FACT: High-Dimensional Random Forests Inference∗

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July 4, 2022

Abstract

Random forests is one of the most widely used machine learning methods over the past decade thanks to its outstanding empirical performance. Yet, because of its black-box nature, the results by random forests can be hard to interpret in many big data applications. Quantifying the usefulness of individual features in random forests learning can greatly enhance its interpretability. Existing studies have shown that some popularly used feature importance measures for random forests suffer from the bias issue. In addition, there lack comprehensive size and power analyses for most of these existing methods. In this paper, we approach the problem via hypothesis testing, and suggest a framework of the self-normalized feature-residual correlation test (FACT) for evaluating the significance of a given feature in the random forests model with bias-resistance property, where our null hypothesis concerns whether the feature is conditionally independent of the response given all other features. Such an endeavor on random forests inference is empowered by some recent developments on high-dimensional random forests consistency. The vanilla version of our FACT test can suffer from the bias issue in the presence of feature dependency. We exploit the techniques of imbalancing and conditioning for bias correction. We further incorporate the ensemble idea into the FACT statistic through feature transformations for the enhanced power. Under a fairly general high-dimensional nonparametric model setting with dependent features, we formally establish that FACT can provide theoretically justified random forests feature p-values and enjoy appealing power through nonasymptotic analyses. The theoretical results and finite-sample advantages of the newly suggested method are illustrated with several simulation examples and an economic forecasting application in relation to COVID-19.

Running title: FACT

Key words: Random forests; Nonparametric inference; High dimensionality; Nonasymptotic theory; Size and power; Bias-resistance; Sparsity and conditional independence

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1 Introduction

Reliable statistical inference depends on an accurate modeling for the observed data. In modern applications, the data collected is often high-dimensional and exhibits complex relationships between the response and its explanatory features. Such an involved modeling task can be done by the state-of-the-art machine learning methods. One method of particular interest is the random forests \cite{breiman2001random, breiman1984classification}, which is an ensemble predictive model making predictions by aggregating the individual predictions from a collection of randomized decision trees. Over the past two decades, a vast amount of research has demonstrated that random forests is reliable in applications from diverse disciplines such as economics \cite{chernozhukov2018double, belloni2014lasso, rossi2018least}, finance \cite{christiano2015structural}, bioinformatics \cite{goldberg2002using, reverter2003identification}, biostatistics \cite{liu2015practical}, and multi-source remote sensing \cite{das2011multi}. Theoretical endeavors have also proven the consistency of random forests \cite{poisson2004random, fan2001linear, gilbert2012confidence} under various nonparametric settings, even in the presence of correlated and high-dimensional features \cite{guyon2003false}.

Despite the appealing estimation/prediction accuracy, the results output by the random forests can be hard to interpret because of its black-box nature. Much effort has been made to enhance its interpretability, mainly using the idea of identifying most significant features in explaining the response. Among the endeavors, permutation inference is a popular approach for accessing variable importance; see, for example, \cite{breiman2001random, strobl2007bias}. The methods therein were designed based on the intuition that the importance of a feature can be assessed by checking the change of some appropriately chosen measure before and after randomly permuting some variables, either the feature to be evaluated \cite{strobl2007bias} or the response \cite{breiman2001random}, with the former work focusing on testing the marginal importance of features and the latter one considering both the marginal and conditional importance of features. Both methods output p-values for testing the null hypothesis that a pre-chosen feature is unimportant based on some heuristic arguments without formal theoretical guarantees. Another hypothesis test based approach is the prediction difference test proposed in \cite{liu2012feature}, which assesses the significance of an explanatory feature based on the prediction difference between the full model and the reduced model without using the feature to be tested. There exist only limited theoretical justifications on the proposed tests along this line of work.

