estimated bandwidth matrix $\hat{\mathbf{H}}$ and directions $\hat{\mathbf{L}}_1$ can be calculated immediately by the singular value decomposition of $\hat{\mathbf{M}}$.

The detailed estimation procedure for the proposed CVML method is summarised in Algorithm 1. This procedure is free of local pairwise constraints that are required in many other metric learning method. Moreover, the procedure to simultaneously estimate the effective directions and the bandwidths avoids the bias problem arising from two separate cost functions for the estimation of the directions and the link function in many popular methods; see Hall (1989); Härdle and Stoker (1989); Carroll et al. (1997).

Algorithm 1: Estimation of directions and bandwidth

Data: $\mathbf{X}$, $\mathbf{y}$, r

Result: $\hat{\mathbf{L}}_1$, $\hat{\mathbf{H}}$

1 Get $\hat{\mathbf{A}}$ by minimizing (2.2) with the gradient (2.4);

2 Calculate $\hat{\mathbf{M}} = \hat{\mathbf{A}}\hat{\mathbf{A}}^\top$;

3 Singular value decomposition $\hat{\mathbf{M}} = \hat{\mathbf{L}}_1\hat{\boldsymbol{\Lambda}}\hat{\mathbf{L}}_1^\top$;

4 $\hat{\mathbf{H}} = \hat{\boldsymbol{\Lambda}}^{-1/2}$;

Remark 1. It is known that Härdle et al. (1993) first applied cross-validation technique to estimate the single-index model ($r_0 = 1$) and the estimator is shown to have good asymptotic properties. Our proposal, however, is similar to but substantially distinguishing from their method. It is not off-the-shelf to extend the idea of cross-validation method to multiple index models, because they used a grid search algorithm to estimate directions and bandwidths, which would be inefficient and costly in a higher dimensional settings. Also, instead of estimating the bandwidths and directions separately as they performed, we simply regard the fusion matrix $\mathbf{M}$ as a Mahalanobis metric.A relevant work to Algorithm 1 is Weinberger and Tesauro (2007). Nonetheless, the bandwidth and directions in the CMS are not studied in their setup, and no theoretical justification on the properties of $\hat{\mathbf{M}}$ was established. They did not consider how to estimate the desired dimensionality when it is unknown. Different from Weinberger and Tesauro (2007) and Noh et al. (2017), we study in depth the structure of $\hat{\mathbf{M}}$ (eigenvalues and eigenvectors) in a statistical way and attempt to apply it to multiple-index models.

Remark 2. Different from some SIR based methods (Li, 1991, 1992; Cook, 1998), the proposal gets free of the linearity condition and constant covariance condition; see condition (C1) in Appendix. Methods such as the seminal MAVE and SA methods, usually perform a non-parametric kernel estimation procedure to estimate the link function or its derivative, which concerns selecting bandwidths to be used in estimating effective directions. This is not needed in the proposed CVML approach, since it directly obtains a data-driven bandwidth. For all large n, the estimated bandwidth is shown to be at the same rate as the theoretically optimal bandwidth in the sense of minimizing the mean weighted integrated squared errors

$$\int_{\mathbf{x}\in\mathbb{R}^p} E\{\hat{f}_n(\mathbf{x}) - f(\mathbf{x})\}^2 w(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x}. \tag{2.5}$$

Here and after, $\|\mathbf{A}\|$ denotes the Frobenius norm for matrix $\mathbf{A}$; $\dot{g}(\mathbf{x})$ and $\ddot{g}(\mathbf{x})$ denote the first and second derivative of $g(\cdot)$ at $\mathbf{x}$, respectively.

Theorem 1 (Consistency)**.** *Suppose that the true dimension r_0 of the CMS is known and conditions (C1)–(C5) in Appendix hold. Define $\mathbf{h} = (h_1, \ldots, h_{r_0})^\top$. If $\|\mathbf{h}\| \to 0$ and $h_1 h_2 \cdots h_{r_0} > n^{-\delta}$ for some $0 < \delta < 1$, then $\hat{\mathbf{L}}_1 \to \mathbf{L}^*$ in probability as $n \to \infty$, where $\mathcal{S}(\mathbf{L}^*) = \mathcal{S}(\mathbf{L}_0)$.*

Theorem 1 tells that under certain conditions, the estimated direction $\hat{\mathbf{L}}_1$ converges to the directions in the true CMS. In other words, the CVML method is able to estimate the directions in CMS consistently. To figure out the convergence rate, we first present the asymptotic expansion of $\mathrm{CM}_n(\mathbf{M})$. Let

$$R_1(K)\mathbf{I}_{r_0} = \int_{\mathbf{s}\in\mathbb{R}^{r_0}} \mathbf{s}\mathbf{s}^\top K(\|\mathbf{s}\|^2) d\mathbf{s},\ R_2(K) = \int_{\mathbf{s}\in\mathbb{R}^{r_0}} K^2(\|\mathbf{s}\|^2) d\mathbf{s}.$$

