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Variable Screening via Conditional Martingale Difference Divergence

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Abstract: Variable screening has been a useful research area that deals with ultrahigh-dimensional data. When there exist both marginally and jointly dependent predictors to the response, existing methods such as conditional screening or iterative screening often suffer from instability against the selection of the conditional set or the computational burden, respectively. In this article, we propose a new independence measure, named **conditional martingale difference divergence** ($\text{CMD}_{\mathcal{H}}$), that can be treated as either a conditional or a marginal independence measure. Under regularity conditions, we show that the *sure screening property* of $\text{CMD}_{\mathcal{H}}$ holds for both marginally and jointly active variables. Based on this measure, we propose a kernel-based model-free variable screening method, which is efficient, flexible, and stable against high correlation among predictors and heterogeneity of the response. In addition, we provide a data-driven method to select the conditional set. In simulations and real data applications, we demonstrate the superior performance of the proposed method.

Key words and phrases: Independence measure; Reproducing kernel Hilbert space; Sure screening property; Conditional screening; Dimension reduction.

1. Introduction

Variable screening has been a research area that deals with ultrahigh-dimensional data, where high-dimensional methods may fail due to the curse of dimensionality, as Fan et al. (2009) suggested. Fan and Lv (2008)'s seminal work suggests to screen the ultrahigh-dimensional

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data before conducting variable selection. They proposed a sure independent screening (SIS) method for linear models to screen out inactive variables based on Pearson correlation. After that, variable screening receives more attention since it only requires that the selected set of variables covers the set of active variables, which is referred to as the *sure screening property* (Fan and Lv, 2008). Screening methods with this property suffer less from *instability* (Yu, 2013) that is seen in many variable selection methods.

Various model-based screening methods have been developed. For linear regression models, screening methods have been proposed based on different measures, including marginal Pearson correlation (Fan and Lv, 2008), forward regression (Wang, 2009), marginal empirical likelihood ratio (Chang et al., 2013), and Kendall's rank correlation (Li et al., 2012a). For linear quantile regression, screening methods based on quantile partial correlation (Ma et al., 2017) and conditional quantile correlation (Zhang and Zhou, 2018) have been proposed to handle heterogeneous data. In the context of generalized linear models, screening methods based on the maximum marginal likelihood or its estimate (Fan and Song, 2010), the sparsity-restricted maximum likelihood estimator (Xu and Chen, 2014), and Kolmogorov-Smirnov statistic (Mai and Zou, 2013) have also been proposed. Other screening methods include model settings such as linear regression models with interactions (Hao and Zhang, 2014; Fan et al., 2016; Kong et al., 2017), Cox models (Zhao and Li, 2012), varying coefficient models (Cheng et al., 2014; Song et al., 2014), and additive models (Fan et al., 2011).

An alternative approach is the model-free screening method, which recently has gained popularity due to its less stringent assumptions. Zhu et al. (2011) proposed a sure independence ranking and screening approach (SIRS) for index models. Li et al. (2012b) proposed a screening method (DC-SIS) based on distance correlation, which can be applied to grouped

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variables. Cui et al. (2015) proposed a model-free screening method (MV-SIS) based on empirical conditional distribution function for discriminant analysis. Shao and Zhang (2014) proposed the use of martingale difference correlation (MDC), which can be applied to mean and quantile screening. Mai and Zou (2015) proposed the fused Kolmogorov filter that works with different types of response variables and high covariate correlation. Nandy et al. (2022) proposed a screening method based on covariate information number (CIN) motivated by Fisher information. Han (2019) developed a screening framework from the perspective of loss functions and proposed a screening method based on conditional strictly convex losses. Based on *ball correlation*, Pan et al. (2019) proposed a generic screening method for biomedical discovery.

As pointed out by Li et al. (2012b); Shao and Zhang (2014); Tian and Feng (2023), screening methods based on marginal measures (e.g., the marginal correlation between the response and each predictor) will possibly miss the marginally but not jointly independent predictors. Two types of approaches have been developed to handle this issue. One approach is *conditional screening*, a screening procedure based on a given set of variables. For example, Barut et al. (2016) proposed conditional sure independence screening (CSIS) for assessing the conditional (on a given conditional set) contribution of a predictor to the response in generalized linear models. Based on conditional distance correlation, Wen et al. (2018) proposed a method that adjusts for confounding variables. Tong et al. (2023) proposed a conditional independence measure and its corresponding screening method (CIS) with false discovery rate (FDR) control, which also works for heavy-tailed predictors/responses. Another approach is *screening via iterative procedures*. For example, the aforementioned forward regression iteratively selects the variables. Xu and Chen (2014) considered a method

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based on sparse MLE, where the algorithm iteratively updates the coefficients in the link function. Zhou et al. (2020) proposed a model-free forward screening method that iteratively updates the conditional set and is robust to outliers. Tian and Feng (2023) proposed an iterative variable screening method based on random subspace ensembles (RaSE) with a theoretical guarantee for iterative screening procedures.

However, two challenges remain. The first problem is that model-based iterative methods (e.g., iterative SIS) may not work if the underlying model is incorrectly identified. The second problem is that the conditional screening method and its performance becomes unstable if an unreasonable conditional set is selected, especially when no prior knowledge is available to choose the conditioning set. It motivates us to develop a stable model-free screening method that identifies both marginally and jointly dependent variables to the response. We propose a kernel-based measure that captures both conditional and marginal mean-independent relationships. In particular, via Bochner's theorem (Wendland, 2004), we transform the problem of choosing weights, a key element in our independence measure, to the problem of choosing kernels and their bandwidths in reproducing kernel Hilbert space (RKHS). This flexible kernel-based fashion allows our method to perform well in various settings, as illustrated in the synthetic and real data analysis.

The advantages of our method are as follows. First, we propose a kernel-based independence measure ($\text{CMD}_{\mathcal{H}}$) that is able to characterize both conditional and marginal mean independence. Thus, we propose a $\text{CMD}_{\mathcal{H}}$ -based screening method that can detect both marginally and jointly dependent/active variables. Second, the proposed model-free screening method is stable against outliers, data heterogeneity, and high covariate correlation. Third, we show the sure screening property holds for screening both marginally and jointly

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dependent variables under mild regularity conditions. We also suggest selecting a stable data-driven conditional set for conducting conditional screening when no prior information is available. Although the way of selecting conditioning set is in a similar position as CSIS, by “stable” we want to emphasize that 1) our method has better variable screening performance in various simulation settings than the existing methods in the literature; 2) our method is stable against small perturbations to the conditional set, such as the change of its cardinality or a small fraction of inactive variables in it. For the second point, we are not claiming that our method is robust for any conditional set, which is impossible, especially when the conditional set do not contain any useful information about the active predictors.

The rest of the article is organized as follows. Section 2 introduces the proposed independence measure and its theoretical properties. In Section 3, we propose a model-free variable screening procedure and present its sure screening property. The simulation results and two real data examples are reported in Section 4, followed by the conclusion in Section 5. Additional theorems are presented in the appendix. Auxiliary simulation results and technical proofs are included in the supplementary material.

2. General methodology

Notations. Throughout the article, we use upper case (e.g., V) to denote a random variable and use bold font to denote a random vector (e.g., \mathbf{U}). We use $(\mathbf{U}'_1, \mathbf{U}'_2, V')$ and $(\mathbf{U}''_1, \mathbf{U}''_2, V'')$ to denote *i.i.d* copies of $(\mathbf{U}_1, \mathbf{U}_2, V)$.

For a sequence $\{t_{ij}\}$ with double indices $i, j = 1, \dots, n$, we define

$$t_{ij}^* = t_{ij} - \bar{t}_{i.} - \bar{t}_{.j} + \bar{t}_{..}, \quad (2.1)$$

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where $\bar{t}_{.j} = \frac{1}{(n-2)} \sum_{i=1}^n t_{ij}$, $\bar{t}_i = \frac{1}{(n-2)} \sum_{j=1}^n t_{ij}$, and $\bar{t}_{..} = \frac{1}{(n-1)(n-2)} \sum_{i=1}^n \sum_{j=1}^n t_{ij}$. Denote $\langle \mathbf{a}, \mathbf{b} \rangle$ as the inner product of any two vectors \mathbf{a}, \mathbf{b} of the same dimension.

2.1 Conditional Martingale Difference Divergence

A motivating example. Assume two random variables X_1 and X_2 are independent with $E(X_2) = 0$, and let $Y = X_1 X_2$. We have $E(Y|X_1) - E(Y) = E(X_2) \cdot \{X_1 - E(X_1)\} = 0$ as long as $E(X_2) = 0$. The condition “ $E(X_2) = 0$ ” is mild as we can standardize predictors in the dataset to have mean 0 in practice. This example indicates that mean independence measures based on the relationship $E(Y|X_1) - E(Y)$ will misleadingly suggest that X_1 is independent from mean of Y . It was pointed out by Li et al. (2012b) and Shao and Zhang (2014) that the marginal measures/methods such as DC and MDC will possibly miss the variables that only jointly contribute to the response variable. It motivates us to consider the following:

$$E(Y|X_1, X_2) - E(Y|X_2),$$

which equals to $X_2 \cdot \{X_1 - E(X_1)\}$ in this example. More generally, we consider the equality $E(V|\mathbf{U}_1, \mathbf{U}_2) = E(V|\mathbf{U}_1)$, i.e., the response variable V and covariate vector \mathbf{U}_2 given the covariate vector \mathbf{U}_1 . If in addition, \mathbf{U}_1 and \mathbf{U}_2 are independent, we have $E(V|\mathbf{U}_1, \mathbf{U}_2) = E(V|\mathbf{U}_1)$ if and only if $E(Ve^{i\langle \mathbf{t}_1, \mathbf{U}_1 \rangle} | \mathbf{U}_2) = E(Ve^{i\langle \mathbf{t}_1, \mathbf{U}_1 \rangle})$ for any \mathbf{t}_1 (the proof is presented in supplementary material S2 (b)). This motivates us to propose the following independence measure in Definition 1, which can be treated as either a conditional or a marginal (see Remark 2) mean independence measure.

Definition 1. Given a random vector $\mathbf{U}_1 \in \mathbb{R}^p$, the *conditional martingale difference*

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divergence of a random variable V and a random vector $\mathbf{U}_2 \in \mathbb{R}^q$ is defined as

$$\begin{aligned} \text{CMD}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) &= \iint |E\{V e^{i(\langle \mathbf{t}_1, \mathbf{U}_1 \rangle + \langle \mathbf{t}_2, \mathbf{U}_2 \rangle)}\} - E(V e^{i\langle \mathbf{t}_1, \mathbf{U}_1 \rangle}) E(e^{i\langle \mathbf{t}_2, \mathbf{U}_2 \rangle})|^2 w_1(\mathbf{t}_1) w_2(\mathbf{t}_2) d\mathbf{t}_1 d\mathbf{t}_2, \end{aligned}$$

where $w_1(\mathbf{t}_1)$ and $w_2(\mathbf{t}_2)$ are weight functions.