The relative feature importance evaluation is a more general framework than the testing approach reviewed above for measuring the feature importance, where the goal is to find out the relative importance of a feature to other features in predicting the response. Yet, relative importance measures are less informative because they do not quantitatively assess the significance of explanatory features as p-values do. Some popularly used random forests feature importance measures include the mean decrease accuracy (MDA) \cite{breiman2001random}, the mean decrease in impurity (MDI) \cite{genuer2010random}, and the conditional permutation importance (CPI) \cite{robin2007perc}. The MDA and CPI are based on the permutation approach, whereas the MDI evaluates a feature by the contributions of all of its associated tree branch splits toward explaining the variation of the response. These intuitive approaches are popularly used for evaluating the relative feature importance for random forests. To name a few recent works along this line, see, e.g., \cite{steyerberg2015validation, zheng2019importance, zheng2019improving, nelissen2019handling, bennett2020estimation}. Although the MDI and MDA may be intuitive, they can suffer from the bias issue toward spurious features when feature dependence is present, as
Table 1: Spurious effects of random forests feature importance measures and the FACT statistic across different model settings from Section 6.4: I) \((n, p, \lambda) = (300, 200, 0.3)\), II) \((n, p, \lambda) = (300, 200, 0.6)\), III) \((n, p, \lambda) = (500, 200, 0.6)\), and IV) \((n, p, \lambda) = (500, 1000, 0.6)\). The correlations between null and relevant features are around 0.15 and 0.7 respectively when \(\lambda = 0.3\) and 0.6. Each entry represents the fraction of times out of 100 simulation repetitions when the feature importance measure for the null feature \(X_{12}\) is larger than those for relevant features \(X_1\) or \(X_{21}\), respectively. The null feature \(X_{12}\) is correlated with the strong linear component \(X_{11}\) in model (28) introduced in Section 6.1. A larger entry in Table 1 suggests a stronger spurious effect and thus means poorer performance of the corresponding measure.

It is seen that when features are independent (setting I), all four measures behave as expected and well. However, when moderate feature dependence is present, the MDI, MDA, and CPI can be seriously biased toward the spurious feature, with the CPI performing slightly better; higher dimensionality adds additional challenges to all three measures. Our FACT statistic, on the other hand, greatly alleviates such a bias issue. We acknowledge that there exist improved versions of the MDI and MDA. However, they are constructed mostly based on heuristics arguments and/or in some specific model settings. Since an important goal of this paper is to provide a theoretically grounded random forests feature importance measure in general model setting, we opt not to exhaustively compare with these extensions.

Let us now formally introduce our FACT method. We approach the problem of random forests feature importance from the hypothesis testing prospective. Such an approach provides us a mathematically rigorous framework for designing a bias-resistant measure and also makes the statistical interpretations unambiguous. Let \(Y \in \mathbb{R}\) be the response of interest and

|         | MDI  | MDA  | CPI  | FACT |
|---------|------|------|------|------|
|         | \(X_1\) \(X_{21}\) | \(X_1\) \(X_{21}\) | \(X_1\) \(X_{21}\) | \(X_1\) \(X_{21}\) |
| I       | 0.04 | 0.07 | 0.06 | 0.11 |
| II      | 0.74 | 0.71 | 0.76 | 0.74 |
| III     | 0.69 | 0.52 | 0.68 | 0.61 |
| IV      | 0.79 | 0.85 | 0.81 | 0.88 |
\( \mathbf{X} = (X_1, \cdots, X_p)^T \in \mathbb{R}^p \) the \( p \)-dimensional feature vector. We evaluate the importance of the \( j \)th feature by formulating a test statistic and calculating the corresponding p-value for the following null hypothesis

\[
H_0: \text{The } j \text{th feature } X_j \text{ is a null feature,}
\]

where our formal definition of null features is given in Definition 1 in Section 3.1 and focuses on the conditional independence of \( X_j \) with respect to response \( Y \) given all remaining features [15, 48]. It will be made clear later that for our testing procedure, the random forests model is fitted and the observed data is assumed to be high-dimensional and have correlated features to cope with the aforementioned practical applications.

One appealing property of random forests is its flexibility in nonparametric modeling. To maintain such flexibility, we do not assume any parametric data generating model in testing (1). We motivate our test from some observations based on the self-normalized correlation between the \( j \)th feature and the random forests residual vector obtained from fitting with the \( j \)th feature removed. Specifically speaking, let independent and identically distributed (i.i.d.) observations of the response and feature vector \( \{(Y_i, \mathbf{X}_i)\}_{i=1}^n \) be given. To gain some insights, let us temporarily assume an errorless model training where the residuals after model training are \( R_i := Y_i - \mathbb{E}(Y_i|\mathbf{X}_{-ij}) \) for all \( i \), with \( \mathbf{X}_{-ij} \) the \( j \)th observation with the \( j \)th feature \( X_{ij} \) excluded. A simple version of the self-normalized correlation is given by

\[
\frac{\sum_{i=1}^n R_i X_{ij}}{\sqrt{\sum_{i=1}^n (R_i X_{ij} - n^{-1} \sum_{i=1}^n R_i X_{ij})^2}}.
\]