Theorem 2 (Asymptotic expansion)**.** *Suppose that the true dimension r_0 of the CMS is known and conditions (C1)–(C5) in Appendix hold. Let*

$$\mathbf{L} = \begin{pmatrix} \mathbf{L}_1 & \mathbf{L}_2 \end{pmatrix}$$

be a $p \times p$ orthonormal matrix, where $\mathbf{L}_1 \in \mathbb{R}^{p\times r_0}$ and $\mathbf{L}_2$ is the augmented orthonormal basis in $\mathbb{R}^p$ satisfying $\|\mathbf{L}_0^\top \mathbf{L}_2\| \to 0$. Let $f_{r_0}(\cdot)$ be the density of $\mathbf{L}_0^\top \mathbf{X}$. Then, uniformly over $\{\mathbf{h} : \|\mathbf{h}\| \le \delta_n\}$ for any $\delta_n \to 0$, and $h_1 h_2 \cdots h_{r_0} > n^{-\delta}$ for some $0 < \delta < 1$,

$$\begin{aligned} \mathrm{CM}_n(\mathbf{M}) - \eta_0 &= \int_{\mathbf{t}\in\mathbb{R}^p} \{\psi(\mathbf{t},\mathbf{h},\mathbf{L}_1)\}^2 f_{\mathbf{X}}(\mathbf{t}) \frac{w(\mathbf{t})}{f_{r_0}^2(\mathbf{L}_0^\top \mathbf{t})} d\mathbf{t} + \frac{R_2(K)V_0}{nh_1\cdots h_{r_0}} \\ &\quad + o_p\left(\|\mathbf{L}_0^\top \mathbf{L}_2\|^2 + \|\mathbf{h}\|^4 + \frac{1}{nh_1\cdots h_{r_0}} \right), \end{aligned} \tag{2.6}$$

where $\eta_0 = n^{-1}\sum_{i=1}^n w(\mathbf{X}_i)\epsilon_i^2$,

$$\begin{aligned} \psi(\mathbf{t},\mathbf{h},\mathbf{L}_1) &= \dot{g}(\mathbf{L}_0^\top \mathbf{t})^\top \mathbf{L}_0^\top \mathbf{L}_2 \mathbf{b}(\mathbf{L}_0^\top \mathbf{t}) + R_1(K) tr\{\mathbf{H}\mathbf{L}_1^\top \mathbf{L}_0 \mathbf{A}(\mathbf{L}_0^\top \mathbf{t})\mathbf{L}_0^\top \mathbf{L}_1 \mathbf{H}\}, \\ \mathbf{A}(\mathbf{L}_0^\top \mathbf{t}) &= \frac{1}{2}\ddot{g}(\mathbf{L}_0^\top \mathbf{t}) f_{r_0}(\mathbf{L}_0^\top \mathbf{t}) + \dot{g}(\mathbf{L}_0^\top \mathbf{t}) \dot{f}_{r_0}(\mathbf{L}_0^\top \mathbf{t})^\top, \quad \mathbf{t} \in \mathbb{R}^p, \\ \mathbf{b}(\mathbf{L}_0^\top \mathbf{t}) &= E_{\mathbf{u}_2|\mathbf{u}_1}(\mathbf{U}_2 - \mathbf{L}_0^{\perp\top}\mathbf{t} | \mathbf{U}_1 = \mathbf{L}_0^\top \mathbf{t}) f_{r_0}(\mathbf{L}_0^\top \mathbf{t}), \\ V_0 &= \int_{\mathbf{t}\in\mathbb{R}^p} \sigma^2(\mathbf{L}_0^\top \mathbf{t}) \frac{f_{\mathbf{X}}(\mathbf{t}) w(\mathbf{t})}{f_{r_0}(\mathbf{L}_0^\top \mathbf{t})} d\mathbf{t}. \end{aligned}$$

Remark 3. The asymptotic expansion in (2.6) offers some insight into the CVML method by noting that the first term on the right-hand side of (2.6) is the bias term and the second term is the variance term. For instance, when the identifiability condition (C4) in Appendix is violated, there exists a unit vector $\boldsymbol{\ell}_1 \in \mathbb{R}^p$, such that $\boldsymbol{\ell}_1^\top \mathbf{L}_0 \dot{g}(\mathbf{L}_0^\top \mathbf{t}) = 0$ for all $\mathbf{t} \in \mathbb{R}^p$. Then, $\boldsymbol{\ell}_1^\top \mathbf{L}_0 \mathbf{A}(\mathbf{L}_0^\top \mathbf{t}) \mathbf{L}_0^\top \boldsymbol{\ell}_1 = 0$. The bandwidth along the direction $\boldsymbol{\ell}_1$ need not be small. In a special case that $g(\cdot)$ is constant and thus $\mathbf{A}(\mathbf{L}_0^\top \mathbf{t}) = \mathbf{0}$, the bias term is irrelevant to the bandwidth $\mathbf{h}$ and only the variance term $R_2(K)V_0/(nh_1 \cdots h_{r_0})$ plays a role in $\mathrm{CM}_n(\mathbf{M}) - \eta_0$. As a result, the estimated bandwidth tends to be large and the estimate of the link function reduces to a constant.