The measure $\text{CMD}_{\mathcal{H}}$ depends on two ingredients: a mean independence measure of a random vector and a random variable, and an adjusting method of the effect of a third vector. It provides valuable information on the conditional contribution of \mathbf{U}_2 to the mean of V given \mathbf{U}_1 .

Remark 1. We choose the weight function $w_1(\mathbf{t}_1)$ and $w_2(\mathbf{t}_2)$ to be integrable, relaxing the strong assumption of the boundedness of \mathbf{U}_1 and \mathbf{U}_2 as in the literature. The choice of an integrable weight function makes the proposed independence measure more flexible. In particular, we can rewrite $\text{CMD}_{\mathcal{H}}(V, \mathbf{U}_2 | \mathbf{U}_1)$ as a functional of kernel functions in RKHS. See more details in Theorem 1(a) and Remark 3.

We now define a scale-invariant version of the proposed measure.

Definition 2. Let k_1 and k_2 be the two kernel functions that correspond to the weight function $w_1(\mathbf{t}_1)$ and $w_2(\mathbf{t}_2)$, as illustrated in Theorem 1(a). We define the **conditional martingale difference correlation**

$$\text{CMC}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) = \begin{cases} \frac{\text{CMD}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1)}{\sqrt{v(k_2, \mathbf{U}_2)v(k_{1_V}, \mathbf{U}_1)}} & \text{if } v(k_2, \mathbf{U}_2)v(k_{1_V}, \mathbf{U}_1) > 0 \\ 0 & \text{otherwise,} \end{cases}$$

where $v(k, \mathbf{U}) := E\{k^2(\mathbf{U}, \mathbf{U}')\} + E^2\{k(\mathbf{U}, \mathbf{U}')\} - 2E\{k(\mathbf{U}, \mathbf{U}') \cdot k(\mathbf{U}, \mathbf{U}'')\}$ and $k_V(\mathbf{U}, \mathbf{U}') := VV'k(\mathbf{U}, \mathbf{U}')$ for any kernel function k .

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Remark 2. When \mathbf{U}_1 contains no useful information ($\mathbf{U}_1 = \emptyset$, $\mathbf{U}_1 \equiv \mathbf{c}$, or \mathbf{U}_1 is independent from (V, \mathbf{U}_2)), the definition of $\text{CMD}_{\mathcal{H}}$ reduces to a marginal mean independence measure.

That is,

$$\text{MD}_{\mathcal{H}}^2(V, \mathbf{U}_2) := \int |E(V e^{i\langle \mathbf{t}_2, \mathbf{U}_2 \rangle}) - E(V)E(e^{i\langle \mathbf{t}_2, \mathbf{U}_2 \rangle})|^2 w(\mathbf{t}_2) d\mathbf{t}_2.$$

Note that $\text{MD}_{\mathcal{H}}(V, \mathbf{U}_2)$ is a generalized version of MDD (Shao and Zhang, 2014) by kernelizing the L_2 distance of \mathbf{U}_2 and its i.i.d. copy \mathbf{U}'_2 . The standardized version $\text{MC}_{\mathcal{H}}$ is defined similarly as $\text{CMC}_{\mathcal{H}}$.

As will be seen in Theorem 1, the definition of the $\text{CMC}_{\mathcal{H}}$ is more convenient for variable screening purpose since it takes values in $[0, 1]$. More detailed discussion of $\text{CMC}_{\mathcal{H}}$ is included in Section 3. Now we show the theoretical properties of the proposed conditional independence measure.

Theorem 1. Assume $E(V^2) < \infty$, we have the following properties:

(a). We can rewrite $\text{CMD}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1)$ as

$$\begin{aligned} & \text{CMD}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) \\ &= E\{VV'k_1(\mathbf{U}_1, \mathbf{U}'_1)k_2(\mathbf{U}_2, \mathbf{U}'_2)\} + E\{VV'k_1(\mathbf{U}_1, \mathbf{U}'_1)\}E\{k_2(\mathbf{U}_2, \mathbf{U}'_2)\} \\ & \quad - 2E\{VV'k_1(\mathbf{U}_1, \mathbf{U}'_1)k_2(\mathbf{U}_2, \mathbf{U}''_2)\}, \end{aligned}$$

where k_1 and k_2 are RHKS kernel functions determined by $w_1(\mathbf{t}_1)$ and $w_2(\mathbf{t}_2)$ defined in Definition 1, respectively.

(b). $0 \leq \text{CMC}_{\mathcal{H}}(V, \mathbf{U}_2 | \mathbf{U}_1) \leq 1$, and $\text{CMC}_{\mathcal{H}}(V, \mathbf{U}_2 | \mathbf{U}_1) = 0 \Leftrightarrow E(V | \mathbf{U}_1, \mathbf{U}_2) = E(V | \mathbf{U}_1)$ a.s. if $\mathbf{U}_1 \perp \mathbf{U}_2$.

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(c). Given two constants $d \in \mathbb{R}$ and $e \in \mathbb{R}$, $\text{CMC}_{\mathcal{H}}(a+bV, \mathbf{c}+d\mathbf{U}_2|e\mathbf{U}_1) = \text{CMC}_{\mathcal{H}}(V, \mathbf{U}_2|\mathbf{U}_1)$ for any scalars $a, b \in \mathbb{R}$ and $\mathbf{c} \in \mathbb{R}^q$. If the kernels k_1 and k_2 in (a) are scale-invariant, the above equality holds for any scalars d and e as well.

(d). If the random variables $U, V \in \mathbb{R}$ are independent, then

$$\text{MC}_{\mathcal{H}}^2(VU, U) = \frac{E^2(V)}{\text{Var}(V) + E^2(V) + E^2(U)\frac{\text{Var}(V)}{\text{Var}(U)}} \text{MC}_{\mathcal{H}}^2(U, U).$$

Furthermore, if $E(V) = 0$, then $\text{MC}_{\mathcal{H}}(VU, U) = 0$.

Remark 3. If we take non-integrable weight functions $w_1(\mathbf{t}_1)$ and $w_2(\mathbf{t}_2)$ in Definition 1, then k_1 and k_2 in Theorem 1(a) may not be translation-invariant kernels in RKHS (e.g., the Euclidean distance function). See *dCov* (Székely et al., 2007) for an example that adopts a non-integrable weight in its definition.

Remark 4. Property (b) shows the equivalence between the conditional mean independence and $\text{CMC}_{\mathcal{H}}$ being 0, which suggests $\text{CMC}_{\mathcal{H}}$ is a suitable tool for conducting variable screening.

Note that the independence of \mathbf{U}_1 and \mathbf{U}_2 in Property (b) is to ease the proof. Indeed, if we define a new independence measure $\text{CMD}_{\mathcal{H},\text{new}}^2(V, \mathbf{U}_2|\mathbf{U}_1) = \iint |E\{Ve^{i(\langle \mathbf{t}_1, \mathbf{U}_1 \rangle + \langle \mathbf{t}_2, \mathbf{U}_2 \rangle)}|\mathbf{U}_1\} - E(Ve^{i\langle \mathbf{t}_1, \mathbf{U}_1 \rangle}|\mathbf{U}_1)E(e^{i\langle \mathbf{t}_2, \mathbf{U}_2 \rangle}|\mathbf{U}_1)|^2 w_1(\mathbf{t}_1)w_2(\mathbf{t}_2) d\mathbf{t}_1 d\mathbf{t}_2$, then

$$\text{CMD}_{\mathcal{H},\text{new}}(V, \mathbf{U}_2|\mathbf{U}_1) = 0 \text{ a.s.} \Leftrightarrow E(V|\mathbf{U}_1, \mathbf{U}_2) = E(V|\mathbf{U}_1) \text{ a.s.}$$

This removes the independence condition of \mathbf{U}_1 and \mathbf{U}_2 . Then we need to replace our U -statistics estimator with the conditional U -statistics to estimate the new independence measure. Note that this new measure $\text{CMD}_{\mathcal{H},\text{new}}$ is a function of the random vector \mathbf{U}_1 . Such a conditional measure and its associated screening method is left as future work of interest.

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In this article, we stick to our original proposed measure $\text{CMD}_{\mathcal{H}}$. In the simulations, as we see, even \mathbf{U}_1 and \mathbf{U}_2 are not independent (e.g., high variable correlations $\rho = 0.5, 0.8, 0.9$ in Example 1, and nonlinearly associated predictors in Example 4), our variable screening method still performs well, or even outperforms other methods in almost all the simulation settings.

Remark 5. Property (c) shows that the proposed $\text{CMC}_{\mathcal{H}}$ is scale-invariant. Property (d) directly shows the deficiency of marginal-type mean independence measure ($\text{MC}_{\mathcal{H}}$) in interaction screening. Thus we propose the variable screening procedure based on $\text{CMC}_{\mathcal{H}}$.

2.2 Empirical Estimators and Asymptotic Properties

Based on property (a) in Theorem 1, we construct the U -statistic to estimate $\text{CMC}_{\mathcal{H}}$.

Definition 3. Let $(\mathbf{U}_{1i}, \mathbf{U}_{2i}, V_i)_{i=1}^n$ be i.i.d. observations of $(\mathbf{U}_1, \mathbf{U}_2, V)$. Denote $a_{ij} = V_i V_j k_1(\mathbf{U}_{1i}, \mathbf{U}_{1j})$ and $b_{ij} = k_2(\mathbf{U}_{2i}, \mathbf{U}_{2j})$ for $i, j = 1, \dots, n$. Define the corresponding a_{ij}^* and b_{ij}^* as in Equation (2.1). The U -statistic estimator of $\text{CMD}_{\mathcal{H}}^2$ is

$$\widehat{\text{CMD}}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) = \frac{1}{n(n-3)} \sum_{1 \leq i \neq j \leq n} a_{ij}^* b_{ij}^*,$$

and the corresponding estimator of $\text{CMC}_{\mathcal{H}}$ is:

$$\widehat{\text{CMC}}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) = \frac{\sum_{1 \leq i \neq j \leq n} a_{ij}^* b_{ij}^*}{\sqrt{\sum_{1 \leq i \neq j \leq n} a_{ij}^{*2} \sum_{1 \leq i \neq j \leq n} b_{ij}^{*2}}}.$$

Remark 6. Compared to the adoption of V -statistic estimator, we choose the U -statistic because it is unbiased and less computationally expensive.