Observe that \( R_i X_{ij}, \, i = 1, \cdots, n \), are i.i.d. with \( \mathbb{E}(R_1 X_{1j}) = 0 \) under the null hypothesis (see Definition 1). Hence, with regularity conditions assumed, the asymptotic properties of (2) can be derived. We refer to the above idea as the self-normalized feature-residual correlation test (FACT). We acknowledge that test formed using the intuition in (2) has been explored in different problems; see a review in Section 1.1. Although some works are closely related, to our best knowledge, FACT has not been explored formally in random forests learning and inference for assessing feature importance.

We will suggest three versions of feature statistics, the basic FACT test and two improved versions of the test. The basic FACT test is directly based on the intuition from (2) and can suffer from the bias issue in two sources: 1) the potentially slow nonparametric convergence rates of random forests fitting in estimating \( R_i \) and 2) potentially high correlations among feature \( j \) and other features. To overcome these issues, we introduce two ideas for debiasing, where the first idea uses imbalanced training and inference samples and the second one replaces \( X_{ij} \) in (2) with an estimate of \( \mathbb{E}(X_{ij}|\mathbf{X}_{-ij}) \); we refer to the second idea as the method of conditioning for easy reference in this paper\(^1\). We identify theoretical conditions and prove through nonasymptotic analyses that under these conditions, the basic FACT test and the two improved tests have null distributions close to standard normal when the sample size is large.

\(^1\)Right before we submit this paper, we learned that FACT test with conditioning is closely related to a recently studied method, the generalized covariance measure (GCM) in [47]; see Section 1.1 for a comparison.
size is large, enabling us to calculate the p-values and design rejection regions with valid asymptotic sizes.

The basic FACT test and its two debiased versions focus mostly on the size of the test. To improve the power, we further suggest to incorporate the ensemble idea into the FACT test. Note that (2) remains to enjoy the asymptotic standard normality under the null hypothesis when we replace $X_{ij}$ with a transformation $g(X_{ij})$, where $g$ is some user-chosen transformation function. Motivated by this, we suggest an ensemble test statistic that is given by the maximum of the absolute values of multiple FACT statistics (the basic FACT or its debiased versions), each of which is calculated with its own feature transformation. The resulting statistic is named as the FACT test with ensemble. Finally, we integrate all the ingredients above, including the imbalancing, conditioning, and ensemble, to form our general FACT test. We advocate the use of the general FACT test in practical implementation, for its nice balance between the size and power. For the nonasymptotic power analysis, we first introduce some appropriate signal strength measures, and then show that the power of our general FACT test can approach one as sample size increases under some regularity conditions formulated using our signal strength measures. In practical applications with limited sample size, we suggest the out-of-bag (OOB) implementation of the general FACT test and numerically demonstrate its appealing finite-sample properties.

To demonstrate the finite-sample properties of the suggested FACT tests, we provide simulation studies in Section 6. We also compare the empirical performance of our statistic with the MDI, MDA, and CPI in Section 6.4; the results show that the FACT statistics are much more robust in the presence of correlated features than CPI, and that CPI improves upon MDI and MDA in the same model setting. In Section 7, we demonstrate how to apply the FACT test to macroeconomic data FRED-MD [39] for assessing the significance of a set of macroeconomic variables regarding important responses such as the inflation, interest rate, and unemployment rate. In addition, we showcase how to use the rolling-window p-values to study the effects of time frames on the relevance of features in recent years.

To our best knowledge, our work is the first one to provide a fully comprehensive and theoretically grounded analysis on random forests inference for testing feature importance under general high-dimensional nonparametric model settings. Our theoretical results include 1) the nonasymptotic analysis of null distributions (p-value and size calculations), 2) the nonasymptotic power analysis, and 3) the bias-resistance analysis. The broader problem of high-dimensional conditional independence testing has been studied in the literature. We will provide a review of the relevant works and discuss our contributions in the next section.