The following corollary presents the rate of convergence of $\hat{\mathbf{L}}_1$. Define the distance between the subspaces spanned by $\mathbf{L}_0$ and $\hat{\mathbf{L}}_1$ as $m(\hat{\mathbf{L}}_1, \mathbf{L}_0) = \|\mathbf{L}_0^\top(\mathbf{I}_p - \hat{\mathbf{L}}_1\hat{\mathbf{L}}_1^\top)\|$, where $\mathbf{I}_p$ is a $p \times p$ identity matrix.

Corollary 1 (Rate of convergence)**.** *Suppose that the true dimension r_0 of the CMS is known and conditions (C1)–(C5) in Appendix hold. Then,*

$$m(\hat{\mathbf{L}}_1, \mathbf{L}_0) = O_p(\|\mathbf{h}\|^2).$$

Moreover, the resulting bandwidth minimizing (2.6) is at the order of $n^{-1/(r_0+4)}$.

Recall that the theoretically optimal bandwidth for the nonparametric estimation in the sense of minimizing (2.5) is also at the order of $n^{-1/(r_0+4)}$. This implies that we can simultaneously estimate the central mean subspace and the link function with the optimal rate of bandwidth.

On the other hand, it can be seen from the asymptotic expansion (2.6) in Theorem 2 that the esimated directions in CMS is only relevant to the bias term. As a result, the convergence rate of $\hat{\mathbf{L}}_1$ is at the order of $\|\mathbf{h}\|^2$. Intuitively, with narrower bandwidth, the convergence rate would be faster. This finding induces the following correction method that allows faster rate of convergence. Instead of minimizing

$\mathrm{CM}_n(\mathbf{M})$, one can minimize

$$\mathrm{CM}_n(\mathbf{M}) - \frac{R_2(K)\hat{V}_0}{nh_1\cdots h_{r_0}}$$

over $\mathbf{M}$, where $\hat{V}_0$ is an estimate of V_0. Recall that V_0 is related to the density $f_{\mathbf{X}}(\mathbf{x})$ and the variance function $\sigma^2(\mathbf{x})$ that are usually unknown. The density $f_{\mathbf{X}}(\mathbf{x})$ can be estimated by conventional density estimation methods. The variance function $\sigma^2(\cdot)$ can be estimated by referring to Härdle et al. (1993). The correction method improves the rate of convergence and is of theoretical interest.

The following remark provide more insights into the convergence rate and the optimal rate of bandwidth in Corollary 1.

Remark 4. Let $\boldsymbol{\alpha} = (\alpha_1,\ldots,\alpha_{r_0})^\top$, $h_1 = \alpha_1 n^{-1/(r_0+4)},\cdots,h_{r_0} = \alpha_{r_0} n^{-1/(r_0+4)}$, $\mathbf{L}_0^\top\mathbf{L}_1 = \tilde{\mathbf{D}}_{r_0\times r_0}$, which is an orthonormal matrix, and $\mathbf{L}_0^\top\mathbf{L}_2 = n^{-2/(r_0+4)}\mathbf{D}_{r_0\times(p-r_0)}$. The leading term of the right-hand side of (2.6) is

$$n^{-\frac{4}{r_0+4}}\Big\{\int_{\mathbf{t}\in\mathbb{R}^p}\Big[\dot{g}(\mathbf{L}_0^\top\mathbf{t})^\top\mathbf{D}\mathbf{b}(\mathbf{L}_0^\top\mathbf{t}) + R_1(K)\mathrm{tr}\big\{\mathrm{diag}(\boldsymbol{\alpha})\tilde{\mathbf{D}}^\top\mathbf{A}(\mathbf{L}_0^\top\mathbf{t})\tilde{\mathbf{D}}\mathrm{diag}(\boldsymbol{\alpha})\big\}\Big]^2 \times \frac{f_{\mathbf{X}}(\mathbf{t})w(\mathbf{t})}{f_{r_0}^2(\mathbf{L}_0^\top\mathbf{t})}d\mathbf{t} + \frac{R_2(K)V_0}{\alpha_1\cdots\alpha_{r_0}}\Big\}. \tag{2.7}$$

Denote the minimizer of (2.7) as $\boldsymbol{\alpha}_*,\mathbf{D}_*,\tilde{\mathbf{D}}_*$. As a result, the optimal bandwidth $\hat{\mathbf{h}} = n^{-1/(r_0+4)}\boldsymbol{\alpha}_*\{1+o(1)\}$ and $\hat{\mathbf{L}}_1 = (\mathbf{L}_0 - n^{-2/(r_0+4)}\hat{\mathbf{L}}_1^\perp\mathbf{D}_*^\top)\tilde{\mathbf{D}}_*^{-1}\{1+o(1)\}$.

