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A Lack-Of-Fit Test with Screening in Sufficient Dimension Reduction

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Abstract: Researchers often need to infer how the conditional mean of a response varies with the predictors. Sufficient dimension-reduction techniques reduce the dimension by identifying a minimal set of linear combinations of the original predictors, without loss of information. This study tests whether a given small number of linear combinations of the original ultrahigh-dimensional covariates is sufficient to characterize the conditional mean of the response. We first introduce a novel consistent lack-of-fit test statistic for the case when the dimensionality of the covariates is moderate. The proposed test is shown to be n-consistent under the null hypothesis, and root-n-consistent under the alternative hypothesis. A bootstrap procedure is developed to approximate the p-values, and the consistency of the test is studied theoretically. To deal with the ultrahigh dimensionality, we introduce a two-stage lack-of-fit test with screening (LOFTS) procedure, based on a data-splitting strategy. The data are randomly partitioned into two equal halves. In the first stage, we apply the martingale difference correlation-based screening to one half of the data, and select a moderate set of covariates.

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In the second stage, we perform the proposed test, based on the selected covariates, using the second half of the data. The data-splitting strategy is crucial to eliminate the effect of spurious correlations and to prevent an increase in the type-I error rates. We also demonstrate the effectiveness of our two-stage test procedure by means of comprehensive simulations and a real-data application.

Key words and phrases: Bootstrap; Central mean subspace, Data splitting, Lack-of-fit test, Sufficient dimension reduction, Variable Selection.

1. Introduction

Let $\mathbf{x} = (X_1, \ldots, X_p)^{\mathrm{T}} \in \mathbb{R}^p$ be a covariate vector, and $\mathbf{y} = (Y_1, \ldots, Y_q)^{\mathrm{T}} \in \mathbb{R}^q$ be a response vector. Researchers often need to infer how the conditional mean of $\mathbf{y}$ varies with the predictors. Sufficient dimension-reduction techniques have become important and useful in high-dimensional data analyses. Such techniques aim to identify a few linear combinations of the original high-dimensional covariates, while retaining all information about $E(\mathbf{y} \mid \mathbf{x})$. Cook and Li (2002) assumed there exists a $p \times d_0$ matrix $\boldsymbol{\beta}$, such that

$$E(\mathbf{y} \mid \mathbf{x}) = E(\mathbf{y} \mid \boldsymbol{\beta}^{\mathrm{T}}\mathbf{x}), \tag{1.1}$$

which implies that the conditional mean function $E(\mathbf{y} \mid \mathbf{x})$ depends on $\mathbf{x}$ through only d_0 linear combinations $\boldsymbol{\beta}^{\mathrm{T}}\mathbf{x}$. This model not only retains the flexibility of nonparametric modeling, but also enjoys the interpretability

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of parametric modeling. Because $\boldsymbol{\beta}$ is not identifiable, Cook and Li (2002) defined the central mean subspace (CMS), denoted by $\mathcal{S}_{E(\mathbf{y}|\mathbf{x})}$, as the smallest column space of $\boldsymbol{\beta}$. Here, the corresponding smallest column numbers, denoted by d_0, form the structural dimension. To recover $\mathcal{S}_{E(\mathbf{y}|\mathbf{x})}$, Li and Duan (1989) suggested using an ordinary least squares estimator when $\mathbf{x}$ follows an elliptical distribution, particularly when $d_0 = 1$. Cook and Li (2002) proved that the column space of $\{\text{var}(\mathbf{x})\}^{-1}\text{cov}(\mathbf{x}, \mathbf{y})$ belongs to the CMS $\mathcal{S}_{E(\mathbf{y}|\mathbf{x})}$ when $\mathbf{x}$ satisfies the linearity condition. Xia et al. (2002) proposed a minimum average variance estimation (MAVE) that can be applied when the covariates are continuous. Ma and Zhu (2012) developed a semiparametric approach to dimension reduction. Ma and Zhu (2014) further investigated the inference and estimation efficiency of the CMS for sufficient dimension reduction. Zhu and Zhong (2015) estimated the CMS for multivariate response data. Refer to Ma and Zhu (2013a) for a comprehensive review of dimension reduction.

Most works in the dimension-reduction literature have focused on estimating the CMS. However, model diagnostic studies have not received much attention within the context of dimension reduction. Thus, it is fundamental to study whether a given small number of linear combinations of the original high-dimensional covariates is sufficient to characterize the

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conditional mean of $\mathbf{y}$. That is, we test the following null hypothesis, for a given $d_0 \geq 1$:

$$H_0: \quad E(\mathbf{y} \mid \mathbf{x}) = E(\mathbf{y} \mid \boldsymbol{\beta}^{\mathrm{T}}\mathbf{x}), \text{ for some } p \times d_0 \text{ matrix } \boldsymbol{\beta}. \tag{1.2}$$

Some efforts have been devoted to model checking. For example, Stute and Zhu (1998) studied nonparametric tests for the validity of generalized linear models with a given parametric link structure, based on certain empirical processes marked by the residuals. Xia et al. (2004) considered model checking for single-index models. Verzelen and Villers (2010) proposed a new goodness-of-fit test for high-dimensional Gaussian linear models based on the Fisher statistic. Guo, Wang, and Zhu (2016) introduced a model-adaptation concept in lack-of-fit testing, and proposed a dimension-reduction model-adaptive (DRMA) test for checking parametric single-index models. Shah and Buhlmann (2018) developed residual prediction goodness-of-fit tests to assess the validity of high-dimensional linear models. For the choice of the structural dimension d_0, Cook and Li (2004) provided a sequential test procedure. Zhu, Yu, and Zhu (2010) proposed a sparse eigendecomposition strategy by introducing an ℓ_1 penalty to shrink small-sample eigenvalues to zero. Ma and Zhang (2015) considered an information criterion-based method to determine the structural dimension of the reduction model. However, the challenges associated with designing

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a general test for (1.2), especially for ultrahigh-dimensional covariates, are not addressed.

For ultrahigh-dimensional data in which the number of covariates is much higher than the sample size, the aforementioned dimension-reduction methods do not work. This is because their asymptotic normality results may require that the dimensionality divergence rate satisfy $p = o(n^{1/3})$ (Zhu, Zhu, and Feng , 2010). In addition, as pointed by Zhang, Yao, and Shao (2018), testing $H_0 : E(\varepsilon \mid \mathbf{x}) = 0$ almost surely, without assuming a parametric model, is very challenging, because we are targeting a general class of alternatives. In addition, the power may decrease quickly owing to the growing dimension and nonlinear dependence. It is natural and crucial to assume the sparsity principle, which states that only a small set of covariates, denoted by $\mathcal{A}$, truly contribute to the response. Let $\mathbf{x}_{\mathcal{A}} = \{X_k, k \in \mathcal{A}\}$ denote the covariates indexed by $\mathcal{A}$. Under the sparsity assumption, the null hypothesis (1.2) can be written as

$$H_0 : \quad E(\mathbf{y} \mid \mathbf{x}) = E(\mathbf{y} \mid \boldsymbol{\beta}_{\mathcal{A}}^{\mathrm{T}} \mathbf{x}_{\mathcal{A}}), \text{ for some } |\mathcal{A}| \times d_0 \text{ matrix } \boldsymbol{\beta}_{\mathcal{A}}, \quad (1.3)$$

where $|\mathcal{A}|$ represents the cardinality of $\mathcal{A}$. Without loss of generality, we assume $\boldsymbol{\beta} = (\boldsymbol{\beta}_{\mathcal{A}}^{\mathrm{T}}, \mathbf{0}_{d_0 \times (p-|\mathcal{A}|)})^{\mathrm{T}}$, where $\mathbf{0}_{d_0 \times (p-|\mathcal{A}|)}$ denotes a $d_0 \times (p - |\mathcal{A}|)$ matrix of zeros. However, in general, $\mathcal{A}$ is unknown. Sure-independence screening approaches (Fan and Lv , 2008; Zhu et al. , 2011; Li, Zhong, and

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Zhu , 2012) have been developed to screen out irrelevant covariates and estimate $\mathcal{A}$ for ultrahigh-dimensional data. Refer to Liu, Zhong, and Li (2015) for a review of variable screening. In particular, Shao and Zhang (2014) proposed a martingale difference correlation (MDC) that imposes few parametric assumptions on the mean regression form $E(\mathbf{y} \mid \mathbf{x})$, but retains the model-free flavor of sufficient dimension reduction.