1.1 High-dimensional conditional independence testing

High-dimensional conditional independence testing is a broader problem than our formulation in (1). It aims at testing the following null hypothesis

$$H_0 : Z_1 \text{ and } Z_2 \text{ are independent given } Z_3,$$

(3)
where each random vectors $Z_k, k = 1, 2, 3$, can be high-dimensional. It is seen that our formulation (1) is a special case of this problem. The grand problem of high-dimensional conditional independence testing has received increasing attention in recent years; see, e.g., [15, 35, 6, 50, 29, 47, 37, 3] and references therein. In particular, for identifying conditional independence, there exist numerous versions of the conditional randomized test (CRT) [15, 35, 6, 50, 29], feature ordering by conditional independence (FOCI) [3], and generalized covariance measure (GCM) [47, 37]. Among them, the FOCI requires mild dimensionality, and hence is inapplicable to our problem. [29] showed that the test statistic proposed in dCRT [35] is the most powerful CRT test against some semiparametric alternative hypotheses.

Several existing works built their tests based on the similar intuition as (2); for example, the dCRT test [35, 29] and the GCM test [47]. We became aware of the recent work [47] upon finishing the final draft of our paper, and realized that our FACT test with conditioning is a type of their GCM test. [47] provided an in-depth study of problem (3), revealing an interesting and important message that there does not exist a uniformly valid conditional independence test. Thus, tests should be tailored to specific null hypothesis. In particular, they provided a general construction for the conditional independence test, GCM, based on regression procedures, where they regress each univariate $Z_1$ and $Z_2$ on high-dimensional $Z_3$, and form a test based on the covariance of residuals from such regressions. They further established general conditions (not specific to any particular regression method) under which the asymptotic null distribution of the GCM is standard normal, and conducted a power analysis. We compare our results with those in [47] and discuss the connections and differences in various parts of our paper. In particular, one major distinction is that our theoretical results are nonasymptotic, whereas those in [47] are asymptotic. It is also unclear whether the general conditions required in [47] are realistic for random forests.

Existing work provides evidence that a test of form (2) may be useful for our goal in this paper [29, 37, 35]. However, these existing studies have been conducted for generic machine learning methods and are not specific to high-dimensional random forests. The practical random forests inference can be too involved for a direct and primitive application of these existing tests. We will see from the construction of our general FACT test that it is essential to integrate various ideas for achieving the goal of our paper. We will also show that a primitive application of some existing method such as GCM may result in no selection power in a simple regression setting in our power analysis, and that our ensemble idea can improve upon the power (see (24)).

The rest of the paper is organized as follows. Section 2 introduces the model setting and provides a brief overview of high-dimensional random forests consistency. We suggest the framework of the FACT test in different forms for high-dimensional random forests inference of feature importance in Section 3. Section 4 presents the nonasymptotic theory of the FACT test from both perspectives of the size and power. We discuss the comparisons with existing works on random forests feature importance measures in Section 5. Sections 6 and 7 present several simulation and real data examples illustrating the finite-sample performance and utility of our newly suggested method. We discuss some implications and extensions of our work in Section 8. All the proofs and technical details as well as some additional simulation
and real data result are provided in the Supplementary Material.

2 High-dimensional random forests

In this section, we will introduce some necessary technical background on high-dimensional random forests consistency, which will empower the nonasymptotic theory for our framework of the FACT test to be presented in Section 3. Denote by \((\Omega, \mathcal{F}, P)\) the underlying probability space, \(Y\) a scalar response, and \(X := (X_1, \cdots, X_p)^T\) a \(p\)-dimensional random feature vector taking values in the unit hypercube \([0, 1]^p\). Assume that we are given an inference sample of independent and identically distributed (i.i.d.) observations \(\{(X_i, Y_i)\}_{i=1}^n\), where \(X_i := (X_{i1}, \cdots, X_{ip})^T\), \((X_i, Y_i)\) and \((X, Y)\) have the same distribution, and \((X, Y)\) is independent of all the observations. Further, assume that we have an independent training sample \(X_0 = \{(U_i, V_i)\}_{i=1}^N\) from the same distribution as \((X, Y)\), where \(U_i = (U_{i1}, \cdots, U_{ip})^T\).