We now show the strong consistency of the proposed estimators.

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Theorem 2. (Consistency) If $E(V^2) < \infty$, then

$$\lim_{n \rightarrow \infty} \widehat{\text{CMD}}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) = \text{CMD}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) \text{ a.s.}, \quad (2.2)$$

and

$$\lim_{n \rightarrow \infty} \widehat{\text{CMC}}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) = \text{CMC}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) \text{ a.s.} \quad (2.3)$$

In the next theorem, we derive the asymptotic distribution for $\text{CMD}_{\mathcal{H}}(V, \mathbf{U}_2 | \mathbf{U}_1)$. Denote the following functions: $g_{\mathbf{U}_2}(\mathbf{t}_2) := E(e^{i\langle \mathbf{t}_2, \mathbf{U}_2 \rangle})$, $g_{V, \mathbf{U}_1}(\mathbf{t}_1) := E(V e^{i\langle \mathbf{t}_1, \mathbf{U}_1 \rangle})$, and $F(\mathbf{t}_1, \mathbf{t}_2) := E(V^2 e^{i\langle \mathbf{t}_1, \mathbf{U}_1 \rangle} e^{i\langle \mathbf{t}_2, \mathbf{U}_2 \rangle})$. Define the covariance function $\text{cov}_{\Gamma}((\mathbf{t}_1, \mathbf{t}_2), (\mathbf{t}'_1, \mathbf{t}'_2)) := F(\mathbf{t}_1 - \mathbf{t}'_1, \mathbf{t}_2 - \mathbf{t}'_2) + (F(\mathbf{t}_1 - \mathbf{t}'_1, 0) + g_{V, \mathbf{U}_1}(\mathbf{t}_1) \overline{g_{V, \mathbf{U}_1}(\mathbf{t}'_1)}) \{g_{\mathbf{U}_2}(\mathbf{t}_2) \overline{g_{\mathbf{U}_2}(\mathbf{t}'_2)} - g_{\mathbf{U}_2}(\mathbf{t}_2 - \mathbf{t}'_2)\} - F(\mathbf{t}_1 - \mathbf{t}'_1, \mathbf{t}_2) \overline{g_{\mathbf{U}_2}(\mathbf{t}'_2)} - F(\mathbf{t}_1 - \mathbf{t}'_1, -\mathbf{t}'_2) g_{\mathbf{U}_2}(\mathbf{t}_2)$. Define the norm $\|\gamma(\cdot)\|_{\mathcal{H}}^2 = \iint |\gamma(\mathbf{t}_1, \mathbf{t}_2)|^2 w_1(\mathbf{t}_1) w_2(\mathbf{t}_2) d\mathbf{t}_1 d\mathbf{t}_2$ for complex function $\gamma(\cdot)$ defined on $\mathbb{R}^p \times \mathbb{R}^q$.

Theorem 3. Assume $E(V^2) < \infty$, and the weight functions satisfy $\int_{|(\mathbf{t}_1, \mathbf{t}_2)|_{p+q} < \delta} w_1(\mathbf{t}_1) w_2(\mathbf{t}_2) d\mathbf{t}_1 d\mathbf{t}_2 \rightarrow 0$ as $\delta \rightarrow 0$, and $\int_{|(\mathbf{t}_1, \mathbf{t}_2)|_{p+q} > 1/\delta} w_1(\mathbf{t}_1) w_2(\mathbf{t}_2) d\mathbf{t}_1 d\mathbf{t}_2 \rightarrow 0$ as $\delta \rightarrow 0$, where $|\cdot|_{p+q}$ denotes the Euclidean distance in \mathbb{R}^{p+q} . We have the following:

a. If $\mathbf{U}_1 \perp \mathbf{U}_2$ and $\text{CMD}_{\mathcal{H}}(V, \mathbf{U}_2 | \mathbf{U}_1) = 0$, then

$$n \widehat{\text{CMD}}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) \xrightarrow{d} \|\Gamma(s)\|_{\mathcal{H}}^2 \quad (2.4)$$

as $n \rightarrow \infty$, where $\Gamma(\cdot)$ is a complex-valued zero-mean Gaussian random process with covariance function $\text{cov}_{\Gamma}((\mathbf{t}_1, \mathbf{t}_2), (\mathbf{t}'_1, \mathbf{t}'_2))$.

b. If $\mathbf{U}_1 \perp \mathbf{U}_2$ and $\text{CMD}_{\mathcal{H}}(V, \mathbf{U}_2 | \mathbf{U}_1) = 0$ and $E(V^2 | \mathbf{U}_2) = E(V^2)$, then

$$n \widehat{\text{CMD}}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) / S_n \xrightarrow{D} \sum_{j=1}^{\infty} \lambda_j Z_j$$

as $n \rightarrow \infty$, where $S_n = \{\frac{1}{n} \sum_i V_i^2 - \frac{1}{n(n-1)} \sum_{i \neq j} a_{ij}\} \{1 - \frac{1}{n(n-1)} \sum_{i \neq j} b_{ij}\}$, $Z_j \stackrel{i.i.d.}{\sim} \chi_1^2$, and $\{\lambda_j\}_{j=1}^{\infty}$ are nonnegative constants such that $E(\sum_{j=1}^{\infty} \lambda_j Z_j) = 1$.

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c. If $\text{CMD}_{\mathcal{H}}(V, \mathbf{U}_2 | \mathbf{U}_1) > 0$, then $n \cdot \widehat{\text{CMD}}_{\mathcal{H}}^2(V, \mathbf{U}_2 | \mathbf{U}_1) / S_n \xrightarrow{p} \infty$ as $n \rightarrow \infty$.

The properties stated in the theorems of this section motivate us to propose variable screening algorithm based on $\text{CMC}_{\mathcal{H}}$ and its estimate $\widehat{\text{CMC}}_{\mathcal{H}}$.

3. $\text{CMC}_{\mathcal{H}}$ -based Variable Screening

In this section, we show the sure screening property of $\text{CMC}_{\mathcal{H}}$ in Section 3.1. In Section 3.2, we introduce a variable screening algorithm named S- $\text{CMC}_{\mathcal{H}}$ to accommodate the dependence among predictors. The algorithm works reasonably well when the data suffer from outliers, high correlation, and heterogeneity as seen in the numerical studies.

3.1 Sure Screening Property

Without loss of generality, let Y be a univariate continuous response variable and $\mathbf{X} = (X_1, \dots, X_p)^T$ be the predictor vector. Denote the sample as $(X_{1k}, \dots, X_{pk}, Y_k)_{k=1}^n$, where $p \gg n$. For any index set $S \subseteq \{1, \dots, p\}$, denote $\mathbf{X}_S := \{\mathbf{X}_j : j \in S\}$. Given a conditional set \mathbf{X}_S with cardinality d_1 , we define

$$\mathcal{D}_S = \{j : \mathbb{E}(Y | (\mathbf{X}_S, X_j)) \text{ depends on } X_j\}$$

as the index set of dependent/active predictors conditional on \mathbf{X}_S , and

$$\mathcal{I}_S = \{j : \mathbb{E}(Y | (\mathbf{X}_S, X_j)) \text{ is independent from } X_j\}$$

as the index set of independent/inactive predictors conditional on \mathbf{X}_S . Note that \mathcal{D}_S is a subset of $\mathcal{D} := \{j : \mathbb{E}(Y | \mathbf{X}) \text{ depends on } X_j\}$, the set of all dependent predictors. Suppressing S , we denote $\omega_j = \text{CMC}_{\mathcal{H}}^2(Y, X_j | \mathbf{X}_S)$ as the dependence score of X_j given \mathbf{X}_S . Let $\hat{\omega}_j =$

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$\widehat{\text{CMC}}_{\mathcal{H}}^2(Y, X_j | \mathbf{X}_S)$ be the estimator of ω_j and

$$\hat{\mathcal{D}}_S = \{j : \hat{\omega}_j \geq cn^{-\kappa}, \text{ for } j \in S^c\}$$

be the set of selected variables after screening. Before stating the sure screening property, we assume the following conditions.

(A1) There exists a constant $s_0 > 0$ such that $E(\exp(sY^2)) < \infty$ for all $0 < s \leq 2s_0$.

(A2) For any given \mathbf{X}_S , $\min_{j \in \mathcal{D}_S} \omega_j \geq 2cn^{-\kappa}$ for some constant $c > 0$ and $0 \leq \kappa < 1/2$.

Condition (A1) puts constraint on the tail distribution of the response variable and Condition (A2) requires that the conditional active/dependent variables and inactive/independent variables are well separated.

Theorem 4. *Under Condition (A1), for any $0 < \gamma < 1/2 - \kappa$, there exist positive constants c_1 and c_2 such that*

$$P \left\{ \max_{1 \leq j \leq p-d_1} |\hat{\omega}_j - \omega_j| \geq cn^{-\kappa} \right\} \leq O[(p-d_1)\{\exp(-c_1 n^{1-2(\kappa+\gamma)}) + n \exp(-c_2 n^\gamma)\}]. \quad (3.1)$$

If Conditions (A2) also holds, we have

$$P(\mathcal{D}_S \subset \hat{\mathcal{D}}_S) \geq 1 - O[s_n \{\exp(-c_1 n^{1-2(\kappa+\gamma)}) + n \exp(-c_2 n^\gamma)\}] \quad (3.2)$$

for any conditional set \mathbf{X}_S , where s_n is the cardinality of \mathcal{D}_S . In particular, let $\delta = \min_{j \in \mathcal{D}_S} \omega_j - \max_{j \in \mathcal{I}_S} \omega_j$, we have the ranking consistency:

$$P \left\{ \max_{j \in \mathcal{I}_S} \hat{\omega}_j < \min_{j \in \mathcal{D}_S} \hat{\omega}_j \right\} \geq 1 - 2O[(p-d_1)\{\exp(-c'_1 \delta^2 n^{1-2\gamma}) + n \exp(-c_2 n^\gamma)\}] \quad (3.3)$$

for a positive constant c'_1 .