2.2. Determining the dimension of CMS

The true dimension r_0 is crucial to the estimation of the CMS but it is often unknown in practice. Determining r_0 is also a non-trivial task. Many existing approaches to determine the structural dimension of CMS are inspired by the equivalence between dimension reduction and matrix eigen-decomposition. The sequential test methods (Li, 1991; Bura and Cook, 2001b; Cook and Ni, 2005) generally cannot give a consistent $\hat{r}$ due to the type-I error. The bootstrapping methods (Ye and Weiss, 2003; Zhu and Zeng, 2006; Luo and Li, 2016) can determine the dimension in a data-driven manner but are computationally burdensome. The BIC criterion (Zhu et al., 2006; Zhu and Zhu, 2007) and the ratio estimation methods (Luo et al., 2009; Xia et al., 2015; Zhu et al., 2019, 2020) are able to produce consistent estimation of r_0 and are computationally attractive. The sparse eigen-decomposition proposed by Zhu et al. (2010) can estimate directions and the structural dimension of the CMS simultaneously. However, the aforementioned methods rely on a relevant kernel matrix, usually obtained by inverse regression-based estimation procedures, and thus the link function is lost. In nonparametric regression framework, Xia et al. (2002) proposed to determine r_0 through a leave-one-out cross-validation procedure based on MAVE estimated directions. Inspired by the novel ideas of Xia et al. (2002) and the ratio estimation approaches, we propose the CVML method for determining the dimension of CMS.

Proposition 1. *Suppose that the conditions (C1)–(C5) in Appendix hold. Under* *model (1.1), as $n \to \infty$, with probability tending to one,*

(i) $\mathrm{CM}_n(\hat{\mathbf{M}}_r)/\mathrm{CM}_n(\hat{\mathbf{M}}_{r_0}) > 1$, *for all* $1 \leq r < r_0$*;*

(ii) $\mathrm{CM}_n(\hat{\mathbf{M}}_r)/\mathrm{CM}_n(\hat{\mathbf{M}}_{r_0}) \to 1$, *for all* $r_0 \leq r \leq p$.

It is seen from the Proposition 1 that $\mathrm{CM}_n(\hat{\mathbf{M}}_r) > \mathrm{CM}_n(\hat{\mathbf{M}}_{r_0})$ for all $r < r_0$ because of lack of fit. Intuitively, $\mathrm{CM}_n(\hat{\mathbf{M}}_r)$ would decrease as r becomes larger and larger until it arrived at r_0. Therefore, we attempt to track the first time that the ratio $\mathrm{CM}_n(\hat{\mathbf{M}}_r)/\mathrm{CM}_n(\hat{\mathbf{M}}_{r+1})$ hits one and estimate the dimension of CMS as

$$\hat{r} \equiv \min_{0 \leq r \leq p-1} \left\{ r : \left| \frac{\mathrm{CM}_n(\hat{\mathbf{M}}_r)}{\mathrm{CM}_n(\hat{\mathbf{M}}_{r+1})} - 1 \right| < \tau_n \right\},$$

where τ_n is positive and converges to zero at a slow rate and $\mathrm{CM}_n(\hat{\mathbf{M}}_0) = n^{-1}(y_i - \bar{y})^2$. The choice of τ_n is given in Section 3. The estimation procedure are detailed in Algorithm 2.

Remark 5. The estimation procedure is proceeded by ranging r from 1 to p. The method in Xia et al. (2002) involves the calculation of cross-validation errors for all $r \in \{1, \ldots, p\}$. Our proposed approach would stop at certain $r < p$ and thus possibly avoids the computational burden caused by the calculation of $\hat{\mathbf{M}}_r$ for some large r. In real application, to ensure the estimation accuracy, one can require that the procedure stops only when two consecutive ratios close to 1 or equivalently modify the stopping condition as $|\mathrm{CM}_n(\hat{\mathbf{M}}_r)/\mathrm{CM}_n(\hat{\mathbf{M}}_{r+1}) - 1| < \tau_n$ and $|\mathrm{CM}_n(\hat{\mathbf{M}}_{r+1})/\mathrm{CM}_n(\hat{\mathbf{M}}_{r+2}) - 1| < \tau_n$ for some fixed r.

The empirical performance of the proposed method in terms of determining the dimension of CMS are shown in the next section.

Algorithm 2: Determining the dimension of CMS

Data: $\mathbf{X}$, $\mathbf{y}$

Result: $\hat{r}$, $\hat{\mathbf{M}}_{\hat{r}}$

Initialization: τ_n, $r = 1$, $\Delta = 10$, $Err_0 = n^{-1}\sum_{i=1}^{n}(y_i - \bar{y})^2$;

while $|\Delta - 1| > \tau_n$ **do**

  if r=p+1 **then**

    print $\hat{r} = p$, **break**;

  else

    Calculate $\hat{\mathbf{M}}_r$ by Algorithm 1, $Err_1 = \mathrm{CM_n}(\hat{\mathbf{M}}_r)$;

    $\Delta = Err_0/Err_1$, $Err_0 = Err_1$;

    $r = r + 1$;

$\hat{r} = r - 2$.

