We propose a novel varying coefficient model (VCM), called principal varying coefficient model (PVCM), by characterizing the varying coefficients through linear combinations of a few principal functions. Compared with the conventional VCM, PVCM reduces the actual number of nonparametric functions and thus has better estimation efficiency. Compared with the semivarying coefficient model (SVCM), PVCM is more flexible but with the same estimation efficiency when the number of principal functions in PVCM and the number of varying coefficients in SVCM are the same. Model estimation and identification are investigated, and the better estimation efficiency is justified theoretically. Incorporating the estimation with the $L_1$ penalty, variables in the linear combinations can be selected automatically, and hence, the estimation efficiency can be further improved. Numerical experiments suggest that the model together with the estimation method is useful even when the number of covariates is large. Supplementary materials for this article are available online.

KEY WORDS: Local linear estimator; $L_1$ penalty; Principal function; Profile least-squares estimation; Semivarying coefficient model.

1. INTRODUCTION

Let $(Y, X, U)$ be a random triplet, where $Y \in \mathbb{R}^1$ is the response of interest, $X = (X_1, \ldots, X_p)^\top \in \mathbb{R}^p$ is the associated $p$-dimensional predictor, and $U \in \mathbb{R}^1$ is the so-called index variable. The conventional varying coefficient model (VCM; Chen and Tsay 1993; Hastie and Tibshirani 1993) assumes that $Y = X^\top \beta(U) + \varepsilon$, where $\varepsilon$ is the random noise and $\beta(u) = (\beta_1(u), \ldots, \beta_p(u))^\top \in \mathbb{R}^p$ is a vector of unknown smooth functions in $u$, called the varying coefficients. Ever since Chen and Tsay (1993) and Hastie and Tibshirani (1993), VCM has gained a lot of popularity in the literature due to the following three facts. First, VCM is easy to interpret because, conditioned on the index variable $U = u$, VCM reduces to a standard linear regression model that is well understood in practice. Second, VCM allows the varying coefficient $\beta(u)$ to be fully nonparametric. Thus, it has much stronger modeling capability than a standard linear regression model. Finally, because the index variable $U$ is typically univariate, VCM is free of the curse of dimensionality. VCM and its variants have been extensively studied in the literature during the past two decades (Fan and Zhang 1999; Cai, Fan, and Li 2000; Fan and Zhang 2000a,b; Huang, Wu, and Zhou 2002; Zhang, Lee, and Song 2002; Fan and Huang 2005; Fan and Zhang 2008; Kai, Li, and Zou 2011).

It is remarkable that although the estimation of VCM requires only univariate nonparametric smoothing, it is still very unstable when $p$ is large or even moderately large, because there are $p$ nonparametric functions to estimate. To improve the estimation efficiency, some estimation methods have been developed based on either kernel smoothing or splines smoothing, including Fan and Zhang (1999); Cheng and Hall (2003); Wu and Liang (2004); Huang, Wu, and Zhou (2002, 2004); Eubank et al. (2004); and Kai, Li, and Zou (2011); their main idea was to apply different smoothing parameters to different coefficients. However, the improvement based on their idea is limited especially when different coefficients need similar smoothing parameters. Another way to improve the efficiency is through further model specification without losing much information. The semivarying coefficient model (SVCM) proposed by Zhang, Lee, and Song (2002) and Fan and Huang (2005) is a good example. SVCM confines some coefficients to be constant but allows the others to vary with the index variable $U$.

In this article, we consider an extension of SVCM by allowing different varying coefficients to be linearly dependent and thus reduce the actual number of unknown functions in the model. To further illustrate the idea, let us revisit the Boston housing data. The response of interest is the median value of owner-occupied homes (MEDV, in $1000$) with 13 predictors, denoted by $X_1, \ldots, X_{13}$, respectively. More details will be stated in Section 4. As noticed by Fan and Huang (2005), the following varying coefficient model with the lower status of the population ($U = \text{LSTAT}$) being the index variable is appropriate for the data:

$$
\text{MEDV} = \beta_1(U)X_1 + \cdots + \beta_{13}(U)X_{13} + \varepsilon. \tag{1.1}
$$

In (1.1), the varying coefficients can be estimated by the method based on the local linear smoothing; see, for example, Fan and Zhang (1999) and Wu and Liang (2004). The estimated coefficients are shown in the first panel of Figure 1 where the coefficients with large variations are highlighted and labeled; these coefficients are redrawn in the second panel for better visualization. Remarkably similar shapes are discovered after linear transformations as shown in the third panel. The similarity implies that different varying coefficients are likely to be linearly dependent and that the index variable affects these coefficients in a similar manner.

Next, we quantify the above linear dependency among $\beta_1(U), \ldots, \beta_p(U)$ using the principal component analysis. Let $\theta = (\theta_1, \ldots, \theta_p)^\top = E\beta(U)$ with $p = 13$ in the above example and $\Sigma_{\beta} = \text{cov}(\beta(U))$.© 2013 American Statistical Association
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Suppose the eigenvalue-eigenvector decomposition is
\[ \Sigma_\beta = (b_1, \ldots, b_p) \text{diag}(\lambda_1, \ldots, \lambda_p) (b_1, \ldots, b_p)^\top \]
with \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0 \) and \( b_k = (b_{k1}, \ldots, b_{kp})^\top \). Define the principal components for the varying coefficients as
\[
\begin{pmatrix}
g_1(U) \\
g_2(U) \\
\vdots \\
g_p(U)
\end{pmatrix} = (b_1, \ldots, b_p)^\top
\begin{pmatrix}
\beta_1(U) - \theta_1 \\
\beta_2(U) - \theta_2 \\
\vdots \\
\beta_p(U) - \theta_p
\end{pmatrix}.
\]
Then it is easy to see that \( E(g_k(U)) = 0 \) and \( \text{var}(g_k(U)) = \lambda_k \), \( k = 1, 2, \ldots, p \), and that
\[
\beta_k(U) = \theta_k + b_{k1}g_1(U) + b_{k2}g_2(U) + \cdots + b_{kp}g_p(U),
\]
\( k = 1, 2, \ldots, p \). \label{eq:beta_k}