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Remark 7. *The above theorem shows the sure screening property holds for any given conditional set \mathbf{X}_S . Define $\mathcal{M} := \{j : \mathbb{E}(Y|X_j) \text{ depends on } X_j\}$ as the set of marginally dependent/active predictors. For the special case where the conditional set $\mathbf{X}_S = \mathbf{X}$, we have $\mathcal{D}_S = \mathcal{D}$, which is the common sure screening property in the literature. In Appendix B.1, we also show that, similarly to Theorem 4, the sure screening property holds when the conditional set is empty. In that case, $\text{CMC}_{\mathcal{H}}$ reduces to $\text{MC}_{\mathcal{H}}$, and the sure screening property holds for selecting the set \mathcal{D} as well as \mathcal{M} . We discuss more details of selecting the conditional set \mathbf{X}_S in Section 3.2.*

Remark 8. *The error terms $\exp(-c_1 n^{1-2(\kappa+\gamma)})$ and $n \exp(-c_2 n^\gamma)$ in (3.5) comes from estimating the three terms in $\text{CMD}_{\mathcal{H}}$ as in Theorem 1(a). In the proof, take the first term $E\{VV'k_1(\mathbf{U}_1, \mathbf{U}'_1)k_2(\mathbf{U}_2, \mathbf{U}'_2)\} := E(h)$ for example, we decompose it into a bounded term $E[hI(h < M)]$ plus an unbounded term $E[hI(h > M)]$ for some large enough $M > 0$. Similar decomposition is done to the other two terms. Setting $M = n^\gamma$ for some $0 < \gamma < 1/2 - \kappa$, we obtain the two error terms $\exp(-c_1 n^{1-2(\kappa+\gamma)})$ and $n \exp(-c_2 n^\gamma)$ for estimating the sum of the bounded terms and that of the unbounded terms, respectively. The role of the parameter γ is a trade-off of estimating the bounded and unbounded terms. By setting $\gamma = \frac{1-2\kappa}{3}$, we achieve a balance and obtain the optimal convergence rate. As mentioned in Shao and Zhang (2014), their bound (3.5) can be further improved by assuming a stronger moment condition on Y , i.e., $E(\exp(sY^4)) < \infty$ for all $s \in (0, 2s_0]$. Their improved bound is the same as our bound. It is also worth mentioning that we do not impose moment conditions on the variable X as in Shao and Zhang (2014). The reason why our method enjoys a better rate under a weaker condition is that our proposed measure $\text{CMC}_{\mathcal{H}}$ only computes the RKHS kernel functions of X (as shown in Theorem 1 (a)). Such kernels are bounded, which frees us from assuming*

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additional moment conditions on X . In contrast, the Martingale Difference Correlation requires to calculate the Euclidean distance (Theorem 1 (1) in Shao and Zhang (2014)), which is unbounded. Thus, they require the stronger assumptions.

3.2 A Variable Screening Algorithm S-CMC \mathcal{H}

The sure screening property holds for any conditional set. In practice, if the conditional set is not given, we use the top d_1 predictors suggested by $\text{MC}_{\mathcal{H}}$, which also enjoys the sure screening property, as shown in Theorems 9 and 10 in the appendix. We propose to use the following variable screening algorithm S-CMC \mathcal{H} as stated in Algorithm 1. The R code of S-CMC \mathcal{H} is available in <https://github.com/lei-fang-stat/CMDD>.

Algorithm 1 The procedure of the S-CMC \mathcal{H} for variable screening.

Input: The conditional set \mathbf{X}_S (optional) and its cardinality d_1 (optional), the number of variables d_2 to select (optional), and the data $\{(y_i, \mathbf{x}_i)\}_{i=1}^n$.

1. If \mathbf{X}_S is not given, calculate $\widehat{\text{MC}}_{\mathcal{H}}(X_i) := \widehat{\text{MC}}_{\mathcal{H}}(Y, X_i)$ for each $i = 1, \dots, p$. Let the conditional set \mathbf{X}_S be the set of the top d_1 (if not given, $d_1 = \lfloor \sqrt{n/\log n} \rfloor$ where $\lfloor \cdot \rfloor$ is the floor function) predictors with the largest $\widehat{\text{MC}}_{\mathcal{H}}(X_i)$.
2. For each $i \in \{1, \dots, p - d_1\}$, calculate $\widehat{\text{CMC}}_{\mathcal{H}}(X_{c_i}) := \widehat{\text{CMC}}_{\mathcal{H}}(Y, X_{c_i}^\perp | \mathbf{X}_S)$, where each c_i is from S^c and $X_{c_i}^\perp = X_{c_i} - P_{\mathbf{X}_S} X_{c_i}$ with $P_{\mathbf{X}_S}$ being the projection matrix onto the column space of \mathbf{X}_S .
3. Calculate the score $A_i := \max\left\{\frac{\text{MC}_{\mathcal{H}}(X_{c_i})}{\max_{1 \leq i \leq p-d_1} \text{MC}_{\mathcal{H}}(X_{c_i})}, \frac{\text{CMC}_{\mathcal{H}}(X_{c_i})}{\max_{1 \leq i \leq p-d_1} \text{CMC}_{\mathcal{H}}(X_{c_i})}\right\}$ for each $i = 1, \dots, p - d_1$. Keep the top $d_2 - d_1$ predictors with the largest scores. If d_2 is not given, $d_2 = \lfloor n/\log n \rfloor$.

Output: The index set of the d_2 selected variables $\{i_1, \dots, i_{d_2}\} \subseteq \{1, \dots, p\}$ (the d_1 variables selected in Step 1 plus the $d_2 - d_1$ variables selected in Step 3).

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Remark 9. *The parameters d_1 and d_2 are predefined values. In general, larger d_1 will lead to worse performance if the set \mathbf{X}_S contains larger proportion of inactive variables. It will not affect the theoretical performance of $\text{CMC}_{\mathcal{H}}$. However, computationally, the estimation of the expected kernel function of long vectors inside $\text{CMC}_{\mathcal{H}}$ becomes less reliable if the sample size is limited. Thus we recommend to choose small d_1 (e.g., $d_1 = \lfloor \sqrt{n/\log n} \rfloor$) in practice.*

Remark 10. *The adoption of $X_{c_i}^\perp$ is to handle the scenario when the independence assumption of \mathbf{X}_S and X_i is violated. Note that this only removes the linear dependence. See more discussion in Remark 4.*

Remark 11. *In the last step, an alternative way is to use a linear combination $w_1 \frac{\text{MC}_{\mathcal{H}}(X_{c_i})}{\max_{1 \leq i \leq p-d_1} \text{MC}_{\mathcal{H}}(X_{c_i})} + w_2 \frac{\text{CMC}_{\mathcal{H}}(X_{c_i})}{\max_{1 \leq i \leq p-d_1} \text{CMC}_{\mathcal{H}}(X_{c_i})}$ to rank all the predictors. The weights can be adaptively chosen by the data, which we leave as a potential future work.*

3.3 Extension to Quantile Screening

In this section, we extend our method to the quantile screening setting. For a univariate random response Y , denote $Y_\tau = \tau - \mathbf{1}(Y \leq q_\tau)$ as its binary version with $\tau \in (0, 1)$, where q_τ is the τ -th quantile of the distribution of Y . Given *i.i.d.* observations $\{y_k\}_{k=1}^n$ of Y , denote $\hat{Y}_\tau = \tau - \mathbf{1}(Y \leq \hat{q}_\tau)$ as the estimate of Y_τ , where \hat{q}_τ is the sample τ -th quantile. So for each observation y_k , we denote $y_{k_\tau} = \tau - \mathbf{1}(y_k \leq \hat{q}_\tau)$. Let $\omega_j(Y_\tau) = \text{CMC}_{\mathcal{H}}^2(Y_\tau, X_j | \mathbf{X}_S)$ and $\hat{\omega}_j(\hat{Y}_\tau) = \widehat{\text{CMC}}_{\mathcal{H}}^2(\hat{Y}_\tau, X_j | \mathbf{X}_S)$. Similarly, we denote $\mathcal{D}_{q_\tau} = \{j : \mathbb{E}(Y_\tau | (\mathbf{X}_S, X_j)) \text{ depends on } X_j\}$ as the quantile active predictors conditional on \mathbf{X}_S , and denote $\hat{\mathcal{D}}_{q_\tau} = \{j : \hat{\omega}_j(\hat{Y}_\tau) \geq cn^{-\kappa}, \text{ for } j \in S^c\}$ as the selected variables.

Next we show the sure screening property for the quantile version of $\text{CMC}_{\mathcal{H}}$.

Theorem 5. *Under condition (C1) in the appendix, for any $0 < \gamma < 1/2 - \kappa$ and $\kappa \in (0, 1/2)$,*

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there exist positive constants c_1, c_2 such that for any $c > 0$,

$$P\left\{\max_{1 \leq j \leq p-d_1} |\hat{\omega}_j(\hat{Y}_\tau) - \omega_j(Y_\tau)| \geq cn^{-\kappa}\right\} \leq O[(p-d_1)\{\exp(-c_1n^{1-2(\kappa+\gamma)}) + n \exp(-c_2n^\gamma)\}]. \quad (3.4)$$

If Condition (C2) in the appendix holds in addition, we have

$$P(\mathcal{D}_{q_\tau} \subseteq \hat{\mathcal{D}}_{q_\tau}) \geq 1 - O[\tilde{s}_n\{\exp(-c_1n^{1-2(\kappa+\gamma)}) + n \exp(-c_2n^\gamma)\}], \quad (3.5)$$

where \tilde{s}_n is the cardinality of \mathcal{D}_{q_τ} .

4. Numerical Studies

In this section, we evaluate the finite-sample performance of the proposed method $\text{CMC}_{\mathcal{H}}$.

The choice of kernel functions Denote the translation-invariant Gaussian kernel as

$$K(\mathbf{x}_1, \mathbf{x}_2) := \exp\left\{-\frac{1}{h}(\mathbf{x}_1 - \mathbf{x}_2)^T(\mathbf{x}_1 - \mathbf{x}_2)\right\}, \quad (4.1)$$

where $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^t, t \in \mathbb{N}$, and h is the bandwidth. For the proposed $\text{CMC}_{\mathcal{H}}$, we use $K(\mathbf{x}_1, \mathbf{x}_2)$ for both k_1 and k_2 . In our simulations, the performance of $\text{CMC}_{\mathcal{H}}$ for variable screening is robust against the bandwidths of k_1 and k_2 . So we set $h = 2$ for both k_1 and k_2 . For $\text{MC}_{\mathcal{H}}$, we adopt Gaussian kernel and conduct a sensitivity analysis of the bandwidth, the results of which are presented in the supplementary material S1.1. The performance of $\text{MC}_{\mathcal{H}}$ is sensitive to the bandwidth h . In particular, $\text{MC}_{\mathcal{H}}$ with smaller h performs better for selecting covariates that are linearly related to the response variable, while larger h is more suitable for selecting nonlinearly related covariates. To select the conditional set \mathbf{X}_S and avoid cherry-picking, we first calculate the values of $\text{MC}_{\mathcal{H}}$ using two bandwidths $h = 2\hat{\sigma}_{X_i}^2$ and $h = 6\hat{\sigma}_{X_i}^2$ for each predictor X_i , where $\hat{\sigma}_{X_i}^2$ is sample variance of X_i and $i = 1, \dots, p$.