---

3. Simulations

In this section, we examine the performance of the proposed CVML method in terms of estimating the directions in CMS and determining the structural dimension of the CMS, respectively. We adopt the Gaussian type kernel function $K(\mathbf{u}) = \exp(-\frac{1}{2}\mathbf{u}^\top\mathbf{M}\mathbf{u})$. For simplicity, the weight function $w(\mathbf{x})$ is set to be 1, and thus all the observations have equal weights. The CVML approach is implemented with the help of the limited-memory Broyden Fletcher Goldfarb Shanno (BFGS) algorithm in the *lbfgs* package in R. Let ϵ follow the standard normal distribution $N(0,1)$. We generate models from the following cases:

Example 3.1. We generate X_i from the standard normal distribution $N(0,1)$ independently; we generate Y from

$$\text{Model 1: } Y = X_1/\{0.5 + (X_2 + 1.5)^2\} + 0.5\epsilon,$$

$$\text{Model 2: } Y = X_1(X_1 + X_2 + 1) + 0.5\epsilon,$$

where Model 1 and Model 2 were used in the literature, such as Li (1991) and Xia et al. (2002). The sample size is set at $n = 200$ or $n = 400$ and $p = 10$ or $p = 30$. 100 replications are drawn in each case. Let $\boldsymbol{\ell}_1 = (1, 0, \dots, 0)^\top$, $\boldsymbol{\ell}_2 = (0, 1, \dots, 0)^\top$ and $\mathbf{L}_0 = (\boldsymbol{\ell}_1, \boldsymbol{\ell}_2)$.

Example 3.2. We generate X_i from the uniform distribution $U(0,1)$. The response variable Y is generated from

$$\text{Model 3: } Y = \sin(2\pi\boldsymbol{\ell}_1^\top\mathbf{X}) + 4(\boldsymbol{\ell}_2^\top\mathbf{X} - 0.5)^2 + \sigma\epsilon. \tag{3.1}$$

Let $\boldsymbol{\ell}_1 = (1, -1, 1, 0, \dots, 0)^\top/\sqrt{3}$ and $\boldsymbol{\ell}_2 = (1, 1, 0, \dots, 0)^\top/\sqrt{2}$.

Example 3.3. Consider the model:

$$\text{Model 4: } Y = 1 + 2(\boldsymbol{\ell}_1^\top\mathbf{X})(\boldsymbol{\ell}_2^\top\mathbf{X})^2 + 2.5\exp\{-(\boldsymbol{\ell}_3^\top\mathbf{X})^2\} + \sigma\epsilon,$$

where X_i is generated from $U(-1,1)$. Let $\boldsymbol{\ell}_1 = (1,-1,1,0,\ldots,0)^\top/\sqrt{3}$, $\boldsymbol{\ell}_2 = (1,1,0,1,0,\ldots,0)^\top/\sqrt{3}$ and $\boldsymbol{\ell}_3 = (-1,0,1,1,0,\ldots,0)^\top/\sqrt{3}$.

As for estimating the directions in the CMS, we compare the results of the proposed methods with the MAVE, OPG, SIR, SAVE and pHd approaches. The means and standard deviations of estimation error $m(\hat{\mathbf{L}}_1, \mathbf{L}_0)$ for Models 1–4 are presented in Tables 1 and 2. Table 3 summarizes the means of estimated bandwidths for Model 3 with the sample size n varying from 200 to 1600 respectively. It is seen clearly from Table 1 that the estimation errors of the proposed CVML estimates are usually smaller than those of the other alternatives for Models 1 and 2, especially when p is large and n is small. The results in Table 2 also indicate that the CVML method performs comparably with the existing ones in terms of directions estimation of the CMS. In addition, Table 3 shows that the estimated bandwidths obtained by CVML becomes smaller as the sample size increases.

On the other hand, we compare the performance of the proposed method in terms of determining the structural dimension with the MAVE based method (MAVE, Xia et al. 2002), the ridge-type ratio estimation (RRE, Xia et al. 2015) and the BIC criterion (BIC, Zhu et al. 2006). For those methods that involve a tuning parameter, we use the values recommended in the literature. Specially, we take the ridge value $c_n = \log(n)/(10\sqrt{n})$ for RRE and the penalty value $\alpha_n = \sqrt{n}$ for BIC. Based on the limited simulation experiments we have conducted, we recommend

$\tau_n = 2.5n^{-1/3}$ for the CVML method. The frequencies of the estimated dimensions for Models 1–4 are presented in Table 4. Figure 1 presents the boxplots of the ratio $\mathrm{CM}_n(\mathbf{M}_r)/\mathrm{CM}_n(\mathbf{M}_{r+1})$ for Models 3 and 4 with red horizontal straight lines representing $y = 1$. It is seen from the results in Table 4 that the CVML performs comparably with the MAVE and outperforms the other competitors, especially for Model 4 where the true dimension of CMS is 3. Figure 1 verifies the feasibility of the proposed estimation procedure.

Overall, the simulation results support our theoretical results and the proposed CVML works reasonably well in dimension reduction, including estimating both the directions and dimension of the CMS.

Table 1: Means and standard deviations (in parentheses) of $m(\hat{\mathbf{L}}_1, \mathbf{L}_0)$ for Model 1 & 2