Because \( \text{var}(g_k(U)) \) decreases with \( k \), the contribution of \( g_k(U) \) to the coefficient functions also decreases with \( k \). In this example, the five largest eigenvalues are 25.8584, 0.5668, 0.1445, 0.0370, and 0.0126. The rest \( 13 - 5 = 8 \) eigenvalues are very close to 0. It is remarkable that the largest eigenvalue (i.e., 25.8584) by itself can explain about 97% of the total variation of \( \beta_1(U), \ldots, \beta_p(U) \), which suggests that the first principal component contributes dominantly to the variation of \( \beta_k(U) \)'s; the contribution by the other principal components is very small.

This fact motivates us to simplify model (\ref{eq:medv}) into
\[
\text{MEDV} = (\theta_1 X_1 + \cdots + \theta_{13} X_{13}) + \gamma_1(U)(\phi_1 X_1 + \cdots + \phi_{13} X_{13}) + \varepsilon. \label{eq:medv_simplified}
\]

Theoretically, the estimators produced by (\ref{eq:medv_simplified}) are more efficient than those by (\ref{eq:medv}) if the simplification does not lose much information, because only one nonparametric function \( \gamma_1(.) \) needs to be estimated in (\ref{eq:medv_simplified}) but a total of \( p = 13 \) functions need to be estimated in (\ref{eq:medv}). Furthermore, model (\ref{eq:medv_simplified}) identifies two important components given by \( \theta_1 X_1 + \cdots + \theta_{13} X_{13} \) and \( \phi_1 X_1 + \cdots + \phi_{13} X_{13} \). The first component is linearly related to the response, and the second nonlinearly in the sense that it has a nontrivial interaction with index variable \( U \). Thus, model (\ref{eq:medv_simplified}) is also more informative than model (\ref{eq:medv}). See Section 4 for more discussion about this real example.

In this article, we shall discuss a more general model of (\ref{eq:medv_simplified}), called the principal varying coefficient model (PVCM). The rest of the article is organized as follows. The next section introduces the model formally and discusses its identification. Model estimation and selection based on a profile approach is investigated in Section 3 theoretically. Incorporating the estimation with the adaptive \( L_1 \) penalty is studied in Section 4. Simulation studies are presented in Section 5 and the Boston housing data is further analyzed in Section 6. Finally, the article is concluded with a brief discussion in Section 7. All technical details are deferred to the Appendix.
also includes the SVCM of Zhang, Lee, and Song (2002) as a special case if the last \( p - q \) elements in \( \theta_0 \) are zeros and the first \( q \) elements in all \( b_j, k = 1, \ldots, d_0 \), are zeros.

Compared with the conventional VCM (Chen and Tsay 1993; Hastie and Tibshirani 1993; Fan and Zhang 1999, 2008), PVCM reduces the actual number of unknown nonparametric functions and thus has better estimation efficiency. Compared with SVCM (Zhang et al. 2002; Fan and Huang 2005; Fan and Zhang 2008), PVCM is more flexible and informative by allowing a predictor to appear in both linear and nonlinear parts simultaneously. On the other hand, PVCM shares the same estimation efficiency with SVCM when the number of principal functions in PVCM and the number of varying coefficients in SVCM are the same.

Model (2.1) is not uniquely identifiable. For example, let \( C \) be an arbitrary \( d_0 \times d_0 \) orthonormal matrix. Then, by redefining \( B_0 := B_0C \) and \( \gamma_0(u) := C^\top \gamma_0(u) \), model (2.1) still holds. Parameter vector \( \theta_0 \) is also not unique even if \( B_0 \) is fixed. For example, let \( c \in \mathbb{R}^{d_0} \) be an arbitrary constant vector and redefine \( \theta_0 := \theta_0 - B_0c \) and \( \gamma_0(\cdot) := \gamma_0(\cdot) + c \), then model (2.1) is still correct. To fix the identification problem, we can always appropriately select the vector \( c \) such that \( E\gamma_0(U) = 0 \). If further \( \text{cov}(\gamma_0(U)) \) is of full rank, we then have the following identification equations

\[
\theta_0 = E(\beta_0(U)), \quad S(B_0) = S(\text{cov}(\beta_0(U))),
\]

(2.2)

where \( S(A) \) stands for the linear subspace spanned by the column vectors of an arbitrary matrix \( A \). Because \( S(B_0) = S(\Sigma_2) \) with \( \Sigma_2 = \text{cov}(\beta_0(U)) \), we can define \( B_0 = (b_1, \ldots, b_{d_0}) \in \mathbb{R}^{p \times d_0} \) where \( b_j (1 \leq j \leq d_0) \) are the eigenvectors associated with \( \Sigma_2 \)'s \( d_0 \) largest eigenvalues in descending order. In that case, \( \gamma_0(U) = B_0^\top \beta_0(U) - E\beta_0(U) \) with

\[
E(\gamma_0(U)) = 0, \quad \text{cov}(\gamma_0(U)) = \text{diag}(\lambda_1, \ldots, \lambda_{d_0}),
\]

(2.3)

where \( \lambda_1 \geq \cdots \geq \lambda_{d_0} > 0 \). As long as the \( d_0 \) largest eigenvalues are mutually different, \( B_0 \) is uniquely identifiable up to a sign difference. For convenience, we assume hereafter that the nonzero eigenvalues of \( \Sigma_2 \) are different from one another.