We first assume that there exists a surrogate index set $\mathcal{S}$ with a moderate size such that $\mathcal{A} \subseteq \mathcal{S}$. Then, we develop a novel consistent lack-of-fit test statistic for (1.3), based on the moderate covariate set $\mathcal{S}$. We demonstrate that the hypothesis based on $\mathcal{S}$ is equivalent to (1.3), as long as $\mathcal{A} \subseteq \mathcal{S}$ in Theorem 1. The proposed test is shown to be n-consistent under the null hypothesis, and root-n-consistent under the alternative hypothesis. We suggest a bootstrap procedure to approximate the p-values, and show theoretically that this procedure is consistent. Our second goal is to introduce a new two-stage approach, based on a random data-splitting strategy, for testing (1.2) when the dimensionality of the covariates is ultrahigh. Specifically, we first partition the data randomly into two equal halves. In the first stage, we apply MDC screening to one half of the data, and select a moderate set of covariates to estimate the index set $\mathcal{S}$. In the second stage, we perform the proposed test for (1.2), based on the selected

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set, using the second half of the data. Note that the data-splitting strategy is crucial to eliminate the effect of spurious correlations and to prevent the Type-I error rate of the test from increasing. Furthermore, to avoid a potential increase in the type-I error rate when some important covariates are missed with a non-ignorable probability, we provide a multi-splitting strategy as an extension to the proposed procedure.

The rest of this paper is organized as follows. Section 2 introduces the two-stage test procedure. In Section 3, we study the theoretical justification for the test procedure. Section 4 demonstrates the finite-sample performance of the test using comprehensive simulations and a real-data application. We discuss the aforementioned multi-splitting strategy in Section 5. All technical proofs are relegated to the Supplemental Material.

A word on notation. Let $\mathbf{x}_{\mathcal{S}}$ be the covariate vector indexed by $\mathcal{S}$, and let $|c|$ be the absolute value of a generic constant c. For a complex-valued function ψ, $\|\psi\|^2 = \psi^{\mathrm{T}}\overline{\psi}$ and $\overline{\psi}$ is the conjugate of ψ, and for a matrix $\boldsymbol{\beta} \in \mathbb{R}^{p\times d_0}$, $\|\boldsymbol{\beta}\| = \{\mathrm{tr}(\boldsymbol{\beta}^{\mathrm{T}}\boldsymbol{\beta})\}^{1/2}$. In addition, span($\boldsymbol{\beta}$) denotes the column space of $\boldsymbol{\beta}$, $\mathcal{S}_{E(\mathbf{y}|\mathbf{x})}$ and $\mathcal{S}_{E(\mathbf{y}|\mathbf{x}_{\mathcal{S}})}$ denote the CMS of $\mathbf{y}$, given $\mathbf{x}$, and the CMS of $\mathbf{y}$, given $\mathbf{x}_{\mathcal{S}}$, respectively. The sign $\xrightarrow{D}$ denotes convergence in distribution.

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2. A New Testing Procedure

In this section, we first propose a lack-of-fit test statistic at the population level, based on a surrogate index set $\mathcal{S}$ with a moderate size, such that $\mathcal{A} \subseteq \mathcal{S}$. Then, we estimate the test statistic and develop a two-stage lack-of-fit test with a screening procedure.

2.1 A Lack-of-Fit Test Statistic

Under the sparsity assumption, this hypothesis can be formulated as in (1.3), where $\mathcal{A}$ represents the index set of covariates that truly contribute to the response. However, in general, $\mathcal{A}$ is unknown, which makes it practically infeasible to directly propose a test for (1.3). To deal with this issue, we first suppose that there exists a surrogate index set $\mathcal{S}$, with a moderate size, that satisfies that $\mathcal{A} \subseteq \mathcal{S}$. Then, we consider the following null hypothesis:

$$H_0: \quad E(\mathbf{y} \mid \mathbf{x}) = E(\mathbf{y} \mid \boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}} \mathbf{x}_{\mathcal{S}}), \text{ for some } |\mathcal{S}| \times d_0 \text{ matrix } \boldsymbol{\beta}_{\mathcal{S}}. \tag{2.1}$$

The following natural question then arises: is testing (2.1) equivalent to testing (1.3)? The following theorem answers this question.

Theorem 1. *In addition to the sparsity assumption, we assume that both* $\mathcal{S}_{E(\mathbf{y}|\mathbf{x})}$ *and* $\mathcal{S}_{E(\mathbf{y}|\mathbf{x}_{\mathcal{S}})}$ *exist and are uniquely defined. Then testing (2.1) is equivalent to testing (1.3) for an arbitrary index set* $\mathcal{S}$*, as long as* $\mathcal{A} \subseteq \mathcal{S}$*.*

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We emphasize the importance of Theorem 1 because it guarantees that testing (2.1) is equivalent to testing (1.3) as long as $\mathcal{A} \subseteq \mathcal{S}$. This allows us to use the two-stage procedure that is feasible for ultrahigh-dimensional testing problems; see the discussion in the next subsection.

Next, we propose a new consistent lack-of-fit test for (2.1) at the population level, based on the index set $\mathcal{S}$. In a sufficient dimension-reduction context, and without any further regression model assumptions, we define the error term $\boldsymbol{\varepsilon} \stackrel{\text{def}}{=} \mathbf{y} - E(\mathbf{y} \mid \boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})$. The null hypothesis H_0 in (2.1) is equivalent to $E(\boldsymbol{\varepsilon} \mid \mathbf{x}_{\mathcal{S}}) = 0$. It is further equivalent to $\left\| E\{\boldsymbol{\varepsilon}\exp(i\mathbf{s}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})\}\right\|^2 = 0$, for all $\mathbf{s} \in \mathbb{R}^{|\mathcal{S}|\times 1}$, using a Fourier transformation, where i stands for an imaginary unit; that is, $i^2 = -1$. We further note that

$$\left\| E\{\boldsymbol{\varepsilon}\exp(i\mathbf{s}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})\}\right\|^2 = E\Big[\boldsymbol{\varepsilon}_1^{\mathrm{T}}\boldsymbol{\varepsilon}_2\exp\{i\mathbf{s}^{\mathrm{T}}(\mathbf{x}_{1,\mathcal{S}} - \mathbf{x}_{2,\mathcal{S}})\}\Big],$$

where $(\mathbf{x}_{1,\mathcal{S}}, \mathbf{y}_1)$ and $(\mathbf{x}_{2,\mathcal{S}}, \mathbf{y}_2)$ are two independent copies of $(\mathbf{x}_{\mathcal{S}}, \mathbf{y})$. Then, for an arbitrary weight function $\omega(\mathbf{s}) > 0$, testing H_0 in (2.1) is equal to checking whether

$$E\left\{\int_{\mathbb{R}^{|\mathcal{S}|}} \boldsymbol{\varepsilon}_1^{\mathrm{T}}\boldsymbol{\varepsilon}_2\exp\{i\mathbf{s}^{\mathrm{T}}(\mathbf{x}_{1,\mathcal{S}} - \mathbf{x}_{2,\mathcal{S}})\}\omega(\mathbf{s})d\mathbf{s}\right\} = 0, \tag{2.2}$$

where the expectation E is taken with respect to $(\mathbf{x}_{1,\mathcal{S}}, \mathbf{y}_1)$ and $(\mathbf{x}_{2,\mathcal{S}}, \mathbf{y}_2)$. Then, the left-hand side of (2.2) can be considered a test statistic. Borrowing from Székely, Rizzo, and Bakirov (2007) and Shao and Zhang (2014),