Model	p	n	CVML	MAVE	OPG	SIR	pHd	SAVE
1	10	200	0.402	0.552	0.499	0.567	0.551	1.327
			(0.095)	(0.170)	(0.154)	(0.134)	(0.104)	(0.058)
		400	0.223	0.319	0.279	0.375	0.385	1.227
			(0.049)	(0.069)	(0.070)	(0.071)	(0.072)	(0.114)
	30	200	0.581	1.021	1.038	1.030	1.095	1.389
			(0.058)	(0.110)	(0.111)	(0.109)	(0.103)	(0.018)
		400	0.475	0.785	0.779	0.728	0.778	1.400
			(0.051)	(0.168)	(0.182)	(0.089)	(0.098)	(0.011)
2	10	200	0.365	0.390	0.363	0.740	0.811	1.058
			(0.102)	(0.122)	(0.123)	(0.194)	(0.186)	(0.086)
		400	0.240	0.242	0.210	0.484	0.628	0.961
			(0.061)	(0.065)	(0.050)	(0.127)	(0.217)	(0.104)
	30	200	0.511	0.770	0.761	1.165	1.101	1.372
			(0.065)	(0.130)	(0.121)	(0.113)	(0.038)	(0.038)
		400	0.475	0.785	0.779	0.728	0.778	1.400
			(0.051)	(0.168)	(0.182)	(0.089)	(0.098)	(0.011)

Table 2: Means and standard deviations (in parentheses) of $m(\hat{\mathbf{L}}_1, \mathbf{L}_0)$ for Model 3 & 4 with $\sigma = 0.2$.

Model	p	n	CVML	MAVE	OPG	SIR	pHd	SAVE
3	10	200	0.144	0.142	0.143	0.958	0.355	0.983
			(0.064)	(0.039)	(0.039)	(0.090)	(0.069)	(0.078)
		400	0.076	0.091	0.089	0.925	0.249	0.672
			(0.021)	(0.025)	(0.025)	(0.106)	(0.035)	(0.214)
	30	200	0.275	0.354	0.402	1.132	0.753	1.342
			(0.048)	(0.076)	(0.079)	(0.067)	(0.108)	(0.054)
		400	0.168	0.168	0.183	1.043	0.479	1.223
			(0.022)	(0.027)	(0.027)	(0.041)	(0.052)	(0.078)
4	10	200	0.417	0.657	0.619	1.269	1.082	1.183
			(0.125)	(0.273)	(0.298)	(0.099)	(0.127)	(0.115)
		400	0.209	0.222	0.202	1.241	0.999	1.066
			(0.047)	(0.047)	(0.039)	(0.102)	(0.120)	(0.101)
	30	200	0.598	0.968	0.969	1.614	1.224	1.537
			(0.119)	(0.104)	(0.103)	(0.054)	(0.052)	(0.075)
		400	0.499	1.034	1.026	1.475	1.287	1.448
			(0.099)	(0.141)	(0.188)	(0.050)	(0.075)	(0.072)

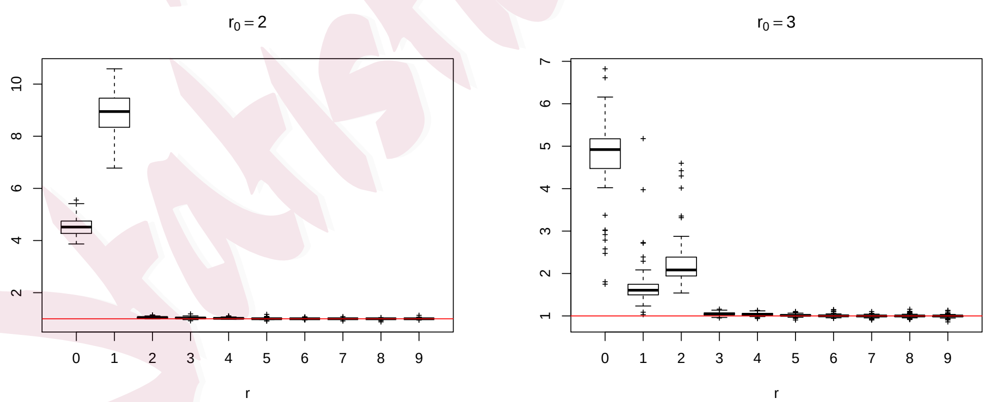
Table 3: Means and standard deviations (in parentheses) of estimated bandwidths for Model 3

p	σ		$n = 200$	$n = 400$	$n = 800$	$n = 1600$
5	0.1	$\hat{h}_1 \times 10$	0.356	0.295	0.285	0.275
			(0.079)	(0.056)	(0.058)	(0.044)
		$\hat{h}_2 \times 10$	0.519	0.420	0.432	0.420
			(0.097)	(0.061)	(0.051)	(0.043)
	0.2	$\hat{h}_1 \times 10$	0.469	0.439	0.397	0.359
			(0.081)	(0.039)	(0.026)	(0.020)
		$\hat{h}_2 \times 10$	0.698	0.609	0.548	0.494
			(0.096)	(0.059)	(0.037)	(0.036)
10	0.1	$\hat{h}_1 \times 10$	0.313	0.291	0.274	0.266
			(0.056)	(0.053)	(0.052)	(0.050)
		$\hat{h}_2 \times 10$	0.452	0.415	0.414	0.404
			(0.072)	(0.048)	(0.047)	(0.040)
	0.2	$\hat{h}_1 \times 10$	0.327	0.323	0.300	0.288
			(0.073)	(0.055)	(0.053)	(0.052)
		$\hat{h}_2 \times 10$	0.483	0.471	0.460	0.443
			(0.099)	(0.056)	(0.043)	(0.034)