Throughout the paper, we consider a single null hypothesis (1) where \(1 \leq j \leq p\) is a pre-chosen covariate index and is fixed over the inference procedure. As mentioned in the Introduction, we will construct random forests estimate of \(E(Y|X_{-j})\) for testing null hypotheses (1), where \(X_{-j} := (X_1, \cdots, X_{j-1}, X_{j+1}, \cdots, X_p)^T\). As shown in Section 3, the inference sample of size \(n\) will be used for calculating the FACT statistics, while the training sample \(X_0\) of size \(N\) will be employed for constructing the underlying random forests estimates. Denote by \(\hat{Y}(X_{-j})\) the random forests estimate of \(E(Y|X_{-j})\) constructed using the independent training sample \(\{(U_{-ij}, V_i)\}_{i=1}^N\), where \(U_{-ij} := (U_{i1}, \cdots, U_{i,j-1}, U_{i,j+1}, \cdots, U_{ip})\). To ensure valid statistical inference using the random forests estimates, we introduce a regularity condition on the random forests consistency in the high-dimensional nonparametric regression setting, and will assume that it holds throughout the paper.

**Condition 1.** Assume that \(E[|E(Y|X_{-j}) - \hat{Y}(X_{-j})|^2] \leq B_1\) for some small \(B_1 > 0\).

There is a growing recent literature on the random forests consistency, which amounts to Condition 1 with null \(X_j\) (see Definition 1 in Section 3.1) and consistency rate \(B_1 = o(1)\) depending on the training sample size \(N\). For example, [46, 17, 49, 31] established the \(L^2\)-consistency of random forests with decision trees grown by the original Breiman’s classification and regression tree (CART) splitting criterion [11, 12] under various settings of the nonparametric regression model

\[
Y = m(X) + \varepsilon, \tag{4}
\]

where \(m(\cdot)\) represents the underlying true regression function and \(\varepsilon\) is the model error that is independent of feature vector \(X\) and has mean zero and finite variance. In particular, by assuming that the true regression function \(m(\cdot)\) and the distribution of feature vector \(X\) satisfy a condition called the sufficient impurity decrease (SID), [17] obtained the high-dimensional random forests consistency rates in a general nonparametric model setting, which ensure that Condition 1 holds with consistency rate \(B_1 = O(N^{-c})\) and feature dimensionality \(p = O(N^{K_0})\) for some constants \(c, K_0 > 0\), allowing for dependent features.
For completeness, let us briefly review the SID condition introduced in [17] below.

**Condition A1. (SID in [17])** Assume that there exists some \( \alpha_1 \geq 1 \) such that for each cell \( t \subset [0,1]^p \), we have

\[
\alpha_1^{-1} \text{Var}(m(X)|X \in t) \leq \text{Var}(m(X)|X \in t) - \inf_{j,x} \left\{ \mathbb{P}(X \in t_1|X \in t)\text{Var}(m(X)|X \in t_1) + \mathbb{P}(X \in t_2|X \in t)\text{Var}(m(X)|X \in t_2) \right\},
\]

where \( t_1 \) and \( t_2 \) represent the two daughter cells of \( t \) after the split \((j,x)\) along feature \( X_j \) and feature value \( x \in \mathbb{R} \), and the infimum is taken over all possible feature and split value combinations \((j,x)\).

In fact, the minimization problem

\[
\inf_{j,x} \left\{ \mathbb{P}(X \in t_1|X \in t)\text{Var}(m(X)|X \in t_1) + \mathbb{P}(X \in t_2|X \in t)\text{Var}(m(X)|X \in t_2) \right\}
\]

on the right-hand side of the inequality in Condition A1 above is the theoretical CART splitting criterion [45, 46, 17], which aims at finding the best split pair \((j,x)\) for minimizing the conditional variance on the cell. Intuitively, the SID condition requires that for each cell in the feature space (i.e., a hyperrectangle that is also referred to as a node or leaf), the conditional impurity decrease on this cell after a CART split, which is the quantity on the right-hand side of the inequality above, is at least in proportion to the total conditional variance on this cell. See [17] for detailed examples of nonparametric regression models that are shown to satisfy the SID condition. In particular, the polynomial growth rate of feature dimensionality \( p = O(N^{K_0}) \) with some constant \( K_0 > 0 \) can suffice for many real applications. In addition to the aforementioned works, the consistency of many variants of random forests has also been investigated in the recent literature. These variants usually consider models of decision trees that are grown by certain splitting protocols other than the original CART criterion; see, e.g., [46, 17, 9] for detailed overviews. Meanwhile, for the proposed test statistics to be useful, it is required that \( B_1 \) should be asymptotically negligible as the inference sample size \( n \) grows, which implicitly requires that \( N \) grows with \( n \). See Sections 3–4 for details of the technical requirements on \( N,n \) and the consistency rates.