Based on (2.2) and (2.3), we can also give another way to identify the linear part. Write \( \delta_0 = (I - B_0\beta_0^\top)b_0B_0^\top \theta_0 \) and \( \tilde{\gamma}_0(U) = \gamma_0(U) + B_0^\top \delta_0 = (\tilde{g}_1(U), \ldots, \tilde{g}_{d_0}(U))^\top \), then we have \( \delta_0 = B_0\delta_0(U) - \tilde{\delta}_0 = B_0\tilde{\gamma}_0(U) - \tilde{\theta}_0 = B_0(\tilde{\gamma}_0(U) - \tilde{B}_0\tilde{\theta}_0) \), such that

\[
B_0^\top \delta_0 = 0, \quad B_0^\top B_0 = I_{d_0}, \quad \text{cov}(\tilde{\gamma}_0(U)) = \text{diag}(\lambda_1, \ldots, \lambda_{d_0}).
\]

(2.4)

By (2.2), it is easy to see that \( \tilde{\theta}_0 \) and \( S(\delta_0) \) satisfying (2.4) are identifiable. This way of identifying the model is preferable because it has less parameters when \( E(\tilde{\beta}_0(U)) \in S(\text{cov}(\tilde{\beta}_0(U))) \), in which case \( \tilde{\theta}_0 = 0 \). This fact will be used in our test for whether there exists a linear combination of \( X \) whose coefficient does not change with \( U \). This fact can also be used to test whether there are constant coefficients in SVCM (Zhang, Lee, and Song 2002). It should be noted that the identification conditions \( E(\gamma_0(U)) = 0 \) in (2.3) and \( B_0^\top \delta_0 = 0 \) in (2.4) should not be used simultaneously. Otherwise, the PVCM might be overspecified.

We end this section by mentioning some work in the literature that is related to principal functions. Factor models or principal component analyses that extract the main informative variables from a large number of variables are powerful approaches toward multivariate analysis. However, most of the existing models are under linear settings or under nonlinear framework; see, for example, Stock and Watson (2002) and Hastie and Stuetzle (1989). Our approach is under a functional framework. On the other hand, the principal components in our model are constructed for unobserved functions which is different from the fact that the usual factor models are proposed for observed data; see, for example, Forni et al. (2000), Forni and Lippi (2001), and Bai (2003).

3. PROFILE LEAST-SQUARE ESTIMATION OF PVCM

In this section, we investigate the model estimation using the kernel smoothing approach. Estimation based on other nonparametric smoothing methods such as splines and penalized polynomial splines can be investigated similarly.

We first consider the estimation of \( \theta_0 \) and \( B_0 \) under the assumption \( d_0 \) is known in advance. The estimation of \( d_0 \) will be addressed later. Equation (2.2) motivates a very convenient way to estimate \( \theta_0 \) and \( B_0 \). Specifically, by the local linear estimation (Fan and Gijbels 1996), we can estimate \( \beta_0(U) \) by \( \hat{\beta}(u) \), where \( \hat{\beta}(u) \) is the minimizer of \( a \) in

\[
\min_{a \in \mathbb{R}^p, b \in \mathbb{R}^p} \sum_{i=1}^n \left[ Y_i - a^\top X_i - b^\top X_i(U_i - u) \right]^2 K_h(U_i - u),
\]

(3.1)

where \( K_h(u) = K(u/h)/h \) and \( K(\cdot) \) is a kernel function. Consequently, we estimate \( \Sigma_2 \) by \( \hat{\Sigma}_2 = n^{-1} \sum (\hat{\beta}(U_i) - \hat{\beta})(\hat{\beta}(U_i) - \hat{\beta})^\top \), where \( \hat{\beta} = n^{-1} \sum \hat{\beta}(U_i) \). We then estimate \( \theta_0 \) by \( \theta(\hat{\beta}) \) with \( \hat{B}(\hat{\theta}) \) defined by \( \hat{B}(\hat{\theta}) = (\hat{B}_1, \ldots, \hat{B}_{d_0}) \), where \( \hat{B}_j \) is the eigenvector associated with the \( j \)th largest eigenvalue of \( \Sigma_2 \) for \( 1 \leq j \leq d_0 \). Let \( A \) be an arbitrary matrix and \( \text{vec}(A) \) stands for a vector constructed by stacking \( A \)'s columns. Denote by \( \|A\| \) the operation norm, that is, the maximal absolute singular value of \( A \). The estimation error for \( B(\hat{\theta}) \) can be then defined as \( \|B(\hat{\theta}) - B_0\|_2 \). We have the following consistency for the estimates.

Theorem 1. Under the conditions (C.1)–(C.4) in the Appendix, we have \( \|\theta(\hat{\beta}) - \theta_0\| = O_p(\sqrt{\log(n)/n^{1/2}}) \) and \( \|\hat{B}(\hat{\theta}) - B_0\|_2 = O_p(\sqrt{\log(n)/n^{1/2}}) \).