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we specifically choose $\omega(\mathbf{s}) = \left(c_0\|\mathbf{s}\|^{1+|\mathcal{S}|}\right)^{-1}$, where $c_0 = \pi^{(1+|\mathcal{S}|)/2}/\Gamma\{(1+|\mathcal{S}|)/2\}$. Then, by $E(\boldsymbol{\varepsilon}_1) = E(\boldsymbol{\varepsilon}_2) = 0$ and Lemma 1 of Székely, Rizzo, and Bakirov (2007), this test statistic has the following closed form:

$$\begin{aligned} T &\overset{\text{def}}{=} E\left[\int_{\mathbb{R}^{|\mathcal{S}|}} \left(c_0\|\mathbf{s}\|^{1+|\mathcal{S}|}\right)^{-1} \boldsymbol{\varepsilon}_1^{\mathrm{T}}\boldsymbol{\varepsilon}_2 \exp\{i\mathbf{s}^{\mathrm{T}}(\mathbf{x}_{1,\mathcal{S}} - \mathbf{x}_{2,\mathcal{S}})\} d\mathbf{s}\right] \\ &= E\left\{\int_{\mathbb{R}^{|\mathcal{S}|}} \left(c_0\|\mathbf{s}\|^{1+|\mathcal{S}|}\right)^{-1} \boldsymbol{\varepsilon}_1^{\mathrm{T}}\boldsymbol{\varepsilon}_2 d\mathbf{s}\right\} \\ &- E\left[\int_{\mathbb{R}^{|\mathcal{S}|}} \left(c_0\|\mathbf{s}\|^{1+|\mathcal{S}|}\right)^{-1} \boldsymbol{\varepsilon}_1^{\mathrm{T}}\boldsymbol{\varepsilon}_2 \left[1 - \cos\{\mathbf{s}^{\mathrm{T}}(\mathbf{x}_{1,\mathcal{S}} - \mathbf{x}_{2,\mathcal{S}})\}\right] d\mathbf{s}\right] \\ &= -E\left(\boldsymbol{\varepsilon}_1^{\mathrm{T}}\boldsymbol{\varepsilon}_2 \|\mathbf{x}_{1,\mathcal{S}} - \mathbf{x}_{2,\mathcal{S}}\|\right). \end{aligned} \tag{2.3}$$

In general, $T \geq 0$. In addition, $T = 0$ if and only if H_0 in (2.1) is true. This motivates us to use a consistent estimator of T as our test statistic for (2.1). Here, larger values of T provide stronger evidence against the null hypothesis (2.1).

2.2 Two-Stage Lack-of-Fit Test with Screening

In order to estimate the test statistic T, we first determine an index set $\mathcal{S}$ that contains the true covariates set $\mathcal{A}$, and estimate the error term $\boldsymbol{\varepsilon} = \mathbf{y} - E(\mathbf{y} \mid \boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})$. To this end, we propose a two-stage testing procedure based on a data-splitting strategy. We partition the random sample $\mathcal{D} \overset{\text{def}}{=} \{(\mathbf{x}_i, \mathbf{y}_i), i = 1, \ldots, n\}$ randomly into two halves. In the first stage, we screen out as many irrelevant covariates as possible based on the first half

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of the data, $\mathcal{D}_1 \overset{\text{def}}{=} \{(\mathbf{x}_i, \mathbf{y}_i), i = 1, \ldots, n_1\}$. As such, we obtain an index set $\mathcal{S}$ with a moderate size, where n_1 is the integer part of $n/2$. In the second stage, we develop a novel consistent lack-of-fit test for (1.3) using the second half of the data, $\mathcal{D}_2 \overset{\text{def}}{=} \{(\mathbf{x}_i, \mathbf{y}_i), i = n_1 + 1, \ldots, n_1 + n_2\}$.

Stage 1: Feature Screening

Feature screening approaches screen out irrelevant covariates and retain those that are truly relevant in a moderate set for ultrahigh-dimensional data. In the first stage, we apply the martingale difference correlation (MDC)-based screening approach proposed by Shao and Zhang (2014) to the first half of the data. In this way, we select a moderate set of covariates.

The martingale difference divergence (MDD) of $\mathbf{y}$, given each covariate X_j, is defined by

$$\text{MDD}(\mathbf{y} \mid X_j)^2 = \frac{1}{c_q} \int_{\mathbb{R}^q} \frac{\|g_{\mathbf{y},X_j}(\mathbf{s}) - E(\mathbf{y}) g_{X_j}(\mathbf{s})\|^2}{\|\mathbf{s}\|^{1+q}} d\mathbf{s}, \tag{2.4}$$

where $g_{\mathbf{y},X_j}(\mathbf{s}) = E(\mathbf{y}e^{i\mathbf{s}^{\mathrm{T}}X_j})$, $g_{X_j}(\mathbf{s}) = E(e^{i\mathbf{s}^{\mathrm{T}}X_j})$, $c_q = \pi^{(1+q)/2}/\Gamma(1+q)/2$, and $\Gamma(\cdot)$ is the gamma function. Note that $\text{MDC}(\mathbf{y} \mid X_j)$ is the normalized version of $\text{MDD}(\mathbf{y} \mid X_j)$. Here, $\text{MDC}(\mathbf{y} \mid X_j) = 0$ if and only if $E(\mathbf{y} \mid X_j) = E(\mathbf{y})$ almost surely, when $E(\|\mathbf{y}\|^2 + X_j^2) < \infty$. That is, when $\text{MDC}(\mathbf{y} \mid X_j) = 0$, the conditional mean of $\mathbf{y}$, given X_j, is independent of X_j. Shao and Zhang (2014) proposed using the estimated MDC of the response, given a covariate, as the marginal utility to rank the importance

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of all covariates. Then, they select a moderate set of covariates from the top ranks. Refer to Shao and Zhang (2014) for the calculation of the sample MDC.

As mentioned by Cook and Li (2002), a regression analysis is primarily concerned with making an inference about the conditional mean of a response, given a set of covariates. This is true of MDC-based screening as well. Furthermore, this approach inherits the model-free flavor of sufficient dimension reduction. We apply MDC-based screening to $\mathcal{D}_1$, the first half of the data. Then, we select the set of covariates defined by

$$\mathcal{S} = \{j : \widehat{\mathrm{MDC}}(\mathbf{y} \mid X_j) \text{ is among the top } s \text{ largest of all } p \text{ sample } \widehat{\mathrm{MDC}} \text{ values}\}.$$

With a slight abuse of notation, we still use $\mathcal{S}$ to represent the set selected by screening. Under some regularity assumptions, the sure-screening property holds for MDC-based screening; that is, $P(\mathcal{A} \subseteq \mathcal{S}) \to 1$ as the sample size approaches infinity. Then, from Theorem 1 and the sure-screening property, it follows that testing (2.1) is asymptotically equivalent to testing (1.3).

Stage 2: A Lack-of-Fit Test

Next, we estimate the test statistic T. First, we suggest using the profile least squares approach to recover $\mathcal{S}_{E(\mathbf{y}|\mathbf{x}_\mathcal{S})}$. This amounts to minimizing the

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profile least squares to obtain the following estimator:

$$\widehat{\boldsymbol{\beta}}_{\mathcal{S},-d_0} \stackrel{\text{def}}{=} \underset{\mathbf{b}\in\mathbb{R}^{(|\mathcal{S}|-d_0)\times d_0}}{\arg\min} \sum_{i=n_1+1}^{n} \|\mathbf{y}_i - \widehat{\mathbf{m}}(\mathbf{x}_{\mathcal{S},d_0,i} + \mathbf{b}^{\mathrm{T}}\mathbf{x}_{\mathcal{S},-d_0,i})\|^2,$$

where $\mathbf{x}_{\mathcal{S},d_0}$ is a vector of the first d_0 elements of $\mathbf{x}_{\mathcal{S}}$, and $\mathbf{x}_{\mathcal{S},-d_0}$ is a vector of the remaining elements. Here, we restrict the upper $d_0 \times d_0$ submatrix of $\boldsymbol{\beta}_{\mathcal{S}}$ to be an identity matrix to ensure that $\boldsymbol{\beta}_{\mathcal{S}}$ itself is identifiable (Ma and Zhu , 2013b) for a given d_0. Then, $\widehat{\boldsymbol{\beta}}_{\mathcal{S},-d_0}$ is a $(|\mathcal{S}| - d_0) \times d_0$ matrix composed of the lower $(|\mathcal{S}| - d_0)$ rows of $\boldsymbol{\beta}_{\mathcal{S}}$. For an arbitrary $\mathbf{b} \in \mathbb{R}^{(|\mathcal{S}|-d_0)\times d_0}$, we estimate $\mathbf{m}(\mathbf{x}_{\mathcal{S},d_0,i} + \mathbf{b}^{\mathrm{T}}\mathbf{x}_{\mathcal{S},-d_0,i})$ using the leave-one-out kernel estimator, defined as