## 3 FACT for high-dimensional random forests inference

In this section, we introduce the main ideas for the FACT framework for high-dimensional random forests inference of feature importance. Specifically, we will propose the basic FACT test and the general FACT test incorporating the ideas of imbalancing, conditioning, and ensemble for debiasing and power enhancement. Hereafter, let \( \Phi(\cdot) \) and \( \Phi^{-1}(\cdot) \) denote respectively the cumulative distribution function of the standard Gaussian distribution and its inverse function, and \( |L| \) be the cardinality of a set \( L \).
3.1 The basic FACT test

Let us begin with presenting the basic FACT test. Recall that \(1 \leq j \leq p\) is a pre-chosen covariate index that is fixed over the inference procedure. Due to the fully nonparametric nature of the random forests model, we adopt the conditional independence definition of the null features below.

**Definition 1.** The \(j\)th feature \(X_j\) is said to be a null feature if \(X_j\) is conditionally independent of response \(Y\) given all remaining features \(X_{-j}\).

Definition 1 above indicates that a null feature \(X_j\) is indeed redundant with respect to the conditional distribution of the response given the feature vector. Correspondingly, each non-null feature will be referred to as an important or relevant feature throughout the paper.

To illustrate the underlying rationale of the basic FACT test, let us consider the population version of an intuitive feature statistic for each feature \(X_j\) given by

\[
n^{-\frac{1}{2}} \sum_{i=1}^{n} \left[ Y_i - m(X_{-ij}) \right] \frac{\{g(X_{ij}) - \mathbb{E}g(X_j)\}}{\sigma_{j0}},
\]

where \(m(X_{-ij})\) denotes a version of the conditional mean \(\mathbb{E}(Y_i|X_{-ij})\) at the population level, \(g(\cdot)\) is some measurable feature transformation that is specified by the user with the identity function \(g(x) = x\) as the default, and \(\sigma^2_{j0} := \text{Var}\{[Y - \mathbb{E}(Y|X_{-j})][g(X_j) - \mathbb{E}g(X_j)]\}\).

Provided that the population objects \(m(\cdot), \sigma_{j0}, \text{and } \mathbb{E}g(X_j)\) were known to us, one could easily implement the feature statistic in (5) and establish its asymptotic standard normality under the null hypothesis (1) with Definition 1 and certain regularity conditions. This is because \(\mathbb{E}\{[Y - \mathbb{E}(Y|X_{-j})][g(X_j) - \mathbb{E}g(X_j)]\} = 0\) under the null and the observations are i.i.d. by assumption.

Meanwhile, it is easy to see that the absolute value of the statistic (5) approaches \(\infty\) in probability as the sample size \(n\) increases when feature \(X_j\) is relevant with \(\mathbb{E}\{[Y - \mathbb{E}(Y|X_{-j})][g(X_j) - \mathbb{E}g(X_j)]\} > c\) for some \(c > 0\) (it is allowed that \(c = c_n \rightarrow 0\) as \(n \rightarrow \infty\); see Section 4.2 for detailed requirement on \(c_n\)). This is because in such a case, the transformed feature \(g(X_j)\) cannot be replaced by the remaining features \(X_{-j}\) in terms of the prediction for response \(Y\). Thus, the feature statistic introduced in (5) can provide a natural starting point for constructing a nonparametric test statistic for testing the null hypothesis (1) that enjoys the appealing asymptotic standard normality under the null hypothesis. The selection power of such a test with respect to relevant features will naturally depend on the underlying nonparametric model setting and the specific choice of feature transformation \(g(\cdot)\).

Yet the ideal version of the feature statistic introduced in (5) cannot be utilized in practice since the population objects \(m(\cdot), \sigma_{j0}, \text{and } \mathbb{E}g(X_j)\) are not immediately available to us. Thus, we suggest below the basic FACT test statistic for the null hypothesis (1)

\[
\text{FACT}_{j0} := n^{-\frac{1}{2}} \sum_{i=1}^{n} \left[ Y_i - \hat{Y}(X_{-ij}) \right] \frac{\{g(X_{ij}) - \mathbb{E}g(X_j)\}}{\hat{\sigma}_{j0}},
\]