Table 4: Frequencies of estimated dimension for Models 1–4 with $p = 10$

Model		$n = 200$			$n = 400$		
		$\hat{r} < r_0$	$\hat{r} = r_0$	$\hat{r} > r_0$	$\hat{r} < r_0$	$\hat{r} = r_0$	$\hat{r} > r_0$
1	CVML	0.04	0.87	0.09	0	1	0
	MAVE	0	0.77	0.23	0	0.99	0.01
	BIC	0	0	1	0	0	1
	RRE	0.44	0.48	0.08	0.27	0.72	0.01
2	CVML	0.24	0.73	0.03	0.05	0.95	0
	MAVE	0.19	0.81	0	0.03	0.97	0
	BIC	0	0	1	0	0	1
	RRE	0.44	0.31	0.25	0.44	0.54	0.02
3	CVML	0	1	0	0	1	0
	MAVE	0	1	0	0	1	0
	BIC	0	0	1	0	0	1
	RRE	0.98	0.01	0.01	0.99	0.01	0
4	CVML	0.16	0.82	0.02	0	1	0
	MAVE	0.92	0.08	0	0.71	0.29	0.01
	BIC	0	0.56	0.44	0	0.15	0.85
	RRE	0.80	0.05	0.15	0.99	0.01	0

Figure 1: Boxplots of the ratio $\mathrm{CM}_n(\mathbf{M}_r)/\mathrm{CM}_n(\mathbf{M}_{r+1})$ for Model 3 (left) and Model 4 (right) with $n = 400$ and $p = 10$



4. Real data illustration

4.1. London air quality dataset

It is known that the air pollution may cause diseases, allergies or death of the human. It occurs when harmful substances including particulates, liquid droplets, gases and chemical molecules produced by human activity are introduced into the atmosphere. Pollutants are classified mainly into primary and secondary substances. Primary pollutants are usually generated from a chemical process, such as the sulfur dioxide released from factories. Secondary pollutants form in the air when primary pollutants react or interact. Ground level ozone (O_3) is a prominent example of the secondary pollutant.

In this study, we attempt to exploit the relationship between the primary pollutants and the secondary pollutant O_3 based on the London air quality data in the R package *openair*. By deleting some missing data, the dataset is collected from May 1, 1998 to September 30, 2004 with hourly updated records of wind speed (x_1), wind direction (x_2), oxides of nitrogen concentration NO_x (x_3), nitrogen dioxide concentration NO_2 (x_4), particulate PM10 in ug/m^3 (x_5), sulfur dioxide concentration SO_2 (x_6), carbon monoxide concentration CO (x_7), particulate PM2.5 in ug/m^3 (x_8) and Ozone concentration (Y). We convert the hourly level data to its daily average for all variables and apply CVML to the treated daily level dataset.

The structural dimension estimated by the CVML procedure is $\hat{r} = 1$. From Table 5, the direction estimated by the CVML approach indicates that NO_x and NO_2 have significant impact on the O_3 concentration. This provides empirical evidence for the claim that the secondary pollutants are usually products of the reactions of the primary pollutants under certain environmental conditions. Nevertheless, the influences of wind speed, wind direction and particulates seem to be not very significant.

Table 5: Estimated directions in CMS for London air quality dataset

Direction	x_1 (ws)	x_2 (wd)	x_3 (NO_x)	x_4 (NO_2)	x_5 (PM10)	x_6 (SO_2)	x_7 (CO)	x_8 (PM2.5)
$\hat{\boldsymbol{\ell}}_1$	−0.045	0.006	0.948	−0.271	0.000	0.012	−0.161	−0.006

4.2. Beijing PM2.5 dataset

Many cities had ever experienced hazy weather in the past few years. The PM2.5—particulate matter less than 2.5 μm in diameter—is known to influence the human health and atmospheric climate. Epidemiological experts concluded that exposure to PM2.5 over a few hours to weeks can cause cardiovascular disease and longer-term exposure increases the risk for cardiovascular mortality and even shortens the life span. In this real data analysis, we intend to investigate the affecting factors for the PM2.5 concentration. We analyse the Beijing PM2.5 dataset collected at Aotizhongxin air-quality monitoring site. The dataset is downloaded from UCI database with the link https://archive.ics.uci.edu/ml/datasets/Beijing+Multi-Site+Air-Quality+Data. The PM2.5 (Y) data ranging from March 2013 to February 2017 are converted to daily averaged records with potential affecting factors PM10 (x_1), SO_2 concentration (x_2), NO_2 concentration (x_3), CO concentration (x_4) and O_3

concentration (x_5) in ug/m^3, temperature (x_6), pressure (x_7), dew point temperature (x_8), precipitation (x_9) and wind speed (x_{10}).

The structural dimension estimated by the CVML method is $\hat{r} = 3$. The three estimated directions are shown in Table 6. Note that the first three eigenvalues of $\hat{\mathbf{M}}$ are 154.447, 36.138 and 9.933. Therefore, the first direction is very important to reveal the relationship between PM2.5 and the potential affecting factors. The first direction in Table 6 clearly indicates that the PM10, the temperature and the dew point temperature are three crucial variables associated with the PM2.5 concentration. The latter two factors were also evidenced by Zhang et al. (2017). The last two directions reveal that the PM2.5 concentration has weak relationship with the pressure and the wind speed but possibly related to NO_2 and CO, which are potential chemical components of PM2.5.