$$\widehat{\mathbf{m}}(\mathbf{x}_{\mathcal{S},d_0,i}+\mathbf{b}^{\mathrm{T}}\mathbf{x}_{\mathcal{S},-d_0,i}) \stackrel{\text{def}}{=} \sum_{j=n_1+1,j\neq i}^{n} \frac{K_h(\mathbf{x}_{\mathcal{S},d_0,j} + \mathbf{b}^{\mathrm{T}}\mathbf{x}_{\mathcal{S},-d_0,j} - \mathbf{x}_{\mathcal{S},d_0,i} - \mathbf{b}^{\mathrm{T}}\mathbf{x}_{\mathcal{S},-d_0,i})\mathbf{y}_j}{K_h(\mathbf{x}_{\mathcal{S},d_0,j} + \mathbf{b}^{\mathrm{T}}\mathbf{x}_{\mathcal{S},-d_0,j} - \mathbf{x}_{\mathcal{S},d_0,i} - \mathbf{b}^{\mathrm{T}}\mathbf{x}_{\mathcal{S},-d_0,i})},$$

where $K_h(\cdot) = K(\cdot/h)/h^{d_0}$, $K(\cdot)$ is the product of d_0 univariate kernel functions, and h is the bandwidth. Then, we estimate T by

$$T_{n_2} \stackrel{\text{def}}{=} \mathrm{tr}\bigg(-\frac{1}{n_2^2} \sum_{i=n_1+1}^{n_1+n_2} \sum_{j=n_1+1}^{n_1+n_2} \widehat{\boldsymbol{\varepsilon}}_i \widehat{\boldsymbol{\varepsilon}}_j^{\mathrm{T}} \|\mathbf{x}_{i,\mathcal{S}} - \mathbf{x}_{j,\mathcal{S}}\| \bigg), \tag{2.5}$$

where $\widehat{\boldsymbol{\varepsilon}} = \mathbf{y} - \widehat{\mathbf{m}}(\widehat{\boldsymbol{\beta}}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})$. In practice, larger values of T_{n_2} provide stronger evidence against H_0 in (2.1).

Because the null hypothesis (2.1) is concerned with studying whether a given small number of linear combinations of covariates is sufficient to characterize the conditional mean of $\mathbf{y}$, the test based on T_{n_2} is essentially

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a lack-of-fit test. Thus, we name this two-stage test procedure the lack-of-fit test with screening (LOFTS) procedure, which is summarized in the following algorithm.

Algorithm 1 The LOFTS Procedure

Step 1. Randomly split the random sample into two even halves, $\mathcal{D}_1$ and $\mathcal{D}_2$.

Step 2. Apply MDC-based screening to $\mathcal{D}_1$ and select the moderate set $\mathcal{S}$.

Step 3. Test (2.1) based on the test statistic T_{n_2} using $\mathcal{D}_2$. The associated p-value can be obtained using the bootstrap procedure (Algorithm 2 in Section 3).

Step 4. Reject (2.1) and (1.3) if p-value$< \alpha$, the significance level.

Remark 1: Note that the data-splitting technique is crucial in the proposed two-stage LOFTS procedure for ultrahigh-dimensional data. If we do not split the data, a naive two-stage procedure is as follows. In the first stage, MDC-screening is applied to the full sample. In the second stage, the proposed test is conducted based on the selected covariates, using the same data. In theory, this method works well, and is even more efficient if, in the first stage, $\mathcal{S}$ happens to be $\mathcal{A}$ exactly. However, this is usually difficult to achieve in ultrahigh-dimensional problems. Often, inactive covariates, which may contribute to the response in a finite sample, are selected in the first screening stage of the naive two-stage procedure. As a result, there is an increase in the type-I error rate when testing (2.1); see the simulation

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results in Section 4. This is the result of spurious correlations inherent in ultrahigh-dimension problems (Fan, Guo, and Hao , 2012). The data-splitting technique can eliminate spurious correlations and further avoid the size increase. Because the two halves of the data set are independent, a covariate that has a large spurious sample correlation with the response over the first half has a small chance of being highly correlated with the response in the second half. Hence, its influence on the size of the test in the second stage is negligible.

Remark 2: Feature screening can efficiently reduce the dimensionality of covariates in the first stage, while retaining the truly important covariates in the asymptotical sense. However, some important covariates may be missed at the finite-sample level. As such, the choice of the reduced model size may be crucial for the screening procedure to work. Fan and Lv (2008) suggested a hard thresholding, where the reduced model size is proportional to $[n/\log n]$. Wu, Boos, and Stefanski (2007), Zhu et al. (2011), and Li, Zhong, Li, and Wu (2014) proposed a soft-thresholding rule by introducing auxiliary variables. To reduce this risk in practice, we may choose a relatively large set $\mathcal{S}$ if we believe that the size of the important covariates is relatively large. Alternatively, we can apply the iterative version of MDC-based screening to avoid missing any important covariates

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that are marginally uncorrelated with the response. Another strategy to enhance the performance of the data-splitting technique is that of multiple data splitting; see Section 5.

REMARK 3: The number of linear combinations of covariates, d_0, in (2.1) is prespecified before the lack-of-fit test procedure. The null hypothesis H_0 (2.1) holds trivially if we specify $d_0 = |\mathcal{S}|$, letting $\boldsymbol{\beta}_{\mathcal{A}}$ be an $|\mathcal{S}| \times |\mathcal{S}|$ identity matrix. We wish to determine the smallest number of linear combinations of covariates that sufficiently capture the regression information of $E(\mathbf{y} \mid \mathbf{x}_{\mathcal{S}})$. For instance, the optimal value of d_0 is one for a general single-index model. For a given dimension d_0, if H_0 is rejected at some level of significance, then we can conclude that $\boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}}$ is not sufficient to characterize the conditional mean $E(\mathbf{y} \mid \mathbf{x}_{\mathcal{S}})$; thus, additional linear combinations of $\mathbf{x}_{\mathcal{S}}$ are needed. In practice, we can perform the two-stage LOFTS procedure sequentially for d_0, from 1 to $|\mathcal{S}|$, until we fail to reject H_0. In this way, we can determine the optimal value of d_0.

3. Theoretical Properties

In this section, we study the theoretical properties of the proposed test, including the asymptotic distribution under the null hypothesis and the asymptotic distributions under the global and local alternative hypotheses.

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We also propose a bootstrap procedure to calculate the associated p-value. The regularity conditions are provided in the Appendix.

Theorem 2 states the asymptotic null distribution of the test statistic under the null hypothesis (2.1).

Theorem 2. *Assume Conditions (C1)–(C5) hold. Then, under H_0 in (2.1),*

$$n_2 T_{n_2} \xrightarrow{D} \|\zeta(\mathbf{s})\|_\omega^2 \stackrel{def}{=} \int_{\mathbf{s}\in\mathbb{R}^{|\mathcal{S}|}} \|\zeta(\mathbf{s})\|^2 (c_0\|\mathbf{s}\|^{1+|\mathcal{S}|})^{-1} d\mathbf{s}, \quad as\ n_2 \to \infty,$$

where $\zeta(\mathbf{s})$ denotes a complex-valued Gaussian random process with mean zero and covariance function $cov\{\zeta(\mathbf{s}), \zeta^T(\mathbf{s}_0)\}$, defined in (S3.1) in the Supplementary Material.

However, the asymptotic distribution of T_{n_2} under H_0 is unfortunately not tractable, because $\|\zeta(\mathbf{s})\|_\omega^2$ hinges upon the unknown joint distribution of $(\mathbf{x}_\mathcal{S}, \mathbf{y})$. In practice, we propose the bootstrap procedure in Algorithm 2 to calculate the associated p-value.

Theorem 3 states the consistency of the bootstrap procedure.

Theorem 3. *Assume Conditions (C1)–(C5) hold. Then, we have that $n_2\widetilde{T}_{n_2} \xrightarrow{D} \|\zeta(\mathbf{s})\|_\omega^2$, as $n_2 \to \infty$.*

Note that although it is not tractable in Theorem 2, it is necessary that we derive the asymptotic distribution of T_{n_2} under H_0, because Theorem 3

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Algorithm 2 The Bootstrap Procedure

Step 1. Obtain $\widehat{\boldsymbol{\beta}}_{\mathcal{S}}$ and $\widehat{\mathbf{m}}(\widehat{\boldsymbol{\beta}}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})$ using the second half $\mathcal{D}_2$, and calculate the residuals $\widehat{\boldsymbol{\varepsilon}}_i = \mathbf{y}_i - \widehat{\mathbf{m}}(\widehat{\boldsymbol{\beta}}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S},i})$, for $i = n_1+1, n_1+2, \ldots, n$. Then, compute the test statistic T_{n_2} in (2.5).

