ESTIMATION IN HIGH-DIMENSIONAL LINEAR MODELS WITH DETERMINISTIC DESIGN MATRICES

BY JUN SHAO1 AND XINWEI DENG

East China Normal University, University of Wisconsin and Virginia Polytechnic Institute and State University

Because of the advance in technologies, modern statistical studies often encounter linear models with the number of explanatory variables much larger than the sample size. Estimation and variable selection in these high-dimensional problems with deterministic design points is very different from those in the case of random covariates, due to the identifiability of the high-dimensional regression parameter vector. We show that a reasonable approach is to focus on the projection of the regression parameter vector onto the linear space generated by the design matrix. In this work, we consider the ridge regression estimator of the projection vector and propose to threshold the ridge regression estimator when the projection vector is sparse in the sense that many of its components are small. The proposed estimator has an explicit form and is easy to use in application. Asymptotic properties such as the consistency of variable selection and estimation and the convergence rate of the prediction mean squared error are established under some sparsity conditions on the projection vector. A simulation study is also conducted to examine the performance of the proposed estimator.

1. Introduction. Consider the following linear model:

\[ y_i = x_i' \beta + \varepsilon_i, \quad i = 1, \ldots, n, \]

where \( y_i \) is an observed response variable, \( x_i \) is a \( p \)-dimensional vector of observed covariates or design points associated with \( y_i \), \( \beta \) is a \( p \)-dimensional vector of unknown parameters and \( \varepsilon_i \)'s are independent and identically distributed unobserved random errors with mean 0 and unknown variance \( \sigma^2 \). The theory of linear models is well established for traditional applications where the dimension \( p \) is fixed and the sample size \( n > p \). With modern

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This is an electronic reprint of the original article published by the Institute of Mathematical Statistics in *The Annals of Statistics*, 2012, Vol. 40, No. 2, 812–831. This reprint differs from the original in pagination and typographic detail.
technologies, however, in many biological, medical, social and economical studies, \( p \) is comparable with, or much larger than, \( n \), and making valid statistical inference is a great challenge.

In the case of \( p < n \), there is a rich literature on variable selection, that is, identifying nonzero components of \( \beta \) in (1). For variable selection in the case of \( p > n \) and statistical inference afterwards, the development of statistical theory started about a decade ago. Some excellent advances in asymptotic theory have been made recently in situations where \( p \) diverges to infinity as the sample size \( n \) increases to infinity with the divergence rate \( O(n^l) \) for some \( l > 0 \) (polynomial-type divergence rate) or \( O(e^{n^\nu}) \) for some \( \nu \in (0,1) \) (ultra-high dimension). See, for example, Fan and Peng (2004), Hunter and Li (2005), Meinshausen and Buhlmann (2006), Zhao and Yu (2006), Zou (2006), Wang, Li and Tsai (2007), Fan and Lv (2008), Zhang and Huang (2008), Meinshausen and Yu (2009), Wang (2009) and a review by Fan and Lv (2010). When \( x_i \)'s are random covariates, under some conditions, some variable selection methods have been shown to be selection-consistent in the sense that, with probability tending to 1 as \( n \to \infty \), the selected variables are exactly those related to the response, where the probability is with respect to the joint distribution of \((y_i, x_i)'s. As Fan and Lv (2008) commented in the end of their stimulating paper, however, no selection-consistency result is available for deterministic \( x_i \)'s and many applications, such as biomedical imaging and signal processing, involve deterministic design points. Another example in which \( x_i \) can be treated as deterministic is an analysis conditional on the observed covariates.

Let \( X \) be the matrix whose \( i \)th row is \( x_i' \), \( i = 1, \ldots, n \). For simplicity, we call \( X \) the design matrix although \( x_i \)'s are not necessarily designed points. When \( p > n \), a key difference between a random \( X \) and a deterministic design matrix is the identifiability of the regression parameter \( \beta \) in (1), caused by the fact that the probabilities under consideration are different. For random \( x_i \)'s that are independent and identically distributed and independent of \( \varepsilon_i \)'s, 

\[
\beta = \left[ \text{cov}(x_i) \right]^{-1} \text{cov}(x_i, y_i).
\]

Hence, even when \( p > n \), components of \( \beta \) can be estimated, and nonzero components of \( \beta \) can be identified consistently with respect to the joint probability distribution of \((y_i, x_i)'s, under some conditions on \text{cov}(x_i) \) and \text{cov}(x_i, y_i). On the other hand, when the design matrix is deterministic or an analysis conditional on \( X \) is considered, the underlying probability is the probability distribution of \((y_1, \ldots, y_n) \) conditional on \( X \), and \( \beta \) is identifiable if and only if it lies in a set having a one-to-one correspondence with \( \mathcal{R}(X) \), the linear space spanned by rows of \( X \). Since the dimension of \( \mathcal{R}(X) \) is at most \( n \), when \( p > n \), \( \beta \) is generally not identifiable with respect to the probability distribution of \((y_1, \ldots, y_n) \) conditional on \( X \). Consequently, with deterministic \( X \) and \( p > n \), it is not realistic to derive consistent estimators of \( \beta \) or consistent variable selection procedures.

Without selection-consistency [as previously described; see definition (7) in Section 4.1], we may still derive consistent estimators of some useful func-
tions of $\beta$ under the $p$-dimensional linear model given by (1) with deterministic $X$ and $p > n$. This is the main focus of the current paper. Although $\beta$ is generally not identifiable when $p > n$, we argue in Section 2 that we may not need to estimate the entire vector $\beta$. For statistical analysis, $\theta$, the projection of $\beta$ onto $\mathcal{R}(X)$, is what we are able to estimate, and perhaps the estimation of $\theta$ is sufficient for valid statistical inference.

To estimate $\theta$, we first consider the ridge regression estimator in Section 3. For any linear combination of the ridge regression estimator, we establish the asymptotic convergence rate of its mean squared error. We also obtain the convergence rate of the expected $L_2$-norm error for the ridge regression estimator of $X\theta$. This expected $L_2$-norm error divided by $n$ is equal to the average prediction mean squared error minus $\sigma^2$.