where \(\hat{Y}(X_{-j})\) (as in Condition 1) denotes the random forests estimate for the conditional
mean $\mathbb{E}(Y|\mathbf{X}_{-j})$, $\hat{\sigma}_{j0}^2 = n^{-1} \sum_{i=1}^n (d_{i1} - n^{-1} \sum_{i=1}^n d_{i1})^2$, and $d_{i1} = |Y_i - \hat{Y}(\mathbf{X}_{ij})| |g(X_{ij}) - \mathbb{E}g(X_j)|$. We see that the basic FACT test statistic introduced in (6) implements the ideal version of the feature statistic in (5) using the corresponding random forests and empirical estimates of the population counterparts. In particular, the specific form of the test statistic in (6) has motivated the name of the self-normalized feature-residual correlation test (FACT). As mentioned in Section 2, the use of the random forests estimate makes our testing method applicable to high-dimensional nonparametric settings, where the feature dimensionality $p$ can exceed the sample size $n$. Moreover, the term “basic” is employed here to emphasize that the simple test statistic in (6) is just a vanilla version of the family of FACT statistics to be introduced later in this section.

It is worth mentioning that the random forests estimate $\hat{Y}$ is typically constructed based on an independent training sample $\mathcal{X}_0$ of size $N$ in order to avoid the dependence of $\hat{Y}$ on the inference sample of size $n$ used in (6). We will discuss in Section 3.5 that the sample splitting or the out-of-bag (OOB) estimation can be exploited for constructing the random forests estimate $\hat{Y}$ when only a single sample is available in practice.

The rejection criterion for the basic FACT test is given as follows: for each given test threshold $t > 0$,

$$\text{we reject the null hypothesis } H_0 \text{ in (1) if } |\text{FACT}_{j,0}| > t,$$

(7)

where the basic FACT test statistic $\text{FACT}_{j,0}$ is given in (6). Thanks to our hypothesis test formulation (1), our result is highly interpretable for characterizing the random forests feature significance. Let $\alpha \in (0, 1)$ be the predetermined desired size. Under the null hypothesis (1) and certain regularity conditions, we will establish in Theorem 1 in Section 4 that with the threshold (i.e., critical value) $t = -\Phi^{-1}(\alpha/2)$, the asymptotic size of the basic FACT test in (7) is at most $\alpha$. For a particular realization of data and its associated value of test statistic $\text{FACT}_{j,0}$, we calculate the p-value utilizing the frequentist’s repeated sampling interpretation. By the same result in Theorem 1, a conservative estimate of the p-value corresponding to the given realization $\text{FACT}_{j,0}$ is $2\Phi(-|\text{FACT}_{j,0}|)$.

3.2 FACT tests via debiasing

The basic form of the FACT test in (7) can be biased unless the features are independent of each other. To gain some insights into the bias issue, assume that $\mathbb{E}g(X_j)$ is known for simplicity. Then the bias of the basic FACT test statistic in (6) under the null hypothesis is given by

$$\text{Bias}_1(N) := \mathbb{E}\left\{ n^{-\frac{1}{2}} \sum_{i=1}^n \left[Y_i - \hat{Y}(\mathbf{X}_{-ij})\right] \left[g(X_{ij}) - \mathbb{E}g(X_j)\right] \right\}$$

$$= \sqrt{n}\mathbb{E}\left\{ \mathbb{E}[Y|\mathbf{X}_{-j}] - \hat{Y}(\mathbf{X}_{-j}) \right\} \left[g(X_j) - \mathbb{E}g(X_j)\right]$$

up to a bounded factor $(\hat{\sigma}_{j0})^{-1}$ in a probabilistic sense. Here, recall that $N$ is the size of independent training sample $\mathcal{X}_0$ for constructing $\hat{Y}(\cdot)$. If $X_j$ is independent of $\mathbf{X}_{-j}$, then it

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is seen that $\text{Bias}_1(N) = 0$, implying that the bias is a result of the feature correlation.

Now, let us assume that Condition 1 holds and $\sup_{x \in [0,1]} |g(x)|$ is bounded. Simple calculations show that

$$\text{Bias}_1(N) \leq 2 \sup_{x \in [0,1]} |g(x)| \sqrt{B_1 n},$$

(8)

where $B_1$ is as in Condition 1. Assuming $N \sim n$, from the above upper bound, $\text{Bias}_1(N)$ of the basic FACT test statistic may not be asymptotically negligible in general because the training sample size is assumed to be $n$ here, leading to the random forests consistency rate $B_1$ much slower than $n^{-1}$ (the parametric rate). In Section 6, we will demonstrate through simulation examples that the bias due to correlated features can make the center of the empirical distribution of the basic FACT statistic $\text{FACT}_{j,0}$ shift away from zero compared to the desired standard Gaussian distribution. We next exploit two ideas of debiasing to alleviate the bias issue of the basic FACT statistic.