Step 2. Draw the weights δ_i independently from $\{1, -1\}$ at random with probability 0.5. Let $\widetilde{\boldsymbol{\varepsilon}}_i = \widehat{\boldsymbol{\varepsilon}}_i\delta_i$ and generate $\widetilde{\mathbf{y}}_i = \widehat{\mathbf{m}}(\widehat{\boldsymbol{\beta}}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S},i}) + \widetilde{\boldsymbol{\varepsilon}}_i$, for $i = n_1+1, n_1+2, \ldots, n$.

Step 3. Repeat Step 1 and calculate the test statistic $\widetilde{T}_{n_2}$ based on (2.5) using the new bootstrapped data set $(\mathbf{x}_i, \widetilde{\mathbf{y}}_i), i = n_1+1, n_1+2, \ldots, n$.

Step 4. Repeat Step 2 and 3 1,000 times to obtain $\widetilde{T}_{n_2}^{(1)}, \widetilde{T}_{n_2}^{(2)}, \ldots, \widetilde{T}_{n_2}^{(1,000)}$. The associated p-value is obtained by $1000^{-1}\sum_{b=1}^{1000} I(\widetilde{T}_{n_2}^{(b)} \geq T_{n_2})$, where $I(\cdot)$ is an indicator function. Reject H_0 if the p-value $< \alpha$, a given significance level.

shows that the asymptotic null distribution of the bootstrapped test statistic is the same as that of the original test statistic. This implies that the bootstrap procedure is able to provide an asymptotically valid inference for the proposed lack-of-fit test.

Next, we consider two alternative hypotheses. The global alternative hypothesis can be specified as follows:

$$H_{1g} : E(\mathbf{y} \mid \mathbf{x}) = E(\mathbf{y} \mid \mathbf{B}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}}), \text{ for some } |\mathcal{S}| \times d_1 \text{ matrix } \mathbf{B}_{\mathcal{S}}, d_0 < d_1 \leq |\mathcal{S}| \quad (3.1)$$

Under H_{1g}, d_0 linear combinations of covariates are not sufficient to recover

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the CMS $\mathcal{S}_{E(\mathbf{y}|\mathbf{x}_\mathcal{S})}$. We also consider a sequence of local alternatives:

$$H_{1l} : \mathbf{y} = \mathbf{m}(\boldsymbol{\beta}_\mathcal{S}^{\mathrm{T}}\mathbf{x}_\mathcal{S}) + C_{n_2}\mathbf{g}(\mathbf{B}_\mathcal{S}^{\mathrm{T}}\mathbf{x}_\mathcal{S}) + \boldsymbol{\varepsilon}, \tag{3.2}$$

$$\text{for some } |\mathcal{S}| \times d_1 \text{ matrix } \mathbf{B}_\mathcal{S}, d_0 < d_1 \leq |\mathcal{S}|,$$

where $\boldsymbol{\beta}_\mathcal{S}$ is a subspace of $\mathbf{B}_\mathcal{S}$, and $C_{n_2} \to 0$ results in H_{1l} becoming local alternatives. Under H_{1l}, we have that $E(\boldsymbol{\varepsilon} \mid \mathbf{x}_\mathcal{S}) = \mathbf{0}$ and $\boldsymbol{\beta}_\mathcal{S}^{\mathrm{T}}\mathbf{x}_\mathcal{S}$ is not sufficient to characterize the conditional mean function $E(\mathbf{y} \mid \mathbf{x}_\mathcal{S})$. However, as $n_2 \to \infty$, H_{1l} approaches H_0. Then, the asymptotic distributions under both the global and the local alternative hypotheses are presented in Theorem 4.

Theorem 4. *Assume conditions (C1)–(C5) in the Appendix hold.*

(i) Under the global alternative in (3.1), as $n_2 \to \infty$,

$$n_2{}^{1/2}(T_{n_2} - T) \xrightarrow{D} N(0, \sigma_0^2),$$

where the variance $\sigma_0^2 \overset{def}{=} 4var(Z_1 + Z_2 + Z_3)$, and Z_1, Z_2, and Z_3 are defined in (S5.1)–(S5.3) of the Supplementary Material, respectively.

(ii) Under the local alternative in (3.2) with $C_{n_2} = n_2^{-1/2}$, as $n_2 \to \infty$,

$$n_2 T_{n_2} \xrightarrow{D} \|\zeta_0(\mathbf{s})\|_\omega^2 \overset{def}{=} \int_{\mathbf{s}\in\mathbb{R}^{|\mathcal{S}|}} \|\zeta_0(\mathbf{s})\|^2 (c_0\|\mathbf{s}\|^{1+|\mathcal{S}|})^{-1} d\mathbf{s},$$

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where $\zeta_0(\mathbf{s})$ denotes a complex-valued Gaussian random process with the mean function defined in (S5.4) and the covariance function $cov\{\zeta_0(\mathbf{s}), \zeta_0(\mathbf{s}_0)\}$ defined in (S3.1) of the Supplementary Material.

4. Numerical Studies

Example 1. We examine the finite-sample performance of the proposed two-stage test procedure using simulations. Consider the following two regression models:

$$\begin{aligned} \text{Model (I)}: \ Y &= (3+\boldsymbol{\beta}_1^{\mathrm{T}}\mathbf{x})^2 + c(\boldsymbol{\beta}_2^{\mathrm{T}}\mathbf{x})^2 + \varepsilon, \\ \text{Model (II)}: \ Y &= \boldsymbol{\beta}_3^{\mathrm{T}}\mathbf{x} + (3+\boldsymbol{\beta}_4^{\mathrm{T}}\mathbf{x})^2 + c(\boldsymbol{\beta}_5^{\mathrm{T}}\mathbf{x})^2 + \varepsilon, \end{aligned}$$

where $\mathbf{x} = (X_1, \ldots, X_p)^{\mathrm{T}}$ is generated from a multivariate normal distribution with mean zero and covariance matrix $\Sigma = (\sigma_{kl})_{p\times p}$, with $\sigma_{kl} = 0.5^{|k-l|}$ for $k, l = 1, \ldots, p$, and $\varepsilon \sim N(0,1)$. Here, we set $\boldsymbol{\beta}_1 = (0.25, 0.25, 0.25, 0.25, 0, \ldots, 0)^{\mathrm{T}}$, $\boldsymbol{\beta}_2 = (0, 1, 0, 0, 0, \ldots, 0)^{\mathrm{T}}$, $\boldsymbol{\beta}_3 = (3, 0, 3, 0, 0, \ldots, 0)^{\mathrm{T}}$, $\boldsymbol{\beta}_4 = (0, 0.5, 0, 0.5, 0, \ldots, 0)^{\mathrm{T}}$, and $\boldsymbol{\beta}_5 = (0, 0, 2, 0, 0, \ldots, 0)^{\mathrm{T}}$. In both models, the value $c = 0$ corresponds to the null hypotheses, and $c \neq 0$ represents the alternatives. Thus, the CMS $\mathcal{S}_{E(Y|\mathbf{x})}$ depends only on $\boldsymbol{\beta}_1^{\mathrm{T}}\mathbf{x}$ under H_0, but on two linear combinations $(\boldsymbol{\beta}_1^{\mathrm{T}}\mathbf{x}, \boldsymbol{\beta}_2^{\mathrm{T}}\mathbf{x})$ under H_1 in Model (I). For Model (II), $\mathcal{S}_{E(Y|\mathbf{x})}$ is two-dimensional under the null, but three-dimensional under the alternative.

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We consider the sample size $n = 200$ and the covariate dimension $p = 2000$. Each sample is divided randomly into two equal halves. We perform the LOFTS procedure in Algorithm 1: Apply MDC-based screening to the first half of the data $\mathcal{D}_1 = \{(\mathbf{x}_i, Y_i), i = 1, \ldots, 100\}$ to obtain a selected model $\mathcal{S}$. Then test hypothesis (2.1) using the second half of the data $\mathcal{D}_2 = \{(\mathbf{x}_{i,\mathcal{S}}, Y_i)$, for $i = 101, \ldots, 200\}$. To compare their empirical performance, we consider the following two procedures: (1) a naive two-stage test procedure, denoted by "NAIVE"; here, we perform both MDC-based screening and the lack-of-fit test on the same full sample; (2) an oracle test procedure, denoted by "Oracle." In the second stage, we conduct the test based on $\{(\mathbf{x}_{i,\mathcal{A}}, Y_i), i = 101, \ldots, 200\}$ directly, because the true model $\mathcal{A}$ is known. We repeat the simulations 1,000 times and summarize their finite-sample performance.