When $\theta$ is sparse in the sense that many of its components are small, we consider in Section 4 a sparse estimator of $\theta$ obtained by thresholding the ridge regression estimator of $\theta$. We show that, with probability tending to 1 at a fast rate, we can eliminate small components of $\theta$ and keep large components of $\theta$, that is, thresholding the ridge regression estimator provides a variable selection procedure, that is, consistent in some sense. This method is computationally much simpler than methods such as the LASSO [Tibshirani (1996)], SCAD [Fan and Li (2001)] and the ENET [Zou and Hastie (2005)], since no numerical minimization is required as the proposed estimator has an explicit form. We show that the convergence rate of the expected $L_2$-norm error or average prediction mean squared error of the thresholded ridge regression estimator is much faster than that of the ridge regression estimator when $\theta$ is sparse. In particular, the thresholded ridge regression estimator is estimation-consistent (defined in Section 4), but the ridge regression estimator may not be.

Thresholding the ridge regression estimator is closely related to the SIS as shown in Fan and Lv (2008). However, its asymptotic behavior for deterministic $X$ is different from that for random $X$, and its consistency also requires very different conditions. For deterministic $X$ and $p > n$, there does not exist any result on the consistency of the LASSO, SCAD or ENET. When $p < n$, Zhang and Huang (2008) showed that the LASSO is estimation-consistent, but the required conditions are more stringent and complicated than those required for the consistency of the thresholded ridge regression estimator.

Some simulation results are presented in Section 5 to study the estimation and prediction performance of the proposed method, the ridge regression, the LASSO and the ENET. All technical proofs are given in Section 6.

2. Identifiability and projection. We consider model (1) with deterministic design matrix $X = (x_1, \ldots, x_n)'$, where the dimension of $x_i$, $p$, is larger than $n$. Let $r = r_n$ be the rank of $X$. From the singular value decomposition, $X = PDQ'$,
where \( P \) is an \( n \times r \) matrix satisfying \( P'P = I_r \), \( Q \) is a \( p \times r \) matrix satisfying \( Q'Q = I_r \), \( I_a \) denotes the identity matrix of order \( a \) and \( D \) is an \( r \times r \) diagonal matrix of full rank. Let \( Q_r \) be a \( p \times (p-r) \) matrix such that \( Q_r'Q_r = 0 \) (the matrix of 0’s with an appropriate order) and \( Q_r'Q_r = I_{p-r} \). Throughout, we denote the \( q \)-dimensional Euclidean space by \( \mathcal{R}^q \) for any positive integer \( q \) and the subspace of \( \mathcal{R}^p \) generated by the rows of \( X \) by \( \mathcal{R}(X) \).

We say that \( \beta \) in (1) is identifiable if \( \beta_1 \in \mathcal{B}, \beta_2 \in \mathcal{B} \) and \( X\beta_1 = X\beta_2 \) imply \( \beta_1 = \beta_2 \), where \( \mathcal{B} \) is the parameter space of \( \beta \). The following lemma gives a sufficient and necessary condition for the identifiability of \( \beta \).

**Lemma 1.** Under model (1) with \( p > r \), \( \beta \) is identifiable if and only if there exists a known function \( \phi \) from \( \mathcal{R}^r \) to \( \mathcal{R}^{p-r} \) such that

\[
\mathcal{B} = \{ \beta : \beta = Q\xi + Q_r\phi(\xi), \xi \in \mathcal{R}^r \}.
\]

Lemma 1 reveals that identifiable \( \beta \)'s must be in a set having a one-to-one correspondence with \( \mathcal{R}(X) = \{ \beta : \beta = Q\xi, \xi \in \mathcal{R}^r \} \). Since the dimension of the set on the right-hand side of (3) is \( r \leq p \) (the minimum of \( n \) and \( p \)), \( \beta \) is typically not identifiable when \( p > n \) and, hence, we are not able to obtain a component-wise consistent estimator of \( \beta \). However, we may not need to estimate the entire vector \( \beta \), that is, if \( X\beta_1 = X\beta_2 \), we can still estimate parameters related to \( X\beta_1 = X\beta_2 \) and make valid inference without trying to distinguish \( \beta_1 \) and \( \beta_2 \). Therefore, we consider the projection of \( \beta \) onto \( \mathcal{R}(X) \), which is what we are able to identify in view of Lemma 1. Define

\[
(XX')^{-1} = PD^{-2}P',
\]

which is \((XX')^{-1}\) if \( r = n \). The projection of \( \beta \) onto \( \mathcal{R}(X) \) is

\[
\theta = X'(XX')^{-1}X\beta = QQ'\beta.
\]

Note that \( \theta \in \mathcal{R}(X) \) and \( \theta = \beta \) if and only if \( \beta \in \mathcal{R}(X) \). Furthermore, \( X\theta = X\beta \) and model (1) can be written as

\[
y_i = x_i'\theta + \varepsilon_i, \quad i = 1, \ldots, n.
\]

Thus, estimating \( \theta \) is enough for inference about parameters \( X\beta = X\theta \) and prediction.

The dimension of \( \theta \) is still \( p \). When \( \beta \) has many zero components, \( \theta \) may not have any zero component. However, \( \theta \) may have many small components. This can be seen from the \( L_2 \)-norms of \( \beta \) and \( \theta \). Since \( \theta = QQ'\beta \) and \( QQ' \) is a projection matrix, we obtain that \( \|\theta\| \leq \|\beta\| \), where \( \|\cdot\| \) denotes the \( L_2 \)-norm. This implies that if \( \beta \) has many zero components so that the order of \( \|\beta\| \) is much smaller than \( O(p) \), then the order of \( \|\theta\| \) is also much smaller than \( O(p) \). Hence, if components of \( \theta \) are nonzero, then many of them must be negligible, and \( \theta \) can be viewed as a sparse vector. More precise descriptions of this sparsity can be found in conditions (C2) in Section 3 and (C4) in Section 4.
3. **The ridge regression estimator of the projection.** Since the dimension of $\theta$ in (4) is $p > n$, we consider the ridge regression estimator of $\theta$ [Hoerl and Kennard (1970)] under model (5).

$$\hat{\theta} = (X'X + h_n I_p)^{-1}X'y,$$

where $y = (y_1, \ldots, y_n)'$ and $h_n > 0$ is an appropriately chosen regularization parameter. The computation of $\hat{\theta}$ involves only inverting an $n \times n$ matrix. This is because (2) implies that

$$\left(X'X + h_n I_p\right)^{-1}X' = X'\left(XX' + h_n I_n\right)^{-1},$$

which also implies that the ridge regression estimator $\hat{\theta}$ is always in $\mathcal{R}(X)$. In fact, if $\hat{\beta}$ is the ridge regression estimator of $\beta$ constructed under model (1), then $\hat{\theta} = X'(XX')^{-1}X\hat{\beta} = \hat{\beta}$. But $\hat{\theta} = \hat{\beta}$ estimates $\theta$, not the nonidentifiable $\beta$ when $p > n$.