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Our experience is that $h = 2\hat{\sigma}_{X_i}^2$ and $h = 6\hat{\sigma}_{X_i}^2$ generally perform well for the simulations. Then we take the maximum of the two $\text{MC}_{\mathcal{H}}$ values for each predictor. One can also use Laplacian kernel and Cauchy kernel in practice. However, in our examples, they yield similar performance to that of the Gaussian kernel.

Criteria of evaluating variable screening performance Following Li et al. (2012b), we consider three criteria for evaluating the variable screening performance: 1) \mathcal{S}_q : the $(100q)$ -th quantile of the minimal model size required to contain all the active predictors. 2) \mathcal{P}_i : the proportion that the predictor X_i is selected, and 3) \mathcal{P}_{all} : the proportion of all active predictors being selected. Essentially, an \mathcal{S}_q closer to the total number of active predictors is preferred. The three criteria are connected in a way that a smaller minimal model size suggests a larger \mathcal{P}_{all} and a larger \mathcal{P}_i for each active variable.

Screening thresholds We compare S-CMC $_{\mathcal{H}}$ with six variable screening methods, including two marginal screening method (DCSIS2 in Kong et al. (2017) and MDC), three conditional screening methods (CSIS in Barut et al. (2016), CDCSIS in Wen et al. (2018) and CIS in ?), and one iterative methods (RaSE $_1$ -eBIC in Tian and Feng (2023)). For each screening method, we keep the top $d_2 = \lfloor n/\log(n) \rfloor$ variables, where n is the sample size. We report the \mathcal{P}_i , \mathcal{P}_{all} and $\mathcal{S}_{0.5}$ values based on 100 repetitions for each example. Since conditional screening methods require a pre-selected conditional set \mathbf{X}_S , we either artificially set up the conditional set based on the variables in the true model or select the top $d_1 = \lfloor \sqrt{n/\log(n)} \rfloor$ variables suggested by $\text{MC}_{\mathcal{H}}$. We also include a sensitivity analysis of using different methods (e.g. SIS, LASSO and forward regression) to choose the conditional set in the supplementary material S1.2.

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4.1 Simulation

Example 1 (Marginally inactive but jointly active predictors). Following the idea of Fan and Lv (2008), we generate samples $\{Y_i, \mathbf{X}_i\}_{i=1}^n$ from the linear regression model

$$Y = X_1 + X_2 + X_3 + X_4 + X_5 - cX_6 + \epsilon,$$

where the coefficient c is designed so that $\text{cov}(X_6, Y) = 0$. That is, the predictor X_6 is marginally independent from the response Y . The predictor vector $\mathbf{X} = (X_1, \dots, X_p) \sim N(\mathbf{0}, \Sigma)$, where Σ has (i, j) -th entry $\sigma_{ij} = \rho^{I\{i \neq j\}}$. The error term $\epsilon \sim N(0, 1)$ and is independent from \mathbf{X} . We set the sample size $n = 200$ and the dimension $p = 3000$. We consider three cases: $(c, \rho) \in \{(2.5, 0.5), (4, 0.8), (4.5, 0.9)\}$. Note that X_6 is dependent with Y if given one or more predictors from $\{X_1, \dots, X_5\}$.

The simulation results are reported in Table 1. The marginal screening method MDC fails to detect the marginally independent predictor X_6 in all cases, while other methods identify X_6 as an active predictor. As the correlation increases from $\rho = 0.5$ to $\rho = 0.9$, the selection proportion \mathcal{P}_i decreases for $i = 1, 2, \dots, 5$. Consequently, \mathcal{P}_{all} decreases as the correlation increases. Note that if the conditional set $\mathbf{X}_{S_1} = \{X_1\}$, the proportion of selecting X_1 is set to 1. We set $d_2 = \lfloor n/\log(n) \rfloor = 37$ in this example. Note that the minimal model size $\mathcal{S}_{0.5}$ is small only in the first case where $\rho = 0.5$, which explains the low values of \mathcal{P}_{all} for all the methods for the high correlation case ($\rho = 0.8$ or 0.9). The three conditional methods: CIS, CSIS and CDC-SIS, fail to detect the active variables X_2, X_3, X_4 and X_5 when the correlation increases to $\rho = 0.9$.

When the conditional set changes from an oracle set \mathbf{X}_{S_1} to a data-dependent set \mathbf{X}_{S_2} , the performances of the three conditional screening methods (CIS, CSIS and CDC-SIS) de-

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	\mathcal{P}_1	\mathcal{P}_2	\mathcal{P}_3	\mathcal{P}_4	\mathcal{P}_5	\mathcal{P}_6	\mathcal{P}_{all}	$\mathcal{S}_{0.5}$
$c = 2.5, \rho = 0.5$								
MDC	0.89	0.94	0.93	0.91	0.90	0.00	0.00	3000.0
CSIS (\mathbf{X}_{S_1})	1.00	0.97	0.98	0.98	0.97	0.87	0.78	14.0
CSIS (\mathbf{X}_{S_2})	0.71	0.75	0.75	0.72	0.72	1.00	0.17	1580.5
CDC-SIS (\mathbf{X}_{S_1})	1.00	0.95	0.95	0.95	0.93	0.16	0.14	708.5
CDC-SIS (\mathbf{X}_{S_2})	0.73	0.76	0.74	0.72	0.72	1.00	0.16	1541.5
CIS(\mathbf{X}_{S_1})	1.00	0.83	0.88	0.87	0.87	0.71	0.34	58.0
CIS(\mathbf{X}_{S_2})	0.97	0.91	0.94	0.94	0.97	0.01	0.01	2997.5
S-CMC $_{\mathcal{H}}$ (\mathbf{X}_{S_1})	1.00	0.94	0.94	0.92	0.92	0.53	0.39	90.5
S-CMC $_{\mathcal{H}}$ (\mathbf{X}_{S_2})	0.91	0.95	0.94	0.93	0.92	1.00	0.72	17.5
RaSE $_1$ -eBIC	0.99	1.00	0.99	0.99	1.00	1.00	0.97	6.0
$c = 4, \rho = 0.8$								
MDC	0.61	0.63	0.64	0.63	0.62	0.00	0.00	3000.0
CSIS (\mathbf{X}_{S_1})	1.00	0.48	0.44	0.40	0.44	1.00	0.10	320.0
CSIS (\mathbf{X}_{S_2})	0.39	0.34	0.36	0.41	0.33	1.00	0.00	2988.5
CDC-SIS (\mathbf{X}_{S_1})	1.00	0.56	0.53	0.54	0.54	0.93	0.06	264.0
CDC-SIS (\mathbf{X}_{S_2})	0.39	0.34	0.36	0.41	0.34	1.00	0.00	2623.5
CIS(\mathbf{X}_{S_1})	1.00	0.39	0.31	0.34	0.42	1.00	0.03	546.0
CIS(\mathbf{X}_{S_2})	0.70	0.59	0.67	0.64	0.69	1.00	0.09	268.0
S-CMC $_{\mathcal{H}}$ (\mathbf{X}_{S_1})	1.00	0.73	0.71	0.66	0.67	1.00	0.26	127.5
S-CMC $_{\mathcal{H}}$ (\mathbf{X}_{S_2})	0.61	0.73	0.72	0.66	0.67	1.00	0.16	156.5
RaSE $_1$ -eBIC	0.80	0.92	0.76	0.79	0.87	1.00	0.35	2312.5
$c = 4.5, \rho = 0.9$								
MDC	0.48	0.40	0.39	0.48	0.40	0.00	0.00	3000.0
CSIS (\mathbf{X}_{S_1})	1.00	0.14	0.09	0.13	0.08	1.00	0.00	2339.0
CSIS (\mathbf{X}_{S_2})	0.28	0.24	0.23	0.24	0.20	1.00	0.00	2992.5
CDC-SIS (\mathbf{X}_{S_1})	1.00	0.29	0.28	0.29	0.28	0.98	0.01	875.0
CDC-SIS (\mathbf{X}_{S_2})	0.28	0.24	0.23	0.24	0.21	1.00	0.00	2875.0
CIS(\mathbf{X}_{S_1})	1.00	0.11	0.08	0.07	0.16	1.00	0.00	2037.5
CIS(\mathbf{X}_{S_2})	0.43	0.44	0.47	0.46	0.41	1.00	0.00	897.0
S-CMC $_{\mathcal{H}}$ (\mathbf{X}_{S_1})	1.00	0.48	0.47	0.51	0.45	1.00	0.07	269.5
S-CMC $_{\mathcal{H}}$ (\mathbf{X}_{S_2})	0.53	0.48	0.47	0.51	0.47	1.00	0.03	338.0
RaSE $_1$ -eBIC	0.62	0.89	0.73	0.65	0.68	1.00	0.19	2316.0

Table 1: The \mathcal{P}_i , \mathcal{P}_{all} and $\mathcal{S}_{0.5}$ in Example 1. The conditional set is either $\mathbf{X}_{S_1} = \{X_1\}$ or $\mathbf{X}_{S_2} = \{\text{the first } d_1 = 6 \text{ predictors selected by MDC}_{\mathcal{H}}\}$.

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teriorate. Our proposed S-CMC \mathcal{H} instead shows robustness against the conditional set. The performance of our method decreases due to the extra cost of selecting X_1 when the conditional set becomes data-dependent.

In this example, from the perspective of the minimal model size $\mathcal{S}_{0.5}$, the minimal model size for RaSE $_1$ -eBIC changes from 6 to 2316 when ρ increases from 0.5 to 0.9. In contrast, the stable performance of S-CMC \mathcal{H} in $\mathcal{S}_{0.5}$ indicates that our method is more robust against the correlation ρ . In terms of \mathcal{P}_{all} and \mathcal{P}_i , RaSE $_1$ -eBIC and S-CMC \mathcal{H} are better than any other method. RaSE $_1$ -eBIC is better than S-CMC \mathcal{H} , which may be due to the good performance of RaSE $_1$ -eBIC in the linear case.

Example 2 (Interaction terms). We consider the following model with interaction terms:

$$Y = X_1 + X_5 + X_{10} + X_1X_{15} + 1.5X_5X_{20} + 2X_{10}X_{25} + \epsilon.$$

The predictor vector $\mathbf{X} = (X_1, \dots, X_p) \sim N(\mathbf{0}, \Sigma)$, where Σ has (i, j) -th entry $\sigma_{ij} = \rho^{|i-j|}$.

We consider two cases: $\rho \in \{0, 0.9\}$. The error term $\epsilon \sim N(0, 1)$ and is independent from \mathbf{X} .

We set the sample size $n = 200$ and the dimension $p = 3000$.