Fix \( B \) and \( \theta \) in model (2.1), and consider the local linear smoother of model (2.1)

\[
\min_{a(u) \in \mathbb{R}^p, \hat{\beta}(u) \in \mathbb{R}^p} \sum_{i=1}^n \left[ Y_i - X_i^\top \theta - a(u)^\top B^\top X_i - b(u)^\top B^\top X_i(U_i - u)/h^2 \right] K_h(U_i - u),
\]

If \( B \) and \( \theta \) are close to the true values, then the minimizer of \( a(u) \) is a local linear estimator of the coefficient functions \( \gamma_0(u) \), denoted by \( \hat{\gamma}(u|B, \theta) \). By Fan and Zhang (1999), we have

\[
\hat{\gamma}(u|B, \theta) = \left( S_n(u, B) \right)^{-1} B^\top \left( L_{n,0}(u) - S_{n,0}(u)\theta \right)
- S_{n,1}(u) B(\theta)^\top S_{n,2}(u) B^{-1} B^\top (L_{n,1}(u) - S_{n,1}(u)\theta),
\]

(3.2)
\[
Y_i \approx X_i^{\top} \theta + X_i^{\top} B \hat{\gamma}(U_i | \theta, B) + \varepsilon_i, \quad i = 1, 2, \ldots, n.
\]

Thus, we consider
\[
Q(\theta, B) = n^{-1} \left\{ Y_i - X_i^{\top} \theta - X_i^{\top} B \hat{\gamma}(U_i | \theta, B) \right\}^2,
\]
and estimate \( \theta_0 \) and \( B_0 \) by
\[
(\hat{\theta}, \hat{B}) = \arg \min_{\theta, B} Q(\theta, B).
\]

Although the minimization is searched over the whole space, as in many model estimations, an initial estimator is sometimes essential. The estimators \( \hat{\theta}(0) \) and \( \hat{B}(0) \) can be used for this purpose. Other robust estimation methods such as the back-fitting method of Wu and Liang (2004) are also helpful in finding initial estimators. To facilitate the theoretical investigation, Theorem 1 allows us to restrict the parameter space in a small range of the true parameters, \( \Theta_n = \{ (\theta, B) : ||\theta - \theta_0|| + ||B - B_0|| \leq M(h^2 + \delta_n) \} \) for some constant \( M > 0 \). In what follows, \( A \otimes B \) denotes the Kronecker product of two matrices \( A \) and \( B \), and the notation \( A^{\otimes 2} \) denotes \( AA^\top \) for any matrix \( A \).

**Theorem 2.** Suppose conditions (C.1)–(C.4) in the Appendix hold. Let \( (\hat{\theta}, \hat{B}) = \arg \min_{\theta, B} Q_n(\theta, B) \). Then
\[
\frac{\sqrt{n}}{\text{vec}(\hat{B} - B_0)} \xrightarrow{D} N(0, \Sigma_0^{-1}(\Sigma_1 + \Sigma_2)\Sigma_0^{-1})
\]
in distribution, where

\[
\begin{align*}
\Sigma_0 & = E \left\{ \left( \begin{array}{cc} X & X \\ \gamma_0(U) \otimes X & \gamma_0(U) \otimes X \end{array} \right)^\top \right\}, \\
\Sigma_1 & = E \left\{ \left( \begin{array}{c} I_p \\ \gamma_0(U) \otimes I_p \\ \gamma_0(U) \otimes W(U) \\ -E \left( \begin{array}{cc} W(U) \\ \gamma_0(U) \otimes W(U) \end{array} \right) V(U) \right) \right\}, \\
\Sigma_2 & = E \left( \begin{array}{c} W(U) \\ \gamma_0(U) \otimes W(U) \end{array} \right) B_0 E \left( \begin{array}{cc} \gamma_0(U) & \gamma_0(U) \end{array} \right) B_0^\top e^\otimes \\
& \times \left( \begin{array}{c} W(U) \\ \gamma_0(U) \otimes W(U) \\ \gamma_0(U) \otimes W(U) \end{array} \right)^\top,
\end{align*}
\]

with \( W(U) = E(XX^\top | U) \) and \( V(U) = B_0(B_0^\top W(U)B_0)^{-1}B_0^\top \).

After \( \hat{\theta}_0 \) and \( B_0 \) are estimated, we can estimate \( \gamma_0(u) \) immediately by \( \hat{\gamma}(u | \hat{\theta}, \hat{B}) \) defined in (3.2) and have the following limiting distribution.

**Theorem 3.** Under regularity conditions (C.1)–(C.4) in the Appendix, we have in distribution
\[
\frac{\sqrt{nh^{-1}}}{\text{vec}(\hat{B} - B_0)} \xrightarrow{D} N(0, \Sigma_0^{-1}(\Sigma_1 + \Sigma_2)\Sigma_0^{-1})
\]

where \( W_2(u) = \int K^2(v) d\nu E(XX^\top | U = u) \), \( \mu_2 = \int u^2 K(v) d\nu \), and \( \hat{f}(u) = n^{-1} \sum_{i=1}^{n} K h(u - U_i) \).

Writing the model as a VCM, the estimated coefficient functions are \( \hat{\beta}_{\text{PVCM}}(u) = \hat{\theta} + \hat{B}(u) \). It follows from Theorems 2 and 3 that
\[
\frac{\sqrt{nh^{-1}}}{\text{vec}(\hat{B} - B_0)} \xrightarrow{D} N(0, \Sigma_{\text{PVCM}}(u)),
\]

where \( \Sigma_{\text{PVCM}}(u) = B_0(B_0^\top W(u)B_0)^{-1}B_0^\top W_2(u)B_0(B_0^\top W(u)B_0)^{-1}B_0^\top \). However, if we treat the model as a VCM in the estimation process and estimate it by the method in Fan and Zhang (1999), then the estimator \( \hat{\beta}_{\text{VCM}}(u) \) has
\[
\frac{\sqrt{nh^{-1}}}{\text{vec}(\hat{B} - B_0)} \xrightarrow{D} N(0, \Sigma_{\text{VCM}}(u)),
\]

indicating that the estimator based on a PVCM is indeed more efficient than that based on a VCM. The smaller the \( d_0 \) is, the more efficient is PVCM compared with VCM.