We now study the bias and variance of $\hat{\theta}$ as an estimator of $\theta$, which is essential for establishing asymptotic properties of $\hat{\theta}$. For the matrix $Q$ given in the singular value decomposition (2), $\Gamma = (QQ')$ is orthogonal, that is, $\Gamma'\Gamma = \Gamma\Gamma' = I_p$. Then

$$\text{bias}(\hat{\theta}) = E(\hat{\theta}) - \theta$$

$$= (X'X + h_n I_p)^{-1}X'X\theta - \theta$$

$$= -(h_n^{-1}X'X + I_p)^{-1}\theta$$

$$= -\Gamma(h_n^{-1}\Gamma'X\Gamma + I_p)^{-1}\Gamma'QQ'\theta$$

$$= -(Q\quad Q')\begin{pmatrix}(h_n^{-1}D^2 + I_r)^{-1} & 0 \\ 0 & I_{p-r}\end{pmatrix}\begin{pmatrix}Q' \\ Q'\end{pmatrix}QQ'\theta$$

$$= -(Q(h_n^{-1}D^2 + I_r)^{-1}Q)\begin{pmatrix}Q'\theta \\ 0\end{pmatrix}$$

$$= -Q(h_n^{-1}D^2 + I_r)^{-1}Q'\theta,$$

where the fourth equality follows from the fact that $\Gamma$ is orthogonal and $\theta = QQ'\beta = QQ'\theta$. The covariance matrix of $\hat{\theta}$ is given by

$$\text{var}(\hat{\theta}) = \sigma^2(X'X + h_n I_p)^{-1}X'X(X'X + h_n I_p)^{-1}$$

$$\leq \sigma^2(X'X + h_n I_p)^{-1}$$

$$\leq \sigma^2 h_n^{-1}I_p,$$

where $A \leq B$ for nonnegative definite matrices $A$ and $B$ means $B - A$ is nonnegative definite.

To study the asymptotic properties of $\hat{\theta}$, we consider $n \to \infty$ and $p = p_n$, a function of $n$. Quantities such as $\beta$, $y$, $x_i$, etc., form triangular arrays, but
the subscript \( n \) is omitted for simplicity. We assume that \( \lambda_{1n} \), the smallest positive eigenvalue of \( X'X \), satisfies

\[
(C1) \quad \lambda_{1n}^{-1} = O(n^{-\eta}), \quad \eta \leq 1 \text{ and } \eta \text{ does not depend on } n.
\]

We also need a sparsity condition on \( \theta \). From the discussion in the end of Section 2, we conclude that, in terms of the \( L_2 \)-norm, the sparsity of \( \beta \) implies the sparsity of \( \theta \). We assume that

\[
(C2) \quad \|\theta\| = O(n^\tau), \quad \tau < \eta \text{ and } \tau \text{ does not depend on } n.
\]

If the number of nonzero components of \( \beta \) is \( O(n^{2\tau}) \), and all absolute values of nonzero components of \( \beta \) are bounded by a constant \( M \), then (C2) holds since \( \|\theta\| \leq \|\beta\| \leq Mn^\tau \).

**Theorem 1.** Assume model (1) and conditions (C1) and (C2).

(i) As \( n \to \infty \), \( E(\theta - \theta)^2 = O(h_n^{-1}) + O(h_n^2n^{-(\eta - \tau)}) \) uniformly over \( p \)-dimensional deterministic vector \( 1 \) with \( \|1\| = 1 \).
(ii) \( n^{-1}E\|X\theta - \theta\|^2 = O(r_n^{-1}) + O(h_n^2n^{-(1+\eta-2\tau)}) \).

Note that these results hold without any condition on the dimension \( p \). Theorem 1(i) shows that the mean squared error of \( Y\theta \) converges to 0 uniformly in \( 1 \) if \( h_n \to \infty \) and \( h_n n^{-(\eta - \tau)} \to 0 \). Theorem 1(ii) gives the convergence rate of the expected \( L_2 \)-norm error \( E\|X\hat{\theta} - \theta\|^2 \) for estimating \( E(y) = X\theta \). Since the dimension of \( X\theta \) is \( n \), we say that an estimator \( \hat{\theta} \) of \( \theta \) is \( L_2 \)-consistent if \( n^{-1}E\|X\hat{\theta} - \theta\|^2 \to 0 \) as \( n \to \infty \). Typically, \( r_n/n \) does not converge to 0 and, hence, \( X\hat{\theta} \) may not be \( L_2 \)-consistent.

To elaborate the motivation of using the expected \( L_2 \)-norm error \( E\|X\hat{\theta} - \theta\|^2 \) as a performance measure for an estimator \( \hat{\theta} \) of \( \theta \), we consider the problem of predicting future \( y \)-values on deterministic \( X \). Let \( y_* \) be independent of \( y \) but with the same distribution as \( y \). For deterministic \( X \), it is typical to assess the accuracy of the prediction \( X\hat{\theta} \) using the average prediction mean squared error \( n^{-1}E\|y_* - X\hat{\theta}\|^2 \). It turns out that

\[
n^{-1}E\|y_* - X\hat{\theta}\|^2 = \sigma^2 + n^{-1}E\|X\hat{\theta} - \theta\|^2.
\]

Hence, having a small expected \( L_2 \)-norm error is equivalent to having a small average prediction mean squared error.

**4. The thresholded ridge regression estimator.** The discussion in the previous section indicates that, although the ridge regression estimator \( \hat{\theta} \) is consistent for the estimation of any linear combination of \( \theta \), it may not be \( L_2 \)-consistent, that is, \( n^{-1}E\|X\theta - X\theta\|^2 \) may not converge to 0. To achieve \( L_2 \)-consistency (and good prediction property) under some sparsity conditions on \( \theta \), we propose to improve the ridge regression estimator by thresholding.
4.1. Variable selection. Let $\mathcal{M}_{\beta,0}$ be the set of indices of nonzero components of $\beta$, and let $\hat{\mathcal{M}}$ be the set of indices of components of $\beta$ selected using a variable selection method. The variable selection method or $\hat{\mathcal{M}}$ is said to be selection-consistent if and only if

$$\lim_{n \to \infty} P(\hat{\mathcal{M}} = \mathcal{M}_{\beta,0}) = 1. \tag{7}$$

Unlike the case of random $X$, for deterministic $X$ with $p > n$, the selection-consistency defined by (7) is generally not achievable because $\beta$ is not identifiable. Some selection-consistency results for the case of $p > n$ and deterministic $X$ published in the literature are based on very strong and sometimes unrealistic conditions on the design matrix $X$ to ensure the identifiability of $\beta$. In fact, when $\beta$ is not identifiable, it is not appropriate to use $\beta$ to describe usefulness of components of $x_i$, since two different $\beta$ may result in the same responses under model (1). Although components of $x_i$ corresponding to zero components of $\beta$ are not related to $y_i$, due to the fact that $\beta$ is unknown and not identifiable, these components of $x_i$ may still be useful in statistical analysis since we have to use model (5) instead of model (1), that is, $\theta$ instead of $\beta$.