The results are reported in Table 2. The three variables X_{15}, X_{20}, X_{25} all jointly contribute to the mean of Y , but are marginally independent of the mean of Y . It is difficult for the marginal screening methods to detect these three terms. Note that X_{25} has a larger coefficient in its interaction term than that of X_{20} or X_{15} . As the signal/coefficient of the interaction term increases, its effect is easier to be detected ($\mathcal{P}_{25} > \mathcal{P}_{20} > \mathcal{P}_{15}$) for all the methods. RaSE $_1$ -eBIC fails in detecting those three variables in this example. This is possibly due to the fact that RaSE $_1$ -eBIC targets additive models. In comparison to the interaction screening method DCSIS2, the proposed method S-CMC \mathcal{H} has a comparable performance

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	\mathcal{P}_1	\mathcal{P}_5	\mathcal{P}_{10}	\mathcal{P}_{15}	\mathcal{P}_{20}	\mathcal{P}_{25}	\mathcal{P}_{all}	$\mathcal{S}_{0.5}$
$\rho = 0$								
MDC	0.94	0.96	0.90	0.01	0.00	0.03	0.00	2662.5
CSIS (\mathbf{X}_{S_1})	1.00	1.00	1.00	0.04	0.03	0.07	0.00	2452.0
CSIS(\mathbf{X}_{S_2})	0.97	0.93	0.90	0.03	0.02	0.04	0.00	2147.0
CDC-SIS (\mathbf{X}_{S_1})	1.00	1.00	1.00	0.01	0.03	0.26	0.00	1637.0
CDC-SIS (\mathbf{X}_{S_2})	0.84	0.86	0.84	0.07	0.17	0.43	0.00	1529.0
DCSIS2	0.40	0.70	0.99	0.11	0.35	0.85	0.00	1372.5
CIS(\mathbf{X}_{S_1})	1.00	1.00	1.00	0.02	0.12	0.45	0.00	566.0
CIS(\mathbf{X}_{S_2})	0.99	0.98	0.96	0.01	0.01	0.02	0.00	2278.0
S-CMC $_{\mathcal{H}}$ (\mathbf{X}_{S_1})	1.00	1.00	1.00	0.18	0.62	0.99	0.09	196.5
S-CMC $_{\mathcal{H}}$ (\mathbf{X}_{S_2})	0.94	0.96	0.91	0.11	0.37	0.77	0.01	851.5
RaSE $_1$ -eBIC	0.87	0.82	0.79	0.01	0.01	0.04	0.00	2295.5
$\rho = 0.9$								
MDC	1.00	1.00	1.00	0.97	0.52	0.14	0.13	350.5
CSIS (\mathbf{X}_{S_1})	1.00	1.00	1.00	0.08	0.15	0.13	0.02	1887.0
CSIS (\mathbf{X}_{S_2})	0.78	0.97	0.74	0.08	0.12	0.13	0.02	1870.0
CDCSIS (\mathbf{X}_{S_1})	1.00	1.00	1.00	0.03	0.04	0.06	0.00	2022.5
CDCSIS(\mathbf{X}_{S_2})	0.52	0.96	0.80	0.86	1.00	1.00	0.40	66.0
DCSIS2	0.93	1.00	1.00	0.87	0.91	0.81	0.62	30.5
CIS(\mathbf{X}_{S_1})	1.00	1.00	1.00	0.28	0.93	1.00	0.27	62.0
CIS(\mathbf{X}_{S_2})	0.78	0.99	0.83	0.43	0.92	0.85	0.2	88.5
S-CMC $_{\mathcal{H}}$ (\mathbf{X}_{S_1})	1.00	1.00	1.00	0.90	1.00	1.00	0.90	25.0
S-CMC $_{\mathcal{H}}$ (\mathbf{X}_{S_2})	1.00	1.00	1.00	0.90	1.00	0.99	0.89	26.0
RaSE $_1$ -eBIC	0.41	0.42	0.37	0.02	0.02	0.01	0.01	2403.0

Table 2: The \mathcal{P}_i , \mathcal{P}_{all} and $\mathcal{S}_{0.5}$ in Example 2. We set the conditional set to be $\mathbf{X}_{S_1}=\{X_1, X_5, X_{10}\}$ or $\mathbf{X}_{S_2}=\{\text{the first } d_1 = 6 \text{ predictors selected by MC}_{\mathcal{H}}\}$.

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in selecting X_{15} , X_{20} and X_{25} for both $\rho = 0$ and $\rho = 0.9$. But S-CMC $_{\mathcal{H}}$ performs better than DCSIS2 in selecting the marginally active variables X_1 , X_5 and X_{10} . What's more, S-CMC $_{\mathcal{H}}$ has the smallest $\mathcal{S}_{0.5}$ among all the methods. Similar to Example 1, the performance of S-CMC $_{\mathcal{H}}$ is stable against the conditional set. We also did a sensitivity analysis against the conditional set. For Examples 1-3, we consider two types of perturbation to the conditional set: change the cardinality of the conditional set or change one inactive variable in the conditional set. We also consider the cases where the correlation is high $\rho = 0.9$ and the noise error distribution is not Gaussian. The results are reported in the supplementary material S1.2, demonstrating a better and more stable performance of S-CMC $_{\mathcal{H}}$ compared to other conditional methods (CSIS, CDC-SIS). Finally, we include a block structure correlation setting where the correlation among active predictors are 0.2 and 0.1 otherwise. We report the result in the supplementary material S1.3, which clearly shows the advantage of S-CMC $_{\mathcal{H}}$.

Example 3 (Heteroscedasticity & Quantile screening). In this example, we demonstrate that our screening method can help in heteroskedastic model specification. We consider the following model:

$$Y = X_1 + X_5 + X_1 X_{10} + 1.5 X_5 X_{15} + \epsilon \cdot \exp(X_{35} + X_{40}).$$

The predictor vector $\mathbf{X} = (X_1, \dots, X_p) \sim N(\mathbf{0}, \Sigma)$, where Σ has (i, j) -th entry $\sigma_{ij} = \rho^{|i-j|}$. We consider two cases: $\rho \in \{0, 0.9\}$. The error term $\epsilon \sim N(0, 1)$ is independent from \mathbf{X} . We set the sample size $n = 400$ and the dimension $p = 3000$. For the purpose of quantile screening, we change the continuous response Y to a binary response $Y_{\tau} = \tau - \mathbf{1}(Y \leq \hat{q}_{\tau})$, where \hat{q}_{τ} is the τ -th sample quantile of the response. Then we apply S-CMC $_{\mathcal{H}}$ and MDC

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on the data (Y_τ, \mathbf{X}) . Note that in fixed design, the population quantile q_τ does not depend on (X_{20}, X_{25}) if and only if $\tau = 0.5$. We consider two choices of the quantile: $\tau = 0.5$ and $\tau = 0.75$.

The results are presented in Table 3 with conditional set selected by $\text{MC}_{\mathcal{H}}$. In this example, we also evaluate the method QaSIS (He et al., 2013), a quantile-adaptive model-free variable screening method for heterogeneous data. Overall, our proposed method $\text{S-CMC}_{\mathcal{H}}$ performs the best across all four combinations of (ρ, τ) . In particular, $\text{S-CMC}_{\mathcal{H}}$ is dominantly better in $\mathcal{S}_{0.5}$ than any other method even under high correlation setting. When there is no correlation among predictors ($\rho = 0$), from the perspective of quantile screening, MDC, CDC-SIS, QaSIS, and $\text{S-CMC}_{\mathcal{H}}$ correctly differentiate the different roles of X_{35} and X_{40} under two values of τ . However, these three methods (MDC, CDC-SIS, QaSIS) fail to identify X_{15} (compared to X_{10}) when $\tau = 0.5$. In contrast, $\text{S-CMC}_{\mathcal{H}}$ has a better performance in separating the active variables from the inactive variables. When high correlation exists among predictors, all methods receive improved performance and $\text{S-CMC}_{\mathcal{H}}$ still remains competitive. This is because the marginal relationship between X_{10} (X_{15}) and the response Y is strengthened by the high correlation among predictors. We also include the scenario when conditional set is $\{X_1, X_5, X_{10}\}$ in the supplementary material S1.4.

Example 4 (Nonlinear case). We consider the following nonlinear case.

$$Y = 3I(X_1 > 0.5)X_2 + 3\sin^2(2\pi X_1)X_3 + 3(X_1^2 - 1)X_4 + \exp(X_1)X_5 + \epsilon,$$

where we first generate $U_1, U_2 \stackrel{i.i.d}{\sim} \text{Unif}[0, 1]$ and then let $X_1 = (U_1 + U_2)/2$ and $X_k = (Z_k + 2U_1)/4$ for $k = 2, 3, \dots, p$. We consider two scenarios, symmetric distribution $Z_k \stackrel{i.i.d}{\sim} N(0, 1)$ and asymmetric distribution $Z_k \stackrel{i.i.d}{\sim} \chi_{(1)}^2$. The error term ϵ is independently drawn from