To make statistical inference, we also need to estimate the variance-covariance matrices in the limiting distributions. These matrices can be estimated simply by their sample versions with the unknown functions and parameters being replaced by their estimators, respectively. By the local linear kernel smoothing, \( W(u) \) can be estimated consistently by

\[
\hat{W}(u) = \frac{\sum_{i=1}^{n} w_{n,h}(U_i - u)X_iX_i^\top}{\sum_{i=1}^{n} w_{n,h}(U_i - u)},
\]

where \( w_{n,h}(U_i - u) = K_h(U_i - u)\sum_{i=1}^{n} K_h(U_i - u)((U_i - u)/h)^2 - K_h(U_i - u)((U_i - u)/h)\sum_{i=1}^{n} K_h(U_i - u)((U_i - u)/h), \) and \( E(XX^\top | U = u) \) by

\[
\sum_{i=1}^{n} w_{n,h}(U_i - u)X_iX_i^\top
\]

As an example of hypothesis testing, we consider whether there is a separate linear part in the model under identification (2.4), that is, whether there exists a linear combination \( \theta_0^\top X \) such that \( \theta_0^\top B_0 = 0 \) and \( \theta_0 \neq 0 \). The corresponding hypothesis is
\[
H_0: \quad (I - B_0B_0^\top)\theta_0 = 0.
\]

With the identification of (2.4), we can construct a test statistic
\[
ST = n(\hat{\theta} - \theta_0^\top) \hat{P} \left( \hat{P} S_{00} \hat{P} \right)^{-1} \hat{P} (\hat{\theta} - \theta_0),
\]
where \( \hat{P} = (I - \hat{B}\hat{B}^\top) \) and \( S_{00} \) is the submatrix of estimated \( \Sigma_{0}^{-1}(\Sigma_{1} + \Sigma_{2})^{-1} \) in its first \( p \) rows and first \( p \) columns, and \( A^\top \) denotes the Moore–Penrose inverse of matrix \( A \).

**Corollary 1.** Under the model assumptions (C.1) and (C.4) and \( H_0 \), with identification (2.4), we have \( ST \xrightarrow{D} \chi^2(p - d_0) \) as \( n \to \infty \).

By Corollary 1, we reject \( H_0 \) if \( ST > \chi^2_{p-d_0}(p - d_0) \) with significance level \( \alpha \).

Next, we consider the estimation of \( d_0 \). To this end, we propose here a Bayesian information criterion (BIC)-type criterion,

\[
\text{BIC}(d) = \log \hat{\sigma}_d^2 + d \times \frac{\log(nh)}{nh}, \tag{3.4}
\]

where \( d \) is the working number of principal functions, \( nh \) is the effective sample size in nonparametric regression, and \( \hat{\sigma}_d^2 \) is given by

\[
\hat{\sigma}_d^2 = n^{-1} \sum_{k=1}^{n} \left( Y_k - X_k^\top \hat{\theta} - \hat{\psi}(U_k) \hat{B}^\top X_k \right)^2,
\]

where estimators \( \hat{\theta}, \hat{B} \), and \( \hat{\psi}(U) \) are all obtained under the working number, \( d \), of principal functions. For the purpose of completeness, define \( \text{BIC}(0) = n^{-1} \sum_{i=1}^{n} (Y_i - \hat{Y})^2 \) with \( \hat{Y} = n^{-1} \sum_{i=1}^{n} Y_i \). Then \( d_0 \) is estimated by \( \hat{d} = \arg \min_{0 \leq d \leq p} \text{BIC}(d) \).

**Theorem 4.** Assuming the technical conditions (C.1)–(C.4) in the Appendix hold, we have \( P(\hat{d} = d_0) \to 1 \).

By Theorem 4, it is also easy to see that Theorems 1–3 still hold if we replace \( d_0 \) by \( \hat{d} \).

### 4. REFINEMENT OF ESTIMATION BASED ON L1 PENALTY

In this section, we estimate the model by incorporating the kernel smoothing with the \( L_1 \) penalty. As well demonstrated in the literature, the \( L_1 \) penalty approach has several advantages. Specifically for PVCM, the \( L_1 \) penalty can achieve the following goals simultaneously: (1) to identify variables that have cross effect with the index variable on the response and those that only have simple linear effect; (2) to identify unimportant variables and automatically remove them from the model, and (3) to improve the estimation efficiency when there is sparsity and the number of covariates is large.

Let \( \alpha = (\alpha_1, \ldots, \alpha_{p(d_0+1)})^\top = (\theta^\top, \text{vec}(B)^\top)^\top \), \( S = \{1, 2, \ldots, p(d_0 + 1)\} \), and \( A = \{s : \alpha_s \neq 0\} \). Then, \( A \) is the index set that contains only nonzero elements in \( \alpha \). Following Zou (2006) and Zhang and Lu (2007), consider the following adaptive LASSO estimation,

\[
\hat{\alpha}^{(n)} = \left\{ \hat{\theta}^\top, \text{vec}(\hat{B}_n)^\top \right\}^\top = \arg \min_{(\theta, B)} Q(\theta, B) + \lambda_n \sum_{i=1}^{p} \left| \hat{w}_i \theta_i \right| + \sum_{j=1}^{d_0} \left| \hat{w}_{ij} B_{ij} \right|
\]

\[
= \arg \min_{\alpha \in \mathbb{R}^{p(d_0+1)}} Q(\alpha) + \lambda_n \sum_{i=1}^{p(d_0+1)} \hat{w}_i |\alpha_s| \tag{4.1}
\]

where \( \hat{w}_s = 1/|\hat{w}_s|^\tau \) with \( \tau > 0 \) and \( \hat{\alpha}_s \) is the estimator of \( \alpha_s \) defined in (3.3). Let \( A_n = \{s \in S : \hat{\alpha}_s^{(n)} \neq 0\} \). Then \( A_n \) is the index set of variables that are selected in either the linear part or nonlinear part of PVCM or both. If a variable is selected neither in the linear nor in the nonlinear part, the variable is unimportant and will be removed automatically from the model.