The previous discussion leads to variable selection in terms of the projection vector $\theta$, since any linear combination $Y'\beta$ is estimable if and only if $Y'\beta = Y'\theta$. However, when $\beta$ contains many zero components, $\theta$ may not have any zero component, although many components of $\theta$ may be close to zero. Small but not exactly zero components of $\theta$ do not contribute much in estimation but add variability. Thus, we would like to carry out variable selection in a more general sense as defined by Zhang and Huang (2008), that is, we try to eliminate small components of $\theta$. Condition (C4) stated later may be used to define whether a component of $\theta$ can be treated as small.

We propose to threshold the ridge regression estimator $\hat{\theta}$. Let $\hat{\theta}_j$ be the $j$th components of $\hat{\theta}$, $j = 1, \ldots, p$. The thresholded ridge regression estimator is defined as $\hat{\theta}$ whose $j$th component $\hat{\theta}_j = \theta_j$ if $|\theta_j| > a_n$ and $\hat{\theta}_j = 0$ if $|\theta_j| \leq a_n$, $j = 1, \ldots, p$, where

$$a_n = C_1 n^{-\alpha}, \quad 0 < \alpha \leq 1/2, C_1 > 0, \tag{8}$$

is the thresholding value with $\alpha$ and $C_1$ not depending on $n$. The computation of $\hat{\theta}$ is easy since it has an explicit form. Thresholding can be viewed as a variable selection procedure; that is, we select components of $\theta$ with indices in $\mathcal{M}_{\theta,a_n}$, the set of indices of nonzero components of $\theta$. We now study the asymptotic behavior of $\mathcal{M}_{\theta,a_n}$ under some conditions and appropriate choices of $a_n$ and $h_n$. A condition on the divergence rate of $p = p_n$ as $n \to \infty$ is

$$(C3) \quad p = O(e^{n^\nu}), \quad 0 < \nu < 1 \text{ and } \nu \text{ does not depend on } n.$$  

If $p = e^{n^\nu}$, it is referred to as the ultra-high dimension [Fan and Lv (2010)].
THEOREM 2. Assume model (1) with normally distributed \( \varepsilon_i \) and conditions (C1)–(C3). Let \( a_n \) be given by (8) with \( \alpha < (\eta - \nu - \tau) / 3 \), \( u_n = 1 + (\log \log n)^{-1} \) and \( h_n = C_2 a_n^{-2}(\log n)^3 \log(n \vee p) \), where \( C_2 > 0 \) is a constant and \( n \vee p \) is the maximum of \( n \) and \( p \). Then, for any constant \( t > 0 \),

\[
P(M_{\theta, u_n} \subset M_{\hat{\theta}, a_n} \subset M_{\theta, u_n}) = 1 - O((n \vee p)^{-t}),
\]

where \( M_{\xi, c_n} \) denotes the set of indices of components of \( \xi \) whose absolute values are larger than \( c_n \).

Result (9) shows that, by thresholding \( \hat{\theta} \), we can eliminate all components of \( \theta \) with absolute values less than \( a_n / u_n \), but keep all components of \( \theta \) with absolute values larger than \( a_n / u_n \), with probability tending to 1 at the rate of \( O((n \vee p)^{-t}) \) for any \( t > 0 \). This rate is at least \( O(n^{-t}) \) for any \( t > 0 \) and it is \( O(e^{-n \nu}) \) for any \( t > 0 \) if \( \log p \) has exactly the order \( n^{\nu} \).

Let \( q_{n-} \) and \( q_{n+} \) be the numbers of elements in \( M_{\theta, u_n} \) and \( M_{\theta, u_n} \), respectively. Then \( q_{n-} \leq q_{n+} \). Since \( u_n \to 1 \), it is often true that \( q_{n+} - q_{n-} \to 0 \) as \( n \to \infty \). Then, result (9) implies that

\[
P(M_{\hat{\theta}, a_n} = M_{\theta, a_n}) = 1 - O((n \vee p)^{-t}),
\]

which will be referred to as the consistency of \( M_{\theta, a_n} \). This consistency is weaker than the selection-consistency given by (7), but the latter may not be achieved.

We now consider nonnormal \( \varepsilon_i \) under model (1), that is, the normality assumption on \( \varepsilon_i \) is replaced by

\[
(M) \quad E(\varepsilon_i^k) < \infty \quad \text{for an even integer } k \text{ not depending on } n,
\]

and condition (C3) is replaced by

\[
(C3') \quad p = O(n^l), \quad 1 \leq l < k/6 \text{ and } l \text{ does not depend on } n,
\]

while the other conditions, (C1) and (C2), remain the same. When the normality condition is relaxed to the moment condition (M), we cannot handle a dimension at the divergence rate given by (C3), although the polynomial-type divergence rate given by (C3') can still be much larger than \( n \). The integer \( k \) in condition (M) has to be sufficiently large so that \( 3l(t + 1)/k < \eta - \tau \), where \( t > 0 \) is in the convergence rate of \( M_{\theta, a_n} \).

THEOREM 2A. Assume model (1) and conditions (M), (C1), (C2) and (C3'). For any \( t > 0 \), let \( a_n \) be given by (8) with \( \alpha \leq (\eta - \xi - \tau) / 3 \) and \( \xi = 3l(t + 1)/k \), and \( u_n = 1 + (\log \log n)^{-1} \). If \( h_n = C_2 a_n^{-2}(\log n)^3(n \vee p)^{2k/(3l)} \), where \( C_2 > 0 \) is a constant, then result (9) holds.