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Method	τ	$\rho = 0$								$\rho = 0.9$							
		\mathcal{P}_1	\mathcal{P}_5	\mathcal{P}_{10}	\mathcal{P}_{15}	\mathcal{P}_{35}	\mathcal{P}_{40}	\mathcal{P}_{all}	$\mathcal{S}_{0.5}$	\mathcal{P}_1	\mathcal{P}_5	\mathcal{P}_{10}	\mathcal{P}_{15}	\mathcal{P}_{35}	\mathcal{P}_{40}	\mathcal{P}_{all}	$\mathcal{S}_{0.5}$
MDC	0.5	1.00	1.00	0.06	0.03	0.04	0.02	0.00	1910.0	1.00	1.00	0.97	0.49	0.06	0.05	0.49	71.0
	0.75	0.99	1.00	0.24	0.38	0.52	0.55	0.03	986.5	1.00	1.00	1.00	1.00	0.91	0.92	0.86	29.5
CSIS	0.5	1.00	0.99	0.01	0.03	0.20	0.16	0.00	2025.5	1.00	1.00	0.19	0.07	0.31	0.24	0.00	1854.5
	0.75	0.97	0.95	0.06	0.14	0.39	0.42	0.00	2207.0	0.86	0.96	0.39	0.11	0.31	0.30	0.00	2138.5
CDC-SIS	0.5	1.00	0.99	0.13	0.28	0.23	0.30	0.04	757.0	1.00	1.00	0.28	0.94	1.00	1.00	0.27	172.5
	0.75	0.96	0.97	0.13	0.51	0.42	0.47	0.04	1159.5	0.88	0.97	0.41	0.87	0.95	0.92	0.25	214.5
QaSIS	0.5	1.00	1.00	0.16	0.16	0.28	0.27	0.03	1085.0	1.00	1.00	1.00	0.90	0.69	0.55	0.90	20.5
	0.75	0.92	0.99	0.14	0.38	0.69	0.72	0.03	600.0	0.99	1.00	1.00	0.97	0.99	0.97	0.92	35.5
DCSIS2	0.5	0.18	0.41	0.04	0.08	0.93	0.90	0.00	1443.5	0.07	0.15	0.06	0.05	1.00	1.00	0.00	918.0
	0.75	0.18	0.41	0.04	0.08	0.93	0.90	0.00	1443.5	0.07	0.15	0.06	0.05	1.00	1.00	0.00	918.0
CIS	0.5	1.00	0.99	0.07	0.04	0.01	0.02	0.01	1982.5	1.00	1.00	0.31	0.89	0.95	0.98	0.29	121.5
	0.75	1.00	0.99	0.06	0.14	0.21	0.3	0.00	2537.5	1.00	0.99	0.47	0.76	0.9	0.91	0.33	129.0
S-CMC \mathcal{H}	0.5	1.00	1.00	0.18	0.80	0.05	0.04	0.13	240.0	1.00	1.00	0.97	0.93	0.34	0.38	0.90	16.0
	0.75	0.99	1.00	0.33	0.67	0.49	0.58	0.05	574.5	1.00	1.00	1.00	0.95	0.97	0.93	0.86	28.0
RaSE $_1$ -eBIC	0.5	0.49	0.31	0.00	0.00	0.03	0.01	0.00	1816.0	0.25	0.07	0.00	0.00	0.04	0.03	0.00	2425.5
	0.75	0.49	0.31	0.00	0.00	0.00	0.00	0.00	2427.0	0.25	0.07	0.00	0.00	0.01	0.02	0.00	2427.0

Table 3: The \mathcal{P}_i , \mathcal{P}_{all} and $\mathcal{S}_{0.5}$ in Example 3 with \mathbf{X}_S selected by $MC_{\mathcal{H}}$.

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	$Z_k \stackrel{i.i.d.}{\sim} N(0, 1)$							$Z_k \stackrel{i.i.d.}{\sim} \chi_{(1)}^2$						
	\mathcal{P}_1	\mathcal{P}_2	\mathcal{P}_3	\mathcal{P}_4	\mathcal{P}_5	\mathcal{P}_{all}	$\mathcal{S}_{0.5}$	\mathcal{P}_1	\mathcal{P}_2	\mathcal{P}_3	\mathcal{P}_4	\mathcal{P}_5	\mathcal{P}_{all}	$\mathcal{S}_{0.5}$
MDC	1.00	0.79	0.84	0.00	0.85	0.00	2974.5	1.00	0.64	0.80	0.00	0.85	0.00	2725.0
CSIS	0.99	0.56	0.55	1.00	0.69	0.17	554.5	1.00	0.61	0.70	1.00	0.81	0.26	100.5
CDC-SIS	0.99	0.62	0.53	0.34	0.68	0.11	1101.5	1.00	0.45	0.60	0.65	0.60	0.11	962.5
DCSIS2	1.00	0.84	0.57	0.00	0.52	0.00	2235.0	1.00	0.90	0.71	0.05	0.70	0.01	1284.5
CIS	1.00	0.95	0.90	0.31	0.94	0.24	153.0	1.00	0.76	0.78	0.42	0.78	0.17	155.0
S-CMC \mathcal{H}	1.00	0.79	0.84	0.95	0.85	0.52	33.5	1.00	0.63	0.78	0.90	0.82	0.35	77.0
RaSE $_1$ -eBIC	0.28	0.60	0.60	0.58	0.74	0.06	2250.0	0.98	0.47	0.63	0.95	0.73	0.18	2253.5

Table 4: The \mathcal{P}_i , \mathcal{P}_{all} and $\mathcal{S}_{0.5}$ in Example 4 with \mathbf{X}_S selected by MC \mathcal{H} .

standard normal distribution. We set the sample size $n = 200$ and the dimension $p = 3000$. The results are reported in Table 4.

In this example, the active predictors are nonlinearly associated with each other. Each element in this model is an interaction effect of two variables. The proposed S-CMC \mathcal{H} demonstrates its competitive performance for selecting all the active predictors with relatively high \mathcal{P}_i and \mathcal{P}_{all} , and smallest $\mathcal{S}_{0.5}$, in both scenarios. The methods DCSIS2 and MDC fail to detect X_4 . It is worth pointing out that the contribution of variable X_4 is also underestimated by the methods CDC-SIS and CIS. This may be because that X_4 's conditional contribution to Y is diffused by the exponential term $\exp(X_1)X_5$, as indicated by the much larger \mathcal{P}_5 in the four methods mentioned above.

4.2 Data Applications

4.2.1 Single Cell Malt Tumor CITE-seq Dataset

The Malt Tumor Cellular Indexing of Transcriptomes and Epitopes by sequencing (CITE-seq) dataset (<http://www.10xgenomics.com>) contains single-cell level sequencing RNA data

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and as well as the surface protein expression count. We are interested in identifying the genes that affect the surface protein level. The dataset contains 33555 genes and proteins from 8412 single cells. Following the data pre-processing procedure in Tong et al. (2023) (filtering out cells with more than 90% zero entries and genes that has zero variance), we obtain a sample of $n = 207$ single cells and $p = 18702$ genes. And we set protein CD8 as the response variable and the protein CD3 as conditional variable. Interested readers are referred to Tong et al. (2023) for detailed scientific explanations of using CD3 as the conditional variable. To evaluate the prediction performance of each screening method, we randomly split the observations into a training set of size 176 and a test set of size 31. We select $d_2 = 38$ variables by the following four conditional methods: CSIS, CDCSIS, CIS and $\text{SCMC}_{\mathcal{H}}$ including CD3. Then a random forest model is fitted with the selected variables and the response, with log transformations on the response and the variables. The mean squared errors (MSE) of the methods on the test set for 100 repetitions are reported in Table 5. In each of the 100 repetitions, we calculate the difference between the MSE of $\text{S-CMC}_{\mathcal{H}}$ and that of each competing method. Then we conducted a one-sided paired two-sample t -test with the alternative hypothesis that our method $\text{S-CMC}_{\mathcal{H}}$ has a smaller average mean squared error (MSE). Our method has the smallest MSE and the p -values of the paired t -test indicates $\text{S-CMC}_{\mathcal{H}}$ outperforms each method in prediction accuracy.

4.2.2 Riboflavin Production Dataset

The dataset (Lee et al., 2001) contains information about riboflavin (vitamin B2) production by $n = 71$ bacillus subtiliswith, where $p = 4088$ gene expression levels are recorded. The dataset is provided by Royal DSM (Switzerland) and is available in the R package `hdi`.

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Method	MSE	paired t -test p -value
CSIS	1.364	$< 2.2 \times 10^{-16}$
CDC-SIS	1.162	$< 2.2 \times 10^{-16}$
CIS	1.268	$< 2.2 \times 10^{-16}$
S-CMC $_{\mathcal{H}}$	0.748	–

Table 5: The prediction accuracy in MALT data.

Our goal is to find which genes are most related in predicting the riboflavin production rate. We randomly split the sample into a training set of size 60 and a test set of size 11. To evaluate the prediction performance of each screening method, we select $d_2 = 16$ variables for each screening method and train a random forest model on the training set. Then we calculate the mean squared error (MSE) of each method on the test set. The average MSE's based on 100 data splittings into training/test sets are reported in Table 6. Similar to Section 4.2.1, we conducted the same one-sided paired two-sample t -test with the alternative hypothesis that our method S-CMC $_{\mathcal{H}}$ has a smaller average mean squared error (MSE). Our method has the smallest MSE and the p -values suggest that it significantly improves the MSE. Without out the such prior knowledge, if we select the conditional set by MC $_{\mathcal{H}}$ with $d_1 = \lfloor \sqrt{n/\log(n)} \rfloor$, unfortunately, it does not contain protein CD3. However, our method still outperforms each method in terms of prediction accuracy as shown in Table 13 in the Supplementary Material S1.5. It is also worth pointing out that all the MSEs are larger than that under the case where the conditional set is selected based on the prior knowledge in Tong et al. (2023), which suggests the advantage of such prior knowledge.

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Method	MSE	paired t -test p -value
MDC	0.301	0.017
CSIS	0.357	2.909×10^{-15}
CDC-SIS	0.323	5.62×10^{-5}
CIS	0.323	5.62×10^{-5}
RaSE ₁ -eBIC	0.293	0.401
S-CMC _{\mathcal{H}}	0.292	–

Table 6: The prediction accuracy in Riboflavin production data. The conditional set \mathbf{X}_S contains the top $d_1 = 4$ variables suggested by MC _{\mathcal{H}} .

5. Conclusion

In this article, we propose the conditional martingale difference divergence (CMD _{\mathcal{H}}) to measure the dependence between a response variable and a predictor vector given a third vector. It is primarily designed to overcome the limitation of marginal independence measures. Based on CMD _{\mathcal{H}} , we develop a new screening procedure called S-CMC _{\mathcal{H}} by combining the merits of the CMC _{\mathcal{H}} and MC _{\mathcal{H}} for selecting both marginal and jointly active variables. The proposed framework can be easily extended to quantile screening. The simulations and real data applications demonstrate that S-CMC _{\mathcal{H}} has a competitive and stable performance under variety model settings for mean or quantile screening. We also provide a data-driven method for selecting the conditional set \mathbf{X}_S . The limitation of this method is that we do need to pre-determine a proper number of variables in conditional set to get a satisfactory performance. Using $\lfloor \sqrt{n/\log n} \rfloor$, as done in our numerical study, may not suffice for the cases when the true underlying model consists jointly only active variables that depends on a large condi-

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tional set. Designing a variable screening method that is free of tuning the cardinality of the conditional set is a challenging future research topic.

Supplementary Material

The online supplementary material contains additional simulation results, and the proofs of theorems and results introduced in the main article.

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6. Appendix

A. Bochner's Theorem

Lemma 1. (*Wendland, 2004, Theorem 6.6*) *A continuous function $k : \mathbb{R}^{p+q} \rightarrow \mathbb{R}$ is positive semi-definite if and only if it is the Fourier transform of a finite nonnegative Borel measure $W(\xi)d\xi$ on \mathbb{R}_{p+q} , that is,*

$$k(z) = \int_{\mathbb{R}^{(p+q)}} e^{-iz^T \xi} W(\xi) d\xi, \quad \forall z \in \mathbb{R}^{p+q}.$$

B. Properties of $\text{MC}_{\mathcal{H}}$

Some important properties of $\text{MD}_{\mathcal{H}}$ and $\text{MC}_{\mathcal{H}}$ are presented as follows.