**Theorem 5.** Under the conditions of Theorem 2 and \( \lambda_n/\sqrt{n} \to 0 \), \( \lambda_n n^{2/7} \to \infty \), we have the following asymptotic properties for the estimators \( \hat{\theta}_n \) and \( \hat{B}_n \).

1. The coefficients with nonzero values in both \( \theta_0 \) and \( B_0 \) can be consistently identified, that is, \( \lim_{n \to \infty} P(A_n = A) = 1 \).
2. The estimated parameters achieve the oracle efficiency where the zero coefficients are known and removed in advance, that is,

\[
\sqrt{n}\left( \hat{\theta} - \theta_0 \right) \xrightarrow{D} \mathcal{N}(0, \Sigma_0^{-1}) \quad \text{and} \quad \sqrt{n}\left( \hat{B} - B_0 \right) \xrightarrow{D} \mathcal{N}(0, ((\Sigma_0 A_0)^{-1} - A_0) \Sigma_0^{-1}), \tag{4.2}
\]

where notation \( M_A \) denotes the submatrix of \( M \) with \( j \)th row (and \( j \)th column if \( M \) is a matrix) being removed for all \( j \in A^c \), complement of set \( A \).

The selection of the tuning parameter \( \lambda_n \) is essential in the estimation. We found that the commonly used BIC criterion works well, which is stated below. To indicate the dependence of the estimators on \( \lambda_n \), write the estimators in (4.1) as \( \hat{\theta}_n \) and \( \hat{B}_n \).

Define

\[
\text{BIC}(\lambda_n) = \log\{Q(\hat{\theta}_n, \hat{B}_n)\} + \log(n) \frac{p_n}{n},
\]

where \( p_n \) is the total number of nonzero values in \( \hat{\theta}_n \) or \( \hat{B}_n \). The asymptotic performance of \( \text{BIC}(\lambda_n) \) in selecting \( \lambda_n \) can be similarly discussed as in Wang and Xia (2008). The details are omitted here.

### 5. SIMULATION STUDIES

Consider two VCMs where the covariates \( X_{ij} \equiv 1 \) and \( X_{ij}'s \) \((1 < j \leq p)\) are simulated from a multivariate normal distribution with \( \text{cov}(X_{ij}, X_{ij}') = 0.5^{[j-(j-1)/2]} \) for any \( j_1, j_2 \geq 2 \), and \( U_i \) is simulated from \( U(0, 1) \), and \( \epsilon_i \) from \( N(0, 1) \). The parameters and principal functions are, respectively,

**Model 1.** \( \theta_0 = b_0, \quad B_0 = b_1, \quad \gamma_{0}(u) = 10u(1-u) - 5/3 \),

**Model 2.** \( \theta_0 = b_0, \quad B_0 = (b_2, b_3), \quad \gamma_{0}(u) = \{\cos(2\pi u), \sin(2\pi u)\}^\top \),

where

\[
b_0 = (1, 1, \ldots, 1, 0, \ldots, 0)^\top,
\]

\[
b_1 = (1, -1, \ldots, 1, -1, 0, \ldots, 0)^\top,
\]

\[
b_2 = (1, \ldots, 1, 0, \ldots, 0)^\top \quad \text{and} \quad \{p-(p-1)/3\}, \quad \{p-(p-1)/3\}
\]

and

\[
b_3 = (0, \ldots, 0, 1, \ldots, 1, 0, \ldots, 0)^\top, \quad \{p-(p-1)/3\}, \quad \{p-(p-1)/3\}
\]
It is easy to see that Model 1 has one principal function ($d_0 = 1$) and Model 2 has two ($d_0 = 2$).

In the following calculation, we use the Newton–Rahpson algorithm to solve the minimization problem in (3.3). For the minimization in (4.1), we use the quadratic norm to approximate the $L_1$ norm and then the Newton–Rahpson algorithm to solve the minimization numerically.

For each model setting, 500 simulation replications are conducted. For each simulation replication, we first estimate the varying coefficients $\hat{\beta}(u)$ according to (3.1) by treating the model as a VCM (see Fan and Zhang (1999) for more details). In the estimation, the bandwidth $h$ is selected by the leave-one-out cross-validation. The same bandwidth is then used throughout the rest of the computational process, except for the estimation of $B_0$ and $\theta_0$ where the bandwidth is multiplied by $n^{-0.1}$ for the purpose of undersmoothing; see Carroll et al. (1997). We then apply the BIC criterion in (3.4) to estimate the number of principal functions, $\hat{d}$. The percentage of replications in which the number of principal functions is correctly estimated is summarized in the third column of Table 1. As we can see, the percentage converges to 100% quickly when sample size increases. This convergency supports the theory that $\hat{d}$ is a consistent estimator of $d_0$.