4.2. \( L_2 \)-consistency. The following result shows that, after the variable selection, the thresholded estimator \( \hat{\theta} \) has asymptotically smaller expected \( L_2 \)-norm error than \( \hat{\theta} \), and it is in fact \( L_2 \)-consistent, under the following
sparsity condition on $\theta$:

\begin{equation}
q_n^+ - q_n^- \to 0, \quad q_n/r_n \to 0 \quad \text{and} \quad a_n v_n \to 0,
\end{equation}

where

$$v_n = \sum_{j : |\theta_j| \leq a_n} |\theta_j|,$$

$\theta_j$ is the $j$th component of $\theta$, $r_n$ is the rank of $X$, $a_n$ is given by (8), and $q_n$, $q_n^-$ and $q_n^+$ are, respectively, the numbers of elements in sets $M_{\theta,a_n}$, $M_{\theta,a_n,u_n}$ and $M_{\theta,a_n/u_n}$ given by (9).

The last two conditions in (C4) are very similar to condition (2.4) in Zhang and Huang (2008); that is, there exist $q_n$ “large” components of $\theta$ with $q_n$ much smaller than the rank of $X$, and $v_n$, the $L_1$ norm of the “small” components of $\theta$, may diverge to $\infty$, but at a rate slower than $a_n^{-1}$.

**Theorem 3.** Assume the conditions in Theorem 2 or 2A. Assume further that (C4) holds and the maximum eigenvalue of $X'X$ is $O(n)$. Then

\begin{equation}
E \|X\hat{\theta} - X\theta\|^2 = O(q_n n^{-1}) + O(v_n a_n) + O(h_n^2 n^{-(1+\eta-2\tau)}).
\end{equation}

Result (11) shows the gain of variable selection by thresholding. The expected $L_2$-norm error $\frac{1}{n} E \|X\hat{\theta} - X\theta\|^2$ is smaller than $\frac{1}{n} E \|X\hat{\theta} - X\theta\|^2$ for sufficiently large $n$. The former converges to 0 at a certain rate and hence $\hat{\theta}$ is $L_2$-consistent, whereas the latter may not converge to 0 when $r_n/n$ does not converge to 0.

If $q_n/n \to 0$, result (11) can also be established with the vector of nonzero components of $\hat{\theta}$ replaced by the ordinary least squares estimator of the sub-vector of $\theta$ indexed by the set $M_{\hat{\theta},a_n}$.

**4.3. Tuning parameters.** To apply thresholding, we need to choose the constants $C_1$ in the thresholding value $a_n$ given by (8) and $C_2$ in the regularization parameter $h_n$ given in Theorem 2 or 2A. Similar to many other problems, $C_1$ and $C_2$ can be viewed as tuning parameters, and there is no optimal way to find their values. Some discussions can be found, for example, in Fan and Lv (2008). It is possible to use a data-driven method to find values of tuning parameters by minimizing the average prediction mean squared error $n^{-1} E \|y_n - X\hat{\theta}\|^2 = \sigma^2 + n^{-1} E \|X\hat{\theta} - X\theta\|^2$.

Let $\psi(C)$ be the average prediction mean squared error when $C = (C_1, C_2)$ is used in $a_n$ and $h_n$. Since $\psi(C)$ is unknown, we minimize the cross-validation estimator

$$\hat{\psi}(C) = \frac{1}{n} \sum_{i=1}^{n} (y_i - x_i' \hat{\theta}(C))_i^2,$$
where $\tilde{\theta}^{(C)}_{-i}$ is the thresholded ridge regression estimator of $\theta$ based on the data set with $(y_i, x_i)$ removed, $i = 1, \ldots, n$. To avoid repeated computation of $\tilde{\theta}^{(C)}_{-i}$, we may use an equivalent formula for $\hat{\psi}(C)$,

$$
\hat{\psi}(C) = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{y_i - x'_i \tilde{\theta}^{(C)}_i}{1 - w_i(C)} \right)^2,
$$

where $w_i(C) = x'_i (X'X + h_n I_p)^{-1} x_i$ and $\tilde{\theta}^{(C)}$ is the thresholded ridge regression estimator based on the whole data set. This method is applied in the simulation study presented in the next section.

5. Simulation results. With deterministic $X$ and $p > n$, we examined the $L_2$-norm errors and the expected $L_2$-norm errors of the ridge regression estimator, the thresholded ridge regression estimator, and the popular LASSO estimator and ENET estimator (for comparison purpose) in four simulation studies. In the first two simulation studies, the design matrix $X$ was generated from a multivariate normal distribution but fixed throughout the simulation, which corresponds to analysis conditional on $X$. In the last two simulation studies, $X$ is a nearly orthogonal Latin hypercube design or a Latin hypercube design.

5.1. Simulation study I. We considered linear model (1) with normally distributed $\varepsilon_i$ and $\sigma = 10$. Three sets of sample and variable sizes were considered, $(n, p) = (30, 100), (100, 500)$ and $(200, 2000)$, with increasing ratio $p/n$. A set of $x_1, \ldots, x_n$ were independently generated with $x_i \sim N(0, \Sigma)$, where the diagonal elements of $\Sigma$ are all equal to 1 and off-diagonal elements of $\Sigma$ are all equal to 0.75. This set of $X$ was fixed throughout the simulation. The first 20 components of $\beta$ are $1 + 0.1j$ for $j = 1, \ldots, 20$, and the rest of the components of $\beta$ are all equal to 0. The $L_2$ cumulative proportion plot of the projection vector $\theta$, that is, $\sum_{j=1}^k \theta^2_{(j)}/\|\theta\|^2$, $k = 1, \ldots, p$, is given in Figure 1, where $\theta^2_{(j)}$ is the $j$th ordered value of $\theta^2_1, \ldots, \theta^2_p$. Although $\beta$ has many zero components, $\theta$ does not have any zero component but many components of $\theta$ are small.

For the thresholded ridge regression estimator, we selected the tuning parameter $C = (C_1, C_2)$ by minimizing $\hat{\psi}(C)$ given by (12). For the ridge regression, LASSO, and ENET estimators, the tuning parameters were selected by a 5-fold cross-validation.

Let $\hat{\theta}$ denote the thresholded ridge regression estimator $\hat{\theta}$, the ridge regression estimator $\hat{\theta}$, the LASSO estimator or the ENET estimator. We independently generated 100 values of $y$ and obtained 100 values of $n^{-1}\|X\beta - X\hat{\theta}\|^2$, the $L_2$-norm error (divided by the sample size). Box plots of 100 values of $n^{-1}\|X\beta - X\hat{\theta}\|^2$ for four estimation methods are given in Figure 1.
The average of 100 values of $n^{-1}\|X\beta - X\hat{\theta}\|^2$, a simulation approximation to the expected $L_2$-norm error $n^{-1}E\|X\beta - X\hat{\theta}\|^2$, is listed in Table 1 for each of the four methods.