REMARK: For simplicity, we test the null hypothesis (2.1) with $d_0 = 1$ for Model (I) and $d_0 = 2$ for Model (II) to compare the performance of the test procedures in the simulations. As a practical byproduct of the two-stage LOFTS procedure, we can perform the procedure for d_0 sequentially, from 1 to $|\mathcal{S}|$. Then, the optimal value of d_0 is determined when the corresponding null hypothesis fails to be rejected at some significance level.

Screening Performance: In the two-stage LOFTS procedure, the first-

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stage screening performance is crucial to the follow-up test, according to Theorem 1. The MDC-based screening method is effective at including almost all truly important covariates in the selected models in this example. However, because this is not the main contribution of this study, we report the screening performance in the Supplementary Material. Refer to Shao and Zhang (2014) for further numerical justifications of MDC-based screening.

Size Performance: Next, we evaluate the size performance of four test procedures for Models (I) and (II) when $c = 0$: the proposed LOFTS procedure, the naive two-stage method, the oracle procedure, and the DRMA procedure proposed by Guo, Wang, and Zhu (2016). Because the DRMA procedure is proposed for a parametric single-index model, we report the results for Model (I) only. The critical values of the lack-of-fit test procedure are determined using the proposed bootstrap procedure in Algorithm 2. We consider four significance levels (i.e., $\alpha = 0.01, 0.02, 0.05$, and 0.10) and two sizes of the selected models, $|\mathcal{S}| = 8$ and 16. The empirical type-I error rates based on 1,000 repetitions for Models (I) and (II) are presented in Table 1. In addition, QQ plots of the empirical p-values and the uniform distribution are shown in Panels (A) and (B), respectively, of Figure 1. It can be clearly seen that the empirical type-I error rates of the LOFTS

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procedure, DRMA procedure, and oracle method are relatively close to the user-specified significance levels. However, the empirical type-I error rates of the naive two-stage method are obviously larger than the significance levels, especially when the selected model size becomes large. The increase in the type-I errors in the naive two-stage procedure is due to spurious correlations between the response and some unimportant covariates in the ultrahigh-dimensional data. The results further support the importance of the data-splitting strategy, which can efficiently eliminate the effect of spurious correlations.

Table 1: The empirical type-I error rates when $c = 0$.

Model	α	LOFTS		NAIVE		Oracle	DRMA	
		$\|\mathcal{S}\| = 8$	$\|\mathcal{S}\| = 16$	$\|\mathcal{S}\| = 8$	$\|\mathcal{S}\| = 16$		$\|\mathcal{S}\| = 8$	$\|\mathcal{S}\| = 16$
(I)	0.01	0.010	0.011	0.021	0.041	0.015	0.011	0.013
	0.02	0.017	0.020	0.044	0.064	0.020	0.020	0.025
	0.05	0.046	0.054	0.096	0.117	0.052	0.051	0.049
	0.10	0.114	0.105	0.152	0.209	0.095	0.098	0.088
(II)	0.01	0.013	0.017	0.021	0.026	0.009	-	-
	0.02	0.026	0.027	0.031	0.039	0.016	-	-
	0.05	0.045	0.049	0.076	0.087	0.054	-	-
	0.10	0.105	0.106	0.118	0.151	0.112	-	-

Power Performance: When $c \neq 0$, the previous null hypotheses are no longer valid. For instance, the response depends on three linear combinations in Model (II) when $c \neq 0$. We consider values of $c = 0.2, 0.4, 0.6, 0.8,$ and 1 to compare the empirical power of the LOFTS and oracle procedures.

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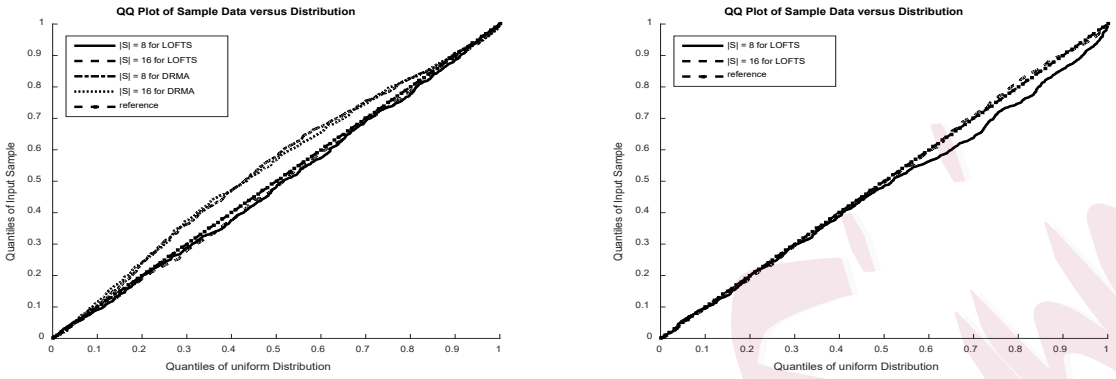

(A) (B)

Figure 1: QQ plots of the empirical p-values and the uniform distribution for Model (I) in Panel (A) and Model (II) in Panel (B) for Example 1.

Note that the "oracle" means we assume that the set of truly important covariates is known in the second test stage. We choose two significance levels (i.e., $\alpha = 0.05$ and 0.10) and two reduced model sizes (i.e., $|\mathcal{S}| = 8$ and 16). Table 2 summarizes the simulation results, which show that the proposed two-stage LOFTS procedure exhibits significant power in terms of detecting the significance of the tests. The empirical power increases with the signal intensity parameter c. Once the true set $\mathcal{A}$ has been identified, a smaller selected model size yields greater empirical power. This further confirms the importance of screening out irrelevant covariates in ultrahigh-dimensional test problems. Note that the superior size and power performance of the oracle procedure also demonstrate the advantage of the proposed lack-of-fit

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test.

Table 2: The empirical power when $c \neq 0$ at $\alpha = 0.05$ or 0.10.

Model	c	LOFTS				Oracle		DRMA			
		$\lvert\mathcal{S}\rvert = 8$		$\lvert\mathcal{S}\rvert = 16$				$\lvert\mathcal{S}\rvert = 8$		$\lvert\mathcal{S}\rvert = 16$	
		0.05	0.10	0.05	0.10	0.05	0.10	0.05	0.10	0.05	0.10
(I)	0.2	0.243	0.369	0.162	0.247	0.572	0.692	0.099	0.160	0.068	0.127
	0.4	0.652	0.756	0.469	0.580	0.965	0.988	0.253	0.343	0.173	0.284
	0.6	0.853	0.908	0.702	0.779	0.995	0.997	0.496	0.620	0.382	0.495
	0.8	0.944	0.976	0.831	0.896	1.000	1.000	0.722	0.806	0.561	0.674
	1.0	0.963	0.980	0.893	0.937	1.000	1.000	0.836	0.906	0.702	0.796
(II)	0.2	0.965	0.977	0.646	0.768	1.000	1.000	-	-	-	-
	0.4	0.999	0.999	0.921	0.971	1.000	1.000	-	-	-	-
	0.6	0.998	0.999	0.963	0.982	1.000	1.000	-	-	-	-
	0.8	1.000	1.000	0.943	0.976	1.000	1.000	-	-	-	-
	1.0	0.997	0.997	0.923	0.965	1.000	1.000	-	-	-	-

Sequential Test Performance: By performing our proposed LOFTS procedure sequentially, we determine the smallest number of linear combinations of covariates that sufficiently capture the regression information of $E(\mathbf{y} \mid \mathbf{x}_{\mathcal{S}})$. The procedure is conducted as follows. Starting with $d_0 = 1$, test the null hypothesis in (1.2) using the LOFTS procedure. If the hypothesis is rejected, increment d_0 by one, and perform the test again. Stop when the first null hypothesis is not rejected in the test series. The corresponding value of d_0, denoted by $\widehat{d}$, is the estimate of d^* that represents the smallest number of linear combinations of covariates that sufficiently recover the CMS. We report the empirical distributions of $\widehat{d}$ at a significance level of

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$\alpha = 0.05$ based, on 1000 simulations, for Models (I) and (II) in Table 3. The results show that the LOFTS sequential tests are able to estimate the true structural dimension correctly with large probabilities, especially when $|\mathcal{S}| = 8$ and $c = 0$ or c is large.