As shown in Theorem 5, the estimation method in (4.1) can also be used for variable selection. To check the performance, we count in each estimation the number of zero rows (i.e., the

![](https://example.com/table1.png)

<table>
<thead>
<tr>
<th>Model and ($p$)</th>
<th>Sample size</th>
<th>Correct $d_0$</th>
<th>Correct (and incorrect) zeros in the rows of $\theta$</th>
<th>Estimation errors (and their standard error)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>$B$</td>
<td>VCM</td>
</tr>
<tr>
<td>I($p = 7$)</td>
<td>100</td>
<td>98%</td>
<td>0.0(0.0)</td>
<td>4.5(0.0)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>100%</td>
<td>0.0(0.0)</td>
<td>4.9(0.0)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>100%</td>
<td>0.0(0.0)</td>
<td>5.0(0.0)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>II($p = 7$)</td>
<td>100</td>
<td>90%</td>
<td>0.0(0.0)</td>
<td>2.9(1.1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>100%</td>
<td>0.0(0.0)</td>
<td>3.0(0.0)</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>100%</td>
<td>0.0(0.0)</td>
<td>3.0(0.0)</td>
</tr>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I($p = 13$)</td>
<td>100</td>
<td>93%</td>
<td>5.9(0.0)</td>
<td>8.8(0.1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>100%</td>
<td>6.0(0.0)</td>
<td>9.0(0.0)</td>
</tr>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>100%</td>
<td>6.0(0.0)</td>
<td>9.0(0.0)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>II($p = 13$)</td>
<td>100</td>
<td>86%</td>
<td>5.3(0.4)</td>
<td>4.9(1.8)</td>
</tr>
<tr>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>97%</td>
<td>5.6(0.0)</td>
<td>5.3(0.3)</td>
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<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>100%</td>
<td>6.0(0.0)</td>
<td>5.0(0.0)</td>
</tr>
<tr>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I($p = 21$)</td>
<td>100</td>
<td>72%</td>
<td>13.8(0.1)</td>
<td>14.4(2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>99%</td>
<td>14.0(0.0)</td>
<td>15.0(0.0)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>100%</td>
<td>14.0(0.0)</td>
<td>15.0(0.0)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>II($p = 21$)</td>
<td>100</td>
<td>84%</td>
<td>12.0(0.4)</td>
<td>9.0(5.7)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>92%</td>
<td>13.5(0.0)</td>
<td>9.0(1.0)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>100%</td>
<td>13.9(0.1)</td>
<td>9.0(0.2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>
rows in which all elements are zeros) in the estimated \( \theta \) and \( B \). The numbers are listed in the fourth and fifth columns of Table 1. Note that if a row of estimated \( \theta \) is zero, it means that the corresponding variable is not selected in the linear part; if all the elements in a row of \( B \) are zero, it means that the corresponding variable is removed from the nonlinear part. By comparing the numbers with true numbers of zeros in \( \theta_0 \) and \( B_0 \) as given in the square brackets of the table, we see that as sample size increases, the estimation method in (4.1) is consistent in selecting the variables in the linear part and nonlinear part.

We evaluate the overall performance of model estimation by checking the estimation error of the coefficients \( \beta(u) \) after rewriting the estimated model as a VCM. With the estimated \( d_0 \), we compute \( \hat{\theta} \) and \( \hat{B} \) and thus \( \hat{\beta}(u_i) = \hat{\theta} + \hat{B}\hat{y}(u_i) \). The estimation error of the whole model is evaluated by

\[
    n^{-1} \sum_{i=1}^{n} |\hat{\beta}(u_i) - \theta_0 - B_0y_0(u_i)|,
\]

where \( |\ell| = (|\ell_1| + |\ell_2| + \cdots + |\ell_p|)/p \) for any vector \( \ell = (\ell_1, \ldots, \ell_p)^T \). The average estimation errors across 500 simulation replications are summarized in columns 6, 7, and 8 of Table 1. In these columns, as the sample size increases, the estimation error steadily shrinks toward 0. These shrinkages support that all the estimators are consistent. However, treating a PVCM as a VCM, the estimation efficiency is very much adversely affected by noticing that column 6 is obviously bigger than column 7. By comparing the eighth column with the seventh column, we can see that imposing the adaptive \( L_1 \) penalty, the estimation efficiency can be substantially improved, especially when the number of covariates is large.

Next, we check the performance of the proposed statistic in Corollary 1 for testing hypothesis on the linear part. We allow the linear part \( \theta_0 \) to change with \( c \), that is, \( \theta_0 = c \times b_0 \). The larger the \( c \) is, the more influential the linear part is. We also vary the signal-to-noise ratios (SNR) by changing the variance of \( \varepsilon \). With significance level \( \alpha = 0.05 \), we calculate the rejection frequencies for \( H_0 : |\theta_0| = 0 \) under model specification (2.4).

In both models, when \( c = 0 \), there are no linear parts, and the rejection frequency should be around 0.05. As \( c \) increases, the rejection frequencies should also increase. For the two models with \( p = 7 \), our simulation results for \( c = 0, 0.05, 0.1, 0.15 \), and 0.2 reported in Figure 2 support our theory quite well, indicating that the hypothesis testing statistic has reasonable power with roughly correct significant level. It is also reasonable to see that as the number of principal functions increases, the power of testing increases.

### 6. A REAL EXAMPLE

The Boston housing data of Harrison and Rubinfeld (1978) has attracted lots of attention in statistics. Various models have been applied to the data, including the linear regression model (Belsley, Kuh, and Welsch 1980), the additive model (Fan and Jiang 2005), and the VCM (Fan and Huang 2006). The response of interest is the MEDV (in $1000) with 13 predictors: lower
status of the population (LSTAT), per capita crime rate (CRIM) by town, average number of rooms per dwelling (RM), full-value property-tax rate per $10,000 (TAX), nitrogen dioxides concentration (NOX, parts per 10 million), pupil-teacher ratio by town (PTRATIO), proportion of owner-occupied units built prior to 1940 (AGE), proportion of residential land zoned for lots over 25,000 square feet (ZN), proportion of nonretail business acres per town (INDUS), Charles River dummy variable (1 if tract bounds river; 0 otherwise; CHAS), weighted distances to five Boston employment centers (DIS), index of accessibility to radial highways (RAD), and 1000($k − 0.63)^2 where $k is the proportion of blacks by town (B).