5.2. Simulation study II. The setting in this study is the same as that in simulation study I except that the values of $x_i$’s were generated with a $\Sigma$ whose $(k,l)$th element is equal to $(0.5)^{|k-l|}$ when $|k - l| \leq 10$ and 0 when $|k-l| > 10$. The $L_2$ cumulative proportion plot of $\theta$ and box plots of values of ...
Table 1
Simulation approximation to the expected $L_2$-norm error

| Study | Method | Study | Method |
|-------|--------|-------|--------|
|       | Thres. Ridge | LASSO | ENET  | Ridge |
| I     |          |       |       |       |
| 30    | 27.34   | 48.46 | 44.56 | 51.48 |
| 100   | 24.72   | 32.01 | 28.46 | 44.32 |
| 200   | 21.86   | 25.37 | 24.17 | 49.37 |
|       | 56.50   | 69.05 | 70.70 | 76.05 |
| II    | 100    | 59.35 | 68.33 | 64.43 | 94.06 |
| 200   | 74.59   | 85.14 | 82.35 | 100.75 |
| III   | 49     | 61.58 | 78.40 | 76.83 | 85.46 |
| 64    | 54.79   | 81.54 | 79.78 | 78.34 |
| IV    | 30     | 43.44 | 55.35 | 49.29 | 59.72 |
| 100   | 46.49   | 56.60 | 52.83 | 65.85 |
| 200   | 48.53   | 51.78 | 56.26 | 71.21 |

$n^{-1}\|X\beta - \hat{X}\hat{\theta}\|^2$ based on 100 simulation runs for four estimation methods are given in Figure 2. The simulation approximations to $n^{-1}E\|X\beta - \hat{X}\hat{\theta}\|^2$ are included in Table 1.

5.3. Simulation study III. Let NOLH$(n,p)$ denote a nearly orthogonal Latin hypercube design with $n$ rows (runs) and $p$ columns (variables). We considered two sets of $n$ and $p$. In the first case, $n = 49, p = 96$ and $X$ is an NOLH$(49,96)$ constructed by using the orthogonal array-based method in Lin, Mukerjee and Tang (2009). In the second case, $n = 64, p = 192$ and $X$ is an NOLH$(64,192)$. In both cases, the first 15 components of $\beta$ are equal to 0.2, 0.4, $\ldots$, 2.8, 3.0, and the rest components of $\beta$ are equal to 0. The standard deviation of $\varepsilon_i$ is 8. The rest of the simulation setting is the same as that in simulation study I. The $L_2$ cumulative proportion plot of $\theta$ and box plots of values of $n^{-1}\|X\beta - \hat{X}\hat{\theta}\|^2$ based on 100 simulation runs for four estimation methods are given in Figure 3. The simulation approximations to $n^{-1}E\|X\beta - \hat{X}\hat{\theta}\|^2$ are included in Table 1.

5.4. Simulation study IV. The setting in this study is the same as that in simulation study I except that $X$ is a deterministic Latin hypercube design [McKay, Beckman and Conover (1979)]: each column of $X$ is a random permutation of $n$ points $6(i/n) - 3$, $i = 1, \ldots, n$, and all columns are generated independently. The $L_2$ cumulative proportion plot of $\theta$ and box plots of values of $n^{-1}\|X\beta - \hat{X}\hat{\theta}\|^2$ based on 100 simulation runs for four estimation methods are given in Figure 4. The simulation approximations to $n^{-1}E\|X\beta - \hat{X}\hat{\theta}\|^2$ are included in Table 1.

5.5. Conclusions based on simulation studies. From Table 1 and Figures 1–4, we conclude that the thresholded ridge regression estimator is
Fig. 2. Study II: $L_2$ cumulative proportion plot of $\theta$ and box plots of $L_2$-norm error for the thresholded ridge regression, LASSO, ENET and ridge regression.

much better than the ridge regression estimator in terms of the $L_2$-norm error or the expected $L_2$-norm error, which supports our asymptotic theory, that is, the thresholded ridge regression estimator is $L_2$-consistent whereas the ridge regression estimator is not. Because the expected $L_2$-norm error is linearly related to the average prediction mean squared error (Section 3), these results show that thresholding ridge regression has better prediction performance. Except for study III, the LASSO performs worse than the ENET and thresholded ridge regression, but better than the ridge regression, and the ENET performs worse than the thresholded ridge regression,
although the difference is small in some cases. Since the ENET uses a combination of $L_1$- and $L_2$-penalty, it is not surprising that its performance is between the LASSO and thresholded ridge regression. However, both LASSO and ENET have large variability in simulation study III. It is well known that the LASSO requires more stringent conditions on the design matrix $X$ [e.g., Zhao and Yu (2006)]. The nearly orthogonal Latin hypercube design in simulation study III may not satisfy these conditions, which results in the poor performance of the LASSO. This also applies to the ENET, since it uses $L_1$-penalty. Furthermore, no result for the $L_2$-consistency of LASSO or ENET is available in the situation of deterministic $X$ and $p > n$.

In terms of the computation, the thresholded ridge regression is much simpler than the LASSO or ENET, especially when $p$ is very large. Because of the identity (6), the computation complexity of the thresholded ridge regression estimator does not increase as $p$ increases.

6. Proofs.

Proof of Lemma 1. Suppose that (3) holds. Let $\beta_j \in B, j = 1, 2$. Then there are $\xi_j \in \mathcal{R}^r$ such that $\beta_j = Q\xi_j + Q_{\perp}\phi(\xi_j), j = 1, 2$. If $X\beta_1 = X\beta_2$, 

The figure shows the $L_2$ cumulative proportion plot of $\theta$ and box plots of $L_2$-norm error for the thresholded ridge regression, LASSO, ENET and ridge regression.
then, by (2), $P D \xi_1 = P D \xi_2$ and, thus, $\xi_1 = \xi_2$, which implies $\beta_1 = \beta_2$. This shows that the parameter $\beta$ in (1) is identifiable.