Table 6: Estimated directions in CMS for Beijing PM2.5 data set

Direction	x_1 (PM10)	x_2 (SO_2)	x_3 (NO_2)	x_4 (CO)	x_5 (O_3)	x_6 (temp)	x_7 (pres)	x_8 (dewp)	x_9 (preci)	x_{10} (ws)
$\hat{\boldsymbol{\ell}}_1$	−0.540	0.002	0.079	−0.128	−0.029	0.410	−0.034	−0.717	0.025	0.003
$\hat{\boldsymbol{\ell}}_2$	−0.795	−0.139	−0.231	0.040	−0.109	−0.209	−0.034	0.446	−0.193	0.018
$\hat{\boldsymbol{\ell}}_3$	0.091	−0.504	−0.231	−0.492	−0.136	0.403	−0.159	0.250	0.397	−0.125

5. Discussion

In this study, we attempt to reduce the dimension for the multiple-index model in the framework of metric learning. The proposed cross-validation-based metric learning method produces a metric that contains crucial information on both the central mean subspace and the unknown link function. The rate of convergence and the optimal order of bandwidth are derived. A novel algorithm has been proposed to determine the structural dimension of the central mean subspace when it is unknown. For the purpose of prediction, we refer to the work by Conn and Li (2019). They showed that the kernel estimate using a full bandwidth matrix will achieve the optimal rate of convergence for a multiple-index model.

Appendix: Assumptions and remarks

Let $\mathbf{A}^{\perp}$ denotes the space orthogonal to that spanned by the column vectors of the matrix $\mathbf{A}$. The following regularity conditions are imposed.

(C1) [*Design of* $\mathbf{X}$.] The density function $f_{\mathbf{X}}(\mathbf{x})$ of $\mathbf{X}$ is positive, bounded and is continuously differentiable up to order two.

(C2) [*Link function.*] The second-order derivatives of $g(\cdot)$ exist and are bounded away from infinity.

(C3) [*Kernel function.*] The kernel function $K(\cdot)$ is a symmetric univariate density function with bounded derivatives.

(C4) [*Identifiability.*] Let $\mathcal{F} = \{\mathbf{t} \in \mathbb{R}^p : \mathbf{t} \in \mathbf{L}_0^{\perp}\}$. For any $\mathbf{x} \in \mathbb{R}^p$, if $f(\mathbf{x}+c\mathbf{t}) = f(\mathbf{x})$ for all $c \in \mathbb{R}$, then it must have $\mathbf{t} \in \mathcal{F}$.

(C5) [*Moments of errors.*] The error satisfies $E(\epsilon_i|\mathbf{X}_i) = 0$, $E(\epsilon_i^2|\mathbf{X}_i) = \sigma^2(\mathbf{L}_0^{\top}\mathbf{X}_i) = \sigma_i^2$ almost surely and $\sup_i E(|\epsilon_i|^4) < \infty$ for all i, where $\sigma^2(\cdot)$ is bounded and continuous.

Condition (C1) is a relatively weaker assumption on the density of $\mathbf{X}$, compared with the linearity condition in many SIR-based methods. Conditions (C2)–(C3) are common conditions on the nonparametric link function and the kernel function, respectively. Condition (C3) is satisfied by many commonly-used kernel functions, such as the biweight kernel and the quadratic kernel. The subspace $\mathcal{F}$ in Condition (C4) indeed equals to the space orthogonal to $\mathcal{S}(\mathbf{L}_0)$. Hence, Condition (C4) indicates that the dimension r_0 cannot be further reduced and the regression function $f(\mathbf{x})$ remains constant when $\mathbf{x}$ varies in $\mathcal{F}$. For more insights into condition (C4), we consider a toy example in which $\mathbf{t} = (t_1, t_2)^\top$, $r_0 = 2$ and $f(\mathbf{x}) = (x_1 + x_2)^2$. By choosing $t_1 = -t_2$, we have $f(\mathbf{x} + c\mathbf{t}) = f(\mathbf{x})$ for all $c \in \mathbb{R}$ and $\mathbf{t} \in \mathcal{F}$ in this instance. The moment assumption up to the fourth order in condition (C5) is made for technical simplicity.

Supplementary Material

The technical proofs are provided in the online Supplementary Material.

Acknowledgments

The authors are grateful to the Editor, Associate Editor and two anonymous reviewers for their insightful comments and suggestions that have substantially improved the presentation and the content of this paper. Linlin Dai's research was supported by the Fundamental Research Funds for the Central Universities (Grant No. JBK1806002) of China and the National Natural Science Foundation of China (Grant No. 12001441). Kani Chen's research was supported by the Hong Kong Research Grant Council grants 16309816, 16300714, 600813, and 600612. The research of Gang Li was partly supported by National Institute of Health Grants 1P01CA236585-01A1, 5P30CA-16042, UTR001881A and NIH CA211015. Yuanyuan Lin's research was supported by the Hong Kong Research Grants Council (Grant No. 14306219 and 14306620), the National Natural Science Foundation of China grant (Grant No. 11961028) and Direct Grants for Research, The Chinese University of Hong Kong.

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