We also compare the performance of the proposed method with that of the iterative Hessian transformation (IHT) method proposed by Cook and Li (2004) and the validated information criterion (VIC)-based method of Ma and Zhang (2015). Note that, for simplicity, we report only those results when the reduced model size is 8. In addition, because we focus here on the structural dimension of the CMS, we examine the VIC for semiparametric principal Hessian direction estimators only. From Table 4, we can see that our LOFTS procedure outperforms both methods in our limited experiments. The IHT method often underestimates the structural dimension, mainly because the largest estimated eigenvalues tend to dominate the others. Although the estimated dimension using the VIC converges to the true structural dimension in probability, there is no guarantee of its finite-sample performance, especially when the sample size is small and the reduced model size is large. Our LOFTS procedure, however, avoids this problem by using the proposed bootstrap procedure.

Example 2. We apply our proposed two-stage LOFTS procedure to

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Table 3: The empirical distributions of $\widehat{d}$ at the significance level $\alpha = 0.05$.

Model	c	d^*	$\lvert\mathcal{S}\rvert = 8$				$\lvert\mathcal{S}\rvert = 16$			
			1	2	3	4	1	2	3	4
(I)	0	1	**0.954**	0.032	0.002	0.012	**0.946**	0.038	0.004	0.012
	0.2	2	**0.757**	0.218	0.009	0.016	**0.838**	0.128	0.015	0.019
	0.4	2	0.348	**0.607**	0.017	0.028	**0.531**	0.432	0.017	0.020
	0.6	2	0.147	**0.803**	0.022	0.028	0.298	**0.652**	0.018	0.032
	0.8	2	0.056	**0.897**	0.018	0.029	0.169	**0.786**	0.019	0.026
	1.0	2	0.037	**0.907**	0.023	0.033	0.107	**0.844**	0.010	0.039
(II)	0	2	0.000	**0.955**	0.019	0.026	0.003	**0.948**	0.030	0.019
	0.2	3	0.001	0.035	**0.923**	0.041	0.012	0.346	**0.607**	0.035
	0.4	3	0.011	0.001	**0.940**	0.048	0.078	0.073	**0.807**	0.042
	0.6	3	0.050	0.002	**0.907**	0.041	0.234	0.024	**0.705**	0.037
	0.8	3	0.000	0.000	**0.969**	0.031	0.006	0.052	**0.901**	0.041
	1.0	3	0.001	0.003	**0.965**	0.031	0.034	0.059	**0.870**	0.037

Table 4: The empirical distributions of $\widehat{d}$ of IHT and VIC when $\lvert\mathcal{S}\rvert = 8$.

Model	c	d^*	IHT				VIC			
			1	2	3	4	1	2	3	4
(I)	0	1	**0.960**	0.039	0.001	0.000	**0.836**	0.164	0.000	0.000
	0.2	2	**0.926**	0.073	0.001	0.000	**0.830**	0.170	0.000	0.000
	0.4	2	**0.821**	0.168	0.011	0.000	**0.787**	0.213	0.000	0.000
	0.6	2	**0.730**	0.258	0.012	0.000	**0.714**	0.284	0.002	0.000
	0.8	2	**0.583**	0.398	0.019	0.000	**0.601**	0.397	0.002	0.000
	1	2	0.466	**0.514**	0.020	0.000	0.437	**0.563**	0.000	0.000
(II)	0	2	0.395	**0.558**	0.047	0.000	0.105	**0.538**	0.357	0.000
	0.2	3	0.026	**0.941**	0.033	0.000	0.004	**0.858**	0.138	0.000
	0.4	3	0.002	**0.928**	0.070	0.000	0.000	**0.787**	0.213	0.000
	0.6	3	0.000	**0.897**	0.103	0.000	0.000	**0.701**	0.299	0.000
	0.8	3	0.000	**0.857**	0.142	0.001	0.000	**0.613**	0.381	0.006
	1	3	0.000	**0.808**	0.190	0.002	0.000	**0.554**	0.430	0.016

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a rat eye microarray expression data set, which is available from Gene Expression Omnibus, with accession number GSE5680. In this study, 120 12-week-old male rats were selected for tissue harvesting from the eyes, and 31,042 probe sets were measured for the microarray analysis. In Scheetz et al. (2006) and Huang, Ma, and Zhang (2008), 18,976 probes were retained that were considered adequately expressed and that exhibited at least two-fold variation in order to investigate the genetic variation in human eye disease. The response variable TRIM32 at probe 1389163_at, one of the selected 18,976 probes, was recently found to cause Bardet–Biedl syndrome (Chiang et al. , 2006). In our study, we aim to check whether a single linear combination of gene expression levels exists that is sufficient to predict the expression level of the gene TRIM32.

We randomly partition this random sample into two halves, each with 60 observations, and marginally standardize all variables. We perform the MDC-based screening method to reduce the covariate dimension from 18,975 to 8 and 16, respectively. Denote as $\mathbf{x}_{\mathcal{S}_1} = (X_1, \ldots, X_8)^{\mathrm{T}}$ and $\mathbf{x}_{\mathcal{S}_2} = (X_1, \ldots, X_{16})^{\mathrm{T}}$ the covariates retained in the screening stage. We apply the profile least squares approach to estimate $\boldsymbol{\beta}_{\mathcal{S}_1}$ based on $\{(\mathbf{x}_{j,\mathcal{S}_1}, Y_j)$, for $j = 61, \ldots, 120\}$, and $\boldsymbol{\beta}_{\mathcal{S}_2}$ based on $\{(\mathbf{x}_{j,\mathcal{S}_2}, Y_j)$, for $j = 61, \ldots, 120\}$.

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To ensure the identifiability of $\boldsymbol{\beta}_{\mathcal{S}_1}$ and $\boldsymbol{\beta}_{\mathcal{S}_2}$, we fix the coefficient of X_1 as one. Table 5 shows the estimate coefficients (denoted by "coef"), along with their respective standard deviations (denoted by "std") and p-values. With two different model sizes, both estimates agree very well: X_4, X_6, X_7, X_8 and X_1 are important at the significance level $\alpha = 0.05$, X_3 and X_5 are important if only eight covariates are retained, and X_9 becomes important if 16 covariates are selected.

Table 5: The estimated coefficients, standard errors, and p-values when $|\mathcal{S}| = 8$ and $|\mathcal{S}| = 16$, in Example 2.

$\lvert\mathcal{S}\rvert$		$\widehat{\beta}_2$	$\widehat{\beta}_3$	$\widehat{\beta}_4$	$\widehat{\beta}_5$	$\widehat{\beta}_6$	$\widehat{\beta}_7$	$\widehat{\beta}_8$	
8	coef	0.043	1.772	-6.750	-5.762	-6.783	4.364	-3.251	
	std	0.824	0.828	2.794	2.596	2.643	1.848	1.346	
	p-value	0.959	0.037	0.019	0.030	0.013	0.022	0.019	
		$\widehat{\beta}_2$	$\widehat{\beta}_3$	$\widehat{\beta}_4$	$\widehat{\beta}_5$	$\widehat{\beta}_6$	$\widehat{\beta}_7$	$\widehat{\beta}_8$	
16	coef	0.711	0.270	-2.087	-1.191	-1.778	1.990	-1.355	
	std	0.741	0.460	0.914	0.730	0.714	0.893	0.630	
	p-value	0.341	0.559	0.026	0.108	0.016	0.030	0.036	
		$\widehat{\beta}_9$	$\widehat{\beta}_{10}$	$\widehat{\beta}_{11}$	$\widehat{\beta}_{12}$	$\widehat{\beta}_{13}$	$\widehat{\beta}_{14}$	$\widehat{\beta}_{15}$	$\widehat{\beta}_{16}$
	coef	-1.766	-0.941	-0.679	0.964	-0.393	0.764	-0.607	0.115
	std	0.757	0.606	0.919	0.732	0.866	0.635	0.656	0.708
	p-value	0.023	0.126	0.463	0.193	0.652	0.234	0.358	0.872

Next, we check whether a single linear combination of the retained covariates suffices to predict the expression level of TRIM32, based on $\{(\mathbf{x}_{j,\mathcal{S}_1}, Y_j), j = 61, \ldots, 120\}$ and $\{(\mathbf{x}_{j,\mathcal{S}_2}, Y_j), j = 61, \ldots, 120\}$. The p-values obtained by our test procedures are 0.765 and 0.479, respectively, indicating

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that we cannot reject the null hypothesis, and a single linear combination indeed suffices to describe how the expression level of the gene TRIM32 varies with other genes. To further justify this test result, we chart scatterplots of the response versus the standardized $(\mathbf{x}_{j,\mathcal{S}_1}^{\mathrm{T}}\widehat{\boldsymbol{\beta}}_{\mathcal{S}_1})$ and $(\mathbf{x}_{j,\mathcal{S}_1}^{\mathrm{T}}\widehat{\boldsymbol{\beta}}_{\mathcal{S}_2})$ in Panels (A) and (B) of Figure 2, respectively. The solid lines are fitted by local linear approximation, where the bandwidths are decided through leave-one-out cross-validation, and the dashed lines are the 95% pointwise confidence intervals. It is clearly observed that the response is described very well using only one linear combination of the selected covariates.