Suppose now that $B$ is not of the form (3). Then, there exist $\xi \in \mathcal{R}^r$, $\zeta_j \in \mathcal{R}^{p-r}$, $j = 1, 2$, $\xi_1 \neq \xi_2$ and $\beta_j = Q \xi + Q \perp \zeta_j \in B$. Then $\beta_1 \neq \beta_2$, but $X \beta_1 = P D \xi = X \beta_2$. This shows that $\beta$ in (1) is not identifiable. \hfill $\square$

Proof of Theorem 1.

(i) From Section 3, $\text{bias}(\hat{\theta}) = -Q (h_n^{-1} D^2 + I_r)^{-1} Q' \theta$. From the facts that $Q'Q = I_r$, $D^2$ contains positive eigenvalues of $X'X$, and $(h_n^{-1} D^2 + $
which is bounded by 1. Hence, trace $X$ since the proof of (i), $l_j$ in $c$ uniformly over $l$. Also, from Section 3, $\var(\hat{\theta}) \leq \sigma^2 h_n^{-1} I_p$. Hence, $\var(\hat{\theta}) = O(h_n^{-1})$ uniformly over $l$ with $||l|| = 1$. Then, the result follows from $E(\hat{\theta} - \theta^2 = \var(\theta) + [\var(\hat{\theta})]$. 

(ii) Note that $E\|X\hat{\theta} - X\theta\|^2 = \text{trace}[X \var(\hat{\theta}) X'] + \|X \var(\hat{\theta})\|^2$. From the proof of (i),

$$X \var(\hat{\theta}) X' \leq \sigma^2 X (X' X + h_n I_p)^{-1} X' = \sigma^2 P D (D^2 + h_n I_r)^{-1} P' \leq \sigma^2 P P',$$

since $D (D^2 + h_n I_r)^{-1} D$ is a diagonal matrix whose diagonal elements are bounded by 1. Hence, $\text{trace}[X \var(\hat{\theta}) X'] \leq \sigma^2 \text{trace}(P P') = \sigma^2 r_n$. Also,

$$\|X \var(\hat{\theta})\|^2 = \theta' Q (h_n^{-1} D^2 + I_r)^{-1} D^2 (h_n^{-1} D^2 + I_r)^{-1} Q' \theta \leq h_n^2 \lambda_{1n} \|\theta\|^2,$$

which is $O(h_n^2 n^{-(\eta - 2\tau)})$ by (C1) and (C2). This completes the proof. □

Proof of Theorem 2. From the proof of Theorem 1,

$$\text{bias}(\hat{\theta})_j = O(||\theta|| h_n / \lambda_{1n}) = O(h_n / n^{\eta - \tau})$$

uniformly in $j = 1, \ldots, p$. For sufficiently large $n$, $\log \log n > 0$. With $h_n = C_2 a_n^{-2} (\log \log n)^3 \log(n \vee p)$ and condition (C3),

$$\frac{h_n}{n^{\eta - \tau} (u_n - 1) a_n} = \frac{C_2 (\log \log n)^4 \log(n \vee p)}{n^{\eta - \tau} a_n} \leq \frac{c_1 (\log \log n)^4}{n^{\eta - \tau - 3\tau}}$$

for some constant $c_1 > 0$ and, hence, $|\text{bias}(\hat{\theta})_j| / [(u_n - 1) a_n] \to 0$ uniformly in $j$ when $\alpha < (\eta - \nu - \tau) / 3$. Since $\var(\hat{\theta})_j = O(h_n^{-1})$, there is a constant $c_0 > 0$ such that

$$\frac{|\text{bias}(\hat{\theta})_j| - (u_n - 1) a_n}{\var(\hat{\theta})_j^{1/2}} \leq -\sqrt{2c_0} \sqrt{h_n a_n / (\log \log n)}.$$

Let $\Phi$ be the standard normal distribution function. From (1) with normally distributed $\varepsilon_i$,

$$P(|\hat{\theta}_j - \theta_j| > (u_n - 1) a_n) \leq 2\Phi \left( \frac{|\text{bias}(\hat{\theta})_j| - (u_n - 1) a_n}{\var(\hat{\theta})_j^{1/2}} \right) \leq 2\Phi(-\sqrt{2c_0} \sqrt{h_n a_n / (\log \log n)}) \leq \exp \{-c_0^2 h_n a_n^{2} / (\log \log n)^2\},$$
for sufficiently large \(n\), where the last inequality follows from \(2\Phi(-x) \leq e^{-x^2/2}\) for \(x \geq 2\) and the fact that \(h_n a_n^2 / (\log \log n)^2 = C_2 \log \log n \log(n \vee p) \to \infty\). Using the same argument, we also obtain that

\[
P(|\hat{\theta}_j - \theta_j| > (1 - u_n^{-1}) a_n) \leq \exp\{-c_0^2 h_n a_n^2 / (\log \log n)^2\}
\]

for sufficiently large \(n\). Let \(t > 0\) be given. For sufficiently large \(n\), \(c_0^2 C_2 \log \log n - 1 > t\) and, hence,

\[
P(M_{\theta, a_n u_n} \subset M_{\theta, a_n}) \geq 1 - P\left( \bigcup_{j:|\theta_j| > a_n a_n} \{ |\hat{\theta}_j| \leq a_n \} \right)
\]

\[
\geq 1 - P\left( \bigcup_{j:|\theta_j| > u_n a_n} \{ |\hat{\theta}_j - \theta_j| > (u_n - 1) a_n \} \right)
\]

\[
\geq 1 - \sum_{j=1}^{p} P(|\hat{\theta}_j - \theta_j| > (u_n - 1) a_n)
\]

\[
\geq 1 - p \exp\{-c_0^2 h_n a_n^2 / (\log \log n)^2\}
\]

\[
\geq 1 - (n \vee p)^{-t}.
\]