Fan and Huang (2005) fitted the data with an SVCM using $U = \sqrt{\text{LSTAT}}$ as the index variable. However, as the number of covariates $p = 13$ is too big for a VCM to be estimated well, Fan and Huang (2005) only included six variables in their model. With the superior estimation efficiency of PVCM over VCM, however, we are able to include all the variables into a PVCM, which will be further identified as (1.3). We standardize all the variables before fitting the model.

As we mentioned in the first section, after linear transformation, remarkably similar shapes are shared among different coefficient functions. The eigenvalues of the estimated $\Sigma_\beta$ suggest that the number of principal functions is $d_0 = 1$. The BIC defined in (3.4) for $d_0 = 0$ (linear model) and $d_0 = 1, \ldots, 10$ are $−1.1593, −1.7199, −1.6950, −1.5482, −1.4933, −1.2018, −0.8020, −0.5044, −0.2011, and −0.1034. Therefore, the number of principal functions is also selected as 1 by the BIC. The corresponding parameters in the model are estimated and listed in Table 2, where the standard errors of estimators are calculated based on Theorem 5 and are put in the parentheses.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>LSTAT</th>
<th>CRIM</th>
<th>RM</th>
<th>TAX</th>
<th>NOX</th>
<th>PTRATIO</th>
<th>AGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_0$</td>
<td>0.5478</td>
<td>0</td>
<td>0.1968</td>
<td>−0.2335</td>
<td>−0.1325</td>
<td>−0.1756</td>
<td>0</td>
</tr>
<tr>
<td>(0.0586)</td>
<td>(—)</td>
<td>(0.0701)</td>
<td>(0.0482)</td>
<td>(0.0526)</td>
<td>(0.0235)</td>
<td>(—)</td>
<td></td>
</tr>
<tr>
<td>$B_0$</td>
<td>−0.2683</td>
<td>0.3026</td>
<td>0.6068</td>
<td>0</td>
<td>0.2743</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(0.1924)</td>
<td>(0.1999)</td>
<td>(0.1762)</td>
<td>(—)</td>
<td>(0.1292)</td>
<td>(—)</td>
<td>(—)</td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Estimated parameters (and their standard errors in the parentheses) in the model for the Boston housing data

*: the standard error is not available in theory.

To further verify the appropriateness of different models for the data, we consider the prediction error of PVCM and compare it with linear regression model and the conventional VCM. We randomly partition all the 506 observations into a training set and a prediction set. We estimate the PVCM based on the training set and use the estimated model to make prediction for observations in the prediction set. With different sizes of training set and prediction set, the average prediction errors based on 1000 random partitions are listed in Table 3. It is easy to see from Table 3 that VCM has very poor prediction capability and is much worse than the simple linear regression model. However, PVCM with one principal function as identified by the proposed method (3.4) has much better prediction ability than VCM and even substantially better prediction than the linear regression model. The prediction ability can be further improved when the number of principal functions is selected as 1 by the BIC.

<table>
<thead>
<tr>
<th>Size of</th>
<th>Training set</th>
<th>Prediction set</th>
<th>Linear model</th>
<th>VCM</th>
<th>PVCM</th>
<th>PVCM + penalty</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>306</td>
<td>0.3028</td>
<td>0.9312</td>
<td>0.2514</td>
<td>0.2434</td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>206</td>
<td>0.2918</td>
<td>0.8210</td>
<td>0.2349</td>
<td>0.2262</td>
<td></td>
</tr>
<tr>
<td>400</td>
<td>106</td>
<td>0.2866</td>
<td>0.8661</td>
<td>0.2274</td>
<td>0.2215</td>
<td></td>
</tr>
</tbody>
</table>

Table 3. Average prediction errors based on 1000 partitions
$L_1$ penalty is imposed in the estimation, though the primary purpose of imposing the $L_1$ penalty is for variable selection.

7. CONCLUSION
Motivated by the compelling need to improve estimation efficiency of a VCM, especially when $p$ is large, and by practical examples in which different coefficient functions are linearly dependent, this article proposed a new VCM, PVCM, that incorporates the intrinsic patterns in the coefficients. The model possesses superior estimation efficiency over VCM.

The proposed model is a semiparametric model and thus can be estimated based on kernel smoothing and splines smoothing as well. The gain in estimation efficiency is due to further model identification that only a small number of principal functions need to be estimated nonparametrically, regardless of the smoothing method. Though only the estimation method based on kernel smoothing is discussed in this article, the splines smoothing and the penalized splines enjoy many good properties (Wood, 2006; Ruppert, Wand, and Carroll 2009). Thus estimation based on the splines smoothing needs further investigation.

The advantage of PVCM over VCM increases as $p$ increases where the coefficient functions are more likely to be linearly dependent. Incorporating with the $L_1$ penalty, the estimation can automatically select variables in the linear part and the nonlinear part. The estimation efficiency only depends on the number of principal functions and the variables in the linear part and nonlinear part. Theoretaical analysis and data study further confirm the advantages of PVCM. In conclusion, PVCM together with the estimation methods provides a powerful approach toward the analysis of complicated data.

SUPPLEMENTARY MATERIALS
Appendix: Technical details

REFERENCES