Definition 4. *Given i.i.d. observations $(\mathbf{U}_i, V_i)_{i=1}^n$ from the distribution of (\mathbf{U}, V) . Let $a_{ij} = V_i V_j$ and $b_{ij} = k(\mathbf{U}_i - \mathbf{U}_j)$, where k is a kernel in RKHS. The unbiased sample RKHS*

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type martingale difference divergence $\widehat{\text{MD}}_{\mathcal{H}}^2(V, \mathbf{U})$ is defined as

$$\widehat{\text{MD}}_{\mathcal{H}}^2(V, \mathbf{U}) = \frac{1}{n(n-3)} \sum_{i \neq j}^n a_{ij}^* b_{ij}^* \quad (\text{B.1})$$

and the unbiased sample RKHS type martingale difference correlation $\widehat{\text{MC}}_{\mathcal{H}}^2(V, \mathbf{U})$ is defined by

$$\widehat{\text{MC}}_{\mathcal{H}}^2(V, \mathbf{U}) = \begin{cases} \frac{\widehat{\text{MD}}_{\mathcal{H}}^2(V, \mathbf{U})}{\text{var}_n(V) \text{var}_{n\mathcal{H}}(\mathbf{U})} & \text{if } \text{var}_n(V) \text{var}_{n\mathcal{H}}(\mathbf{U}) > 0 \\ 0 & \text{otherwise,} \end{cases} \quad (\text{B.2})$$

where $\text{var}_n(V) = (\frac{1}{n(n-3)} \sum_{i \neq j}^n |a_{ij}^*|^2)^{1/2}$, and $\text{var}_{n\mathcal{H}}(\mathbf{U}) = (\frac{1}{n(n-3)} \sum_{i \neq j}^n |b_{ij}^*|^2)^{1/2}$.

Theorem 6. *The following properties hold if $E(V^2) < \infty$:*

- a. $\text{MD}_{\mathcal{H}}^2(V, \mathbf{U}) = E[\{V - E(V)\}\{V' - E(V')\}k(\mathbf{U} - \mathbf{U}')]$.
- b. $0 \leq \text{MC}_{\mathcal{H}}(V, \mathbf{U}) \leq 1$, and $\text{MC}_{\mathcal{H}}(V, \mathbf{U}) = 0 \Leftrightarrow E(V|\mathbf{U}) = E(V)$ almost surely.
- c. $\text{MC}_{\mathcal{H}}(a + bV, c + \mathbf{U}) = \text{MC}_{\mathcal{H}}(V, \mathbf{U})$ for any scalars $a, b \in \mathbb{R}$ and $c \in \mathbb{R}^q$.

Theorem 7. *If $E(V^2) < \infty$, then*

$$\lim_{n \rightarrow \infty} \widehat{\text{MD}}_{\mathcal{H}}^2(V, \mathbf{U}) = \text{MD}_{\mathcal{H}}^2(V, \mathbf{U}) \text{ a.s.,} \quad (\text{B.3})$$

and

$$\lim_{n \rightarrow \infty} \widehat{\text{MC}}_{\mathcal{H}}^2(V, \mathbf{U}) = \text{MC}_{\mathcal{H}}^2(V, \mathbf{U}) \text{ a.s..} \quad (\text{B.4})$$

Theorem 8. *Assume $E(V^2) < \infty$, we have the following:*

- a. *If $\text{MC}_{\mathcal{H}}(V, \mathbf{U}) = 0$, then*

$$n \widehat{\text{MD}}_{\mathcal{H}}^2(V, \mathbf{U}) \xrightarrow[n \rightarrow \infty]{D} \|\Gamma(s)\|_{\mathcal{H}_k}^2, \quad (\text{B.5})$$

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where $\Gamma(\cdot)$ denotes a complex-valued zero-mean Gaussian random process with covariance function

$$\begin{aligned} \text{cov}_\Gamma(s, s_0) &= F(s - s_0) - g_U(s - s_0)E^2(V) + \{E(V^2) + E^2(V)\}g_U(s)\overline{g_U(s_0)} \\ &\quad - F(s)\overline{g_U(s_0)} - g_U(s)\overline{F(s_0)} \end{aligned}$$

with $s, s_0 \in \mathbb{R}^q$ and $g_U(s) = E(e^{i\langle s, \mathbf{U} \rangle})$, $F(s) = E[V^2 \exp(i\langle \mathbf{U}, s \rangle)]$.

b. If $\text{MC}_\mathcal{H}(V, \mathbf{U}) = 0$ and $E(V^2|\mathbf{U}) = E(V^2)$, then

$$n\widehat{\text{MD}}_\mathcal{H}^2(V, \mathbf{U})/S_n \xrightarrow[n \rightarrow \infty]{D} Q,$$

where $S_n = \{1 - \frac{1}{n(n-1)} \sum_{k \neq l} k(\mathbf{U}_k - \mathbf{U}_l)\} \{\frac{1}{n} \sum_k (V_k - \bar{V}_n)^2\}$, and Q is a nonnegative quadratic form $Q = \sum_{i=1}^\infty \lambda_i Z_i^2$, where Z_i are independent standard normal random variables. $\{\lambda_i\}$ are nonnegative constants that depend on the distribution of (U, V) and $E(Q) = 1$.

c. If $\text{MC}_\mathcal{H}(V, \mathbf{U}) \neq 0$, then $n\widehat{\text{MD}}_\mathcal{H}^2(V, \mathbf{U})/S_n \xrightarrow[n \rightarrow \infty]{P} \infty$.

B.1 Sure Screening Property of $\text{MC}_\mathcal{H}$

Let $\psi_i = \text{MC}_\mathcal{H}(Y, X_i)$ for predictor X_i and $\hat{\psi}_i = \widehat{\text{MC}}_\mathcal{H}(Y, X_i)$. Denote $\widehat{\mathcal{M}} = \{j : \hat{\psi}_j \geq cn^{-\kappa}, \text{ for } 1 \leq j \leq p\}$. Similar to $\text{CMC}_\mathcal{H}$, we need the following two assumptions.

(B1) There exists a positive constant s_0 such that for all $0 < s \leq 2s_0$, then $E\{\exp(sY^2)\} < \infty$.

(B2) The minimum $\text{MC}_\mathcal{H}$ value of active predictors is greater than $2cn^{-\kappa}$, for some constant $c > 0$ and $0 \leq \kappa < \frac{1}{2}$.

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Theorem 9. *Under Assumption (B1), for any $0 < \gamma < 1/2 - \kappa$, there exist positive constants c_1 and c_2 such that*

$$P\left\{\max_{1 \leq j \leq p} |\hat{\psi}_j - \psi_j| \geq cn^{-\kappa}\right\} \leq O[p\{\exp(-c_1 n^{1-2(\kappa+\gamma)}) + n \exp(-c_2 n^\gamma)\}]. \quad (\text{B.6})$$

Under conditions (B1) and (B2), we have that

$$P(\mathcal{M} \subset \widehat{\mathcal{M}}) \geq 1 - O[s_n\{\exp(-c_1 n^{1-2(\kappa+\gamma)}) + n \exp(-c_2 n^\gamma)\}], \quad (\text{B.7})$$

where s_n is the cardinality of \mathcal{M} .

For the sure screening property of quantile screening by $\text{MC}_{\mathcal{H}}$, we require the condition (C1) in the following Section C. Denote $\mathcal{M}_{q_\tau} := \{j : \mathbb{E}(Y_\tau | X_j) \text{ depends on } X_j\}$ and $\widehat{\mathcal{M}}_{q_\tau} := \{j : \hat{\psi}_j(\hat{Y}_\tau) \geq cn^{-\kappa}, \text{ for } 1 \leq j \leq p\}$.

Theorem 10. *Under (C1), for any $0 < \gamma < 1/2 - \kappa$ and $\kappa \in (0, 1/2)$, there exists positive constants c_1, c_2 such that for any $c > 0$,*

$$P\left\{\max_{1 \leq j \leq p} |\hat{\psi}_j(\hat{Y}_\tau) - \psi_j(Y_\tau)| \geq cn^{-\kappa}\right\} \leq O[p\{\exp(-c_1 n^{1-2(\kappa+\gamma)}) + n \exp(-c_2 n^\gamma)\}]. \quad (\text{B.8})$$

If the minimum $\text{MC}_{\mathcal{H}}$ value of active predictors satisfies $\min_{j \in \mathcal{M}_{q_\tau}} \psi_j(Y_\tau) \geq 2cn^{-\kappa}$ for some constant $c > 0$ and $0 \leq \kappa < 1/2$, we can show that

$$P(\mathcal{M}_{q_\tau} \subseteq \widehat{\mathcal{M}}_{q_\tau}) \geq 1 - O[\tilde{s}_n\{\exp(-c_1 n^{1-2(\kappa+\gamma)}) + n \exp(-c_2 n^\gamma)\}], \quad (\text{B.9})$$

where \tilde{s}_n is the cardinality of \mathcal{M}_{q_τ} .

C. Sure Screening Property of Quantile Screening using $\text{CMC}_{\mathcal{H}}$

We require the two assumptions below:

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(C1) The CDF of Y (F_Y) is continuously differentiable in a small neighborhood of $q_\tau = q_\tau(Y)$, say $[q_\tau - \delta_0, q_\tau + \delta_0]$ for $\delta > 0$. Let $G_1(\delta_0) = \inf_{y \in [q_\tau - \delta_0, q_\tau + \delta_0]} f_Y(y)$, and $G_2(\delta_0) = \sup_{y \in [q_\tau - \delta_0, q_\tau + \delta_0]} f_Y(y)$ where f_Y is the density function of Y . Assume that $0 < G_1(\delta_0) \leq G_2(\delta_0) < \infty$.

(C2) The minimum $\text{CMC}_{\mathcal{H}}$ value of active predictors satisfies $\min_{j \in \mathcal{D}_{q_\tau}} \omega_j(Y_\tau) \geq 2cn^{-\kappa}$ for some constant $c > 0$ and $0 \leq \kappa < 1/2$.

The following proposition from Shao and Zhang (2014) is necessary for proving the sure screening property.

Proposition 1. *Under condition (C1), there exists $\epsilon_0 > 0$ and $c_1 > 0$, such that for any $\epsilon \in (0, \epsilon_0)$,*

$$P\left(\frac{1}{n} \sum_{l=1}^n |\hat{y}_{l_\tau} - y_{l_\tau}| > \epsilon\right) \leq 3 \exp(-2nc_1\epsilon^2) \quad (\text{C.1})$$

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