To further examine the prediction performance of single-index models based on the selected covariates, we calculate the mean squared prediction errors based on leave-one-out cross-validation. The errors are 0.3801 based on $\{(\mathbf{x}_{j,\mathcal{S}_1}^{\mathrm{T}}\widehat{\boldsymbol{\beta}}_{\mathcal{S}_1}, Y_j), j = 1, \ldots, 120\}$, and 0.4297 based on $\{(\mathbf{x}_{j,\mathcal{S}_2}^{\mathrm{T}}\widehat{\boldsymbol{\beta}}_{\mathcal{S}_2}, Y_j), j = 1, \ldots, 120\}$. This indicates that the selected covariates are probably truly predictive for the expression level of the gene TRIM32, and that a single linear combination of these covariates is probably sufficient to characterize the conditional mean of the response.

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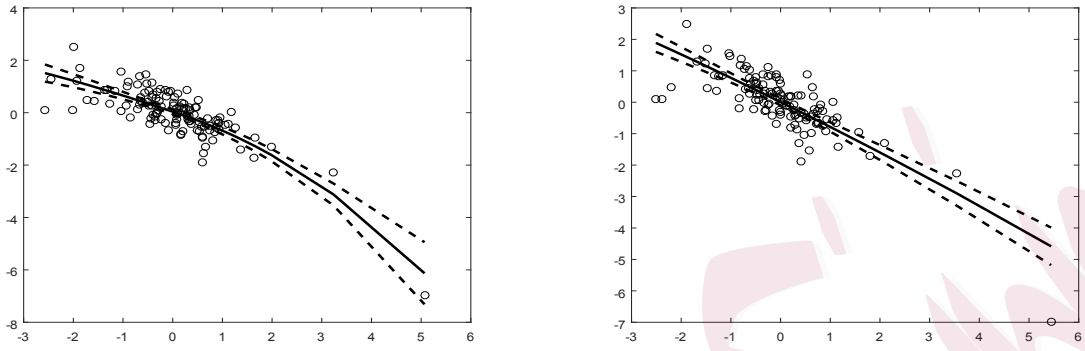

(A) (B)

Figure 2: The scatterplots of the response versus standardized $(\mathbf{x}_{j,\mathcal{S}_1}^{\mathrm{T}}\widehat{\boldsymbol{\beta}}_{\mathcal{S}_1})$ in Panel (A) and versus standardized $(\mathbf{x}_{j,\mathcal{S}_2}^{\mathrm{T}}\widehat{\boldsymbol{\beta}}_{\mathcal{S}_2})$ in Panel (B) in Example 2.

5. An Extension: Multiple Splitting

In the proposed two-stage testing procedure, the sure-screening property that $\mathcal{A} \subseteq \mathcal{S}$ with probability tending to one is crucial to guaranteeing that testing (2.1) is asymptotically equivalent to testing (1.3). However, at the sample level, important variables may be missed in the first screening stage, owing to a limitation of the sample size, a violation of some assumption, or data randomness. In this case, the empirical type-I error rates may be inflated. To deal with this issue, we can use the iterated MDC-based screening procedure to reduce the risk of missing important variables. Another efficient solution is the multi-splitting strategy Meinshausen, Meier, and Bühlmann (2009). Here, we divide the sample repeatedly (B times), and

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obtain one p-value from each sample split using the LOFTS procedure. For all p-values, denoted by $p_1, \ldots, p_B$, we define

$$Q(\gamma) = \min \left[1, q_\gamma \left(\{p_i/\gamma\} \right) \right],$$

for $\gamma \in (\gamma_{\min}, 1)$, where $q_\gamma \left(\{p_i/\gamma\} \right)$ is the γth quantile of $\{p_i/\gamma\}$, for $i = 1, \ldots, B$. Here, $\gamma_{\min} \in (0, 1)$ is a lower bound for γ, typically 0.05 or $1/B$, in practice. The adjusted p-value is then given by $Q(\gamma)$ for any fixed γ. However, a proper selection of γ may be difficult in practice. An adaptive version is defined as follows: Let $\gamma_{\min} \in (0, 1)$ be a lower bound for γ, typically 0.05, and

$$Q^*(\gamma) = \min \left\{ 1, (1 - \log\gamma_{\min}) \inf_{\gamma \in (\gamma_{\min}, 1)} Q(\gamma) \right\}.$$

With the adjusted p-value and the adaptive version of the p-value, the type-I error remains controlled at level α, asymptotically. This result is presented in the following theorem.

Theorem 5. *Assume* $\lim_{n\to\infty} P(\mathcal{A} \subset \mathcal{S}_i) = 1$*, where* $\mathcal{S}_i$ *is the selected model in the screening stage, based on the* i*th sample split. Then,*

$$\lim_{n\to\infty} \sup P\left\{ Q(\gamma) \le \alpha \right\} \le \alpha, \quad \lim_{n\to\infty} \sup P\left\{ Q^*(\gamma) \le \alpha \right\} \le \alpha.$$

We also perform a toy example to illustrate how the the type-I error remains controlled at level α when some important covariates are missed with

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a non-ignorable probability. We generate Y from the following regression model:

$$Y = X_1 + X_2 + X_3 + 0.5X_4 + \varepsilon,$$

where $\mathbf{x} = (X_1, \ldots, X_p)^{\mathrm{T}}$, other than X_4, are drawn from a multivariate normal distribution with mean zero and covariance matrix $\mathbf{\Sigma} = (\rho_{kl})_{p\times p}$, with $\rho_{kl} = 0.5^{|k-l|}, k, l = 1, \ldots, p$; X_4 is generated from the regression model $X_4 = (0.5 - X_1 - X_3)^2 + \varepsilon_1$. In addition, ε follows the standard normal distribution and is independent of $\mathbf{x}$, and ε_1 is an independent copy of ε. The sample size is set to 200, the dimensionality of the covariates is 1000, the reduced model size $|\mathcal{S}| = 5$, and the proposed bootstrap procedure is repeated 300 times, for simplicity. In addition, the multi-splitting procedure is repeated 50 times. In our simulations, X_4 is missed 204 times out of 1000 replicates, which means the corresponding type-I error is inflated. From Table 6, we can see that the multi-splitting strategy outperforms the single-splitting technique and maintains the empirical type-I errors at the nominal levels of $\alpha = 0.05$ and $\alpha = 0.10$.

Supplementary Material

All technical proofs and the screening performance in the simulation are included in the online Supplementary Material.

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Table 6: The empirical type-I errors for different splitting techniques.

	single-splitting				multi-splitting			
nominal	0.01	0.02	0.05	0.10	0.01	0.02	0.05	0.10
empirical	0.054	0.077	0.135	0.220	0.001	0.002	0.037	0.095

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Appendix: Regularity Conditions

(C1) *(The Kernel Function)* The univariate kernel function $K(\cdot)$ is a density function with compact support. It is symmetric about zero and

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Lipschitz continuous. In addition, it satisfies

$$\int K(v)dv = 1, \quad \int v^i K(v)dv = 0, 1 \leq i \leq t-1, \quad 0 \neq \int v^t K(v)dv < \infty.$$

(C2) *(The Density)* The probability density function of $\boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}}$, denoted by $f(\boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})$ is bounded away from 0 to infinity.

(C3) *(The Derivatives)* The $(t-1)$th derivatives of the mean function $\mathbf{m}(\boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})$, the density function $f(\boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})$ and $\mathbf{m}(\boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})f(\boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}})$ are locally Lipschitz-continuous with respect to $\boldsymbol{\beta}_{\mathcal{S}}^{\mathrm{T}}\mathbf{x}_{\mathcal{S}}$.

(C4) *(The Bandwidth)* The bandwidth h satisfies $h = O(n^{-\kappa})$, for some κ which satisfies $(2t)^{-1} < \kappa < (2d)^{-1}$.

(C5) *(The Moment)* The covariates used in the test stage statisfy that $E\left(\|\mathbf{x}_{\mathcal{S}}\|^2\right)/|\mathcal{S}| < \infty$.

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