Similarly, for any \(t > 0\),

\[
P(M_{\theta, a_n u_n} \subset M_{\theta, a_n / u_n}) \geq P\left( \bigcap_{j:|\theta_j| \leq a_n / u_n} \{ |\hat{\theta}_j| \leq a_n \} \right)
\]

\[
\geq 1 - P\left( \bigcup_{j:|\theta_j| \leq a_n / u_n} \{ |\hat{\theta}_j - \theta_j| > (1 - u_n^{-1}) a_n \} \right)
\]

\[
\geq 1 - p \exp\{-c_0^2 h_n a_n^2 / (\log \log n)^2\}
\]

\[
\geq 1 - (n \vee p)^{-t}.
\]

for sufficiently large \(n\). This completes the proof. □

**Proof of Theorem 2A.** From the proof of Theorem 1, we still have \(\text{bias}(\hat{\theta}_j) = O(h_n / n^{\eta-\tau})\) uniformly in \(j = 1, \ldots, p\). Let \(\zeta_j\) be the \(j\)th component of \((X'X + h_n I_p)^{-1} \sum_{i=1}^{n} x_i (y_i - X_i' \theta)\). Then, for \(u_n = 1 + (\log \log n)^{-1}\),

\[
P(|\hat{\theta}_j - \theta_j| > (u_n - 1) a_n) \leq \frac{E(|\hat{\theta}_j - \theta_j|^k)}{[u_n - 1] a_n^k}
\]

\[
= O\left( \left| \text{bias}(\hat{\theta}_j)^k + E(\zeta_j^k) \right| / [u_n - 1] a_n^k \right)
\]

\[
= O\left( \frac{h_n^k \log n^k}{n^{k(\eta-\tau)} a_n^k} \right) + O\left( \frac{(\log \log n)^k}{h_n^{k/2} a_n^k} \right),
\]
where the last equality follows from $E(\zeta^k) = O(h_n^{-k/2})$ [Whittle (1960), Theorem 2]. Similarly,

$$P(|\hat{\theta}_j - \theta_j| > (1 - u_n^{-1})a_n) = O\left(\frac{(n \log n)^{k}}{h_n^{k(\eta - \tau)}a_n^k}\right) + O\left(\frac{(n \log n)^{k}}{h_n^{k/2}a_n^k}\right).$$

Using $h_n = C_2 a_n^{-2}(\log \log n)^{2(n \vee p)}^{2k/(3l)}$, we obtain that

$$P\left(M_{\hat{\theta},a_n} \subset M_{\theta,a_n / u_n}\right) \geq 1 - \sum_{j=1}^{p} P(|\hat{\theta}_j - \theta_j| > (1 - u_n^{-1})a_n)$$

$$= 1 - O\left(\frac{p(n \log n)^{k}}{n^{k(\eta - \tau)}a_n^k}\right) - O\left(\frac{p(n \log n)^{k}}{h_n^{k/2}a_n^k}\right)$$

$$= 1 - O\left(\frac{p(n \log n)^{k}}{n^{k(\eta - \tau)}a_n^k}\right) - O\left(\frac{p}{(n \log n)^{k/(3l)}}\right)$$

$$= 1 - O\left(\frac{p(n \log n)^{k}}{n^{k(\eta - \tau)}a_n^k}\right) - O\left(\frac{1}{(n \log n)^{t}}\right)$$

$$= 1 - O((n \log n)^{k/(3l)}) = 1 - O((n \log n)^{k/(3l)})$$

since $k(\eta - \tau)/3l = t + 1$ and $\alpha \leq (\eta - \xi - \tau)/3$. Similarly,

$$P\left(M_{\theta,a_n / u_n} \subset M_{\hat{\theta},a_n}\right) \geq 1 - O((n \log n)^{k/(3l)})$$

Hence, result (9) follows. □

**Proof of Theorem 3.** Let $A_n = \{M_{\hat{\theta},a_n} = M_{\theta,a_n}\}$ and $A'_n$ be its complement. On the set $A_n$, the number of nonzero components of $\hat{\theta}$ is the same as $q_n$. Let $\theta_1$ be $\theta$ with its components smaller than $a_n$ in absolute value set to 0. Under condition (C4) and the condition that $X'X$ has a maximum eigenvalue bounded by $cn$ for a constant $c$,

$$n^{-1}\|X\theta_1 - X\theta\|^2 \leq c\|\theta_1 - \theta\|^2$$

$$= c \sum_{j: |\theta_j| \leq a_n} \theta_j^2$$
\[ \leq c a_n \sum_{j:|\theta_j| \leq a_n} |\theta_j| = O(v_n a_n). \]

Hence,
\[ n^{-1} E \| \hat{X} \hat{\theta} - X \theta \| ^2 \leq 2 n^{-1} (E \| \hat{X} \hat{\theta} - X \theta_1 \| ^2 + \| X \theta_1 - X \theta \| ^2) = 2 n^{-1} E \| \hat{X} \hat{\theta} - X \theta_1 \| ^2 + O(v_n a_n). \]

Then, it remains to show that
\[ n^{-1} E \| \hat{X} \hat{\theta} - X \theta_1 \| ^2 = O(q_n n^{-1}) + O(v_n a_n) + O(h_n n^{-1}(1+\eta-2\tau)). \]

Following the proof of Theorem 1 we obtain that
\[ n^{-1} E[\| \hat{X} \hat{\theta} - X \theta_1 \| ^2 I_{A_n}] = O(q_n n^{-1}) + O(h_n n^{-1}(1+\eta-2\tau)), \]
where \( I_A \) is the indicator of the set \( A \). From
\[ \| \hat{X} \hat{\theta} - X \theta_1 \| ^2 I_{A_n} \leq 2 \| \hat{X} \hat{\theta} - X \hat{\theta} \| ^2 I_{A_n} + 2 \| X \hat{\theta} - X \theta_1 \| ^2 I_{A_n} \]
and Theorem 1, result (13) follows if we can show that
\[ n^{-1} E \| \hat{X} \hat{\theta} - X \hat{\theta} \| ^2 I_{A_n} = o(q_n n^{-1}) \bigvee h_n n^{-1}(1+\eta-2\tau)). \]

Since
\[ \| \hat{X} \hat{\theta} - X \hat{\theta} \| ^2 = (\hat{\theta} - \hat{\theta})' X' X (\hat{\theta} - \hat{\theta}) \leq O(n) \| \hat{\theta} - \theta \| ^2 \leq O(a_n^2 pm), \]
the result follows from \( P(A_n^c) = O((n \bigvee p)^{-t}) \) for any \( t > 0 \) according to Theorem 2 or 2A. This completes the proof. \( \square \)

Acknowledgments. The authors would like to thank a referee and an Associate Editor for their helpful comments and suggestions.

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School of Finance and Statistics
East China Normal University
500 Dongchuan Rd.
Shanghai, 200241
China

and

Department of Statistics
University of Wisconsin
1300 University Ave.
Madison, Wisconsin 53706
USA

E-mail: shao@stat.wisc.edu

Zou, H. (2006). The adaptive lasso and its oracle properties. *J. Amer. Statist. Assoc.* 101:1418–1429. MR2279469

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Department of Statistics
Virginia Polytechnic Institute and State University
211 Hutcheson Hall
Blacksburg, Virginia 24061
USA

E-mail: xdeng@vt.edu