### 3.2.1 FACT test with imbalancing

The observation in (8) motivates a natural idea of debiasing with imbalancing that employs a relatively larger independent training sample $X_0$ of size $N$ for the construction of the random forests estimate $\hat{Y}(X_{-j})$ and a relatively smaller inference sample of size $n$ for constructing the test statistic. When $N$ with $N \gg n$ is sufficiently large, the random forests consistency rate $B_1$ may become asymptotically negligible compared to $n^{-1}$. We demonstrate empirically in Section 6 that the choice of $n = O((\log N)^{-1} N)$ can lead to appealing finite-sample performance of the FACT test incorporating the imbalancing idea. In addition, the theoretical requirements on $n$ and $N$ are discussed in Remark 4 in Section 4.

Let us define the FACT test statistic with imbalancing for each feature $X_j$ as

$$\text{FACT}_{jN/n} = \text{FACT}_{j,0} \text{ with } \hat{\sigma}_{jN/n} = \hat{\sigma}_{j0},$$

(9)

where we explicitly write out the training/inference split “$N/n$” to emphasize the use of imbalanced samples with $n = o(N)$, and all the notation is the same as in (6). The testing procedure with the test statistic (9) is given as follows: for each given test threshold $t > 0$,

$$\text{we reject the null hypothesis } H_0 \text{ in (1) if } |\text{FACT}_{jN/n}| > t.$$

(10)

Under the null hypothesis (1) and certain regularity conditions, Theorem 2 in Section 4 shows that with the threshold $t = -\Phi^{-1}(\alpha/2)$, the asymptotic size of the FACT test with imbalancing in (10) is at most $\alpha$, and for a given realization of the test statistic $\text{FACT}_{jN/n}$, the p-value can be conservatively estimated as $2\Phi(-|\text{FACT}_{jN/n}|)$.

As shown in Theorem 2, the debiasing idea of imbalancing can indeed relax the stringent assumption of zero bias that is needed for the asymptotic theory of the basic FACT test. We also provide simulation results showing how the imbalancing idea can help alleviate the bias issue empirically.
3.2.2 FACT test with conditioning

Let us turn to the second idea of debiasing with conditioning. Formally, we define the FACT test statistic with conditioning for each feature $X_j$ as

$$ \text{FACT}_{j|X_{-j}} := n^{-\frac{1}{2}} \sum_{i=1}^{n} \frac{Y_i - \hat{Y}(X_{-ij}) - g(X_{ij}) + \hat{g}(X_{-ij})}{\hat{\sigma}_{j|X_{-j}}}, $$

(11)

where $\hat{Y}(X_{-ij})$ and $\hat{g}(X_{-ij})$ are the random forests estimates of the conditional means $E(Y|X_{-j})$ and $E\{g(X_j)|X_{-j}\}$, respectively, that are constructed based on a common independent training sample $X_0$ of size $N$, $\hat{\sigma}_{j|X_{-j}}^2 = n^{-1} \sum_{i=1}^{n} (d_{ij} - n^{-1} \sum_{i=1}^{n} d_{ij})^2$, and $d_{ij} = [Y_i - \hat{Y}(X_{-ij})] [g(X_{ij}) - \hat{g}(X_{-ij})]$. Observe that the FACT test statistic with conditioning suggested in (11) is similar to the basic FACT test statistic in (6), but with the empirical average $n^{-1} \sum_{i=1}^{n} g(X_{ij})$ replaced by the random forests estimate $\hat{g}(X_{-j})$. In particular, we use the subscript “$|X_{-j}$” to stress the idea of debiasing with conditioning. We acknowledge that (11) is a type of GCM test in [47]. We provide more discussions on the connections and differences of our conditions and results with those in [47] in Section 4.

The testing procedure with the conditioning version of the FACT statistic (11) is given as follows: for each given test threshold $t > 0$,

$$ \text{we reject the null hypothesis } H_0 \text{ in (1) if } |\text{FACT}_{j|X_{-j}}| > t. $$

(12)

Under the null hypothesis (1) and certain regularity conditions, we will show in Theorem 3 in Section 4.1 that conservative estimates of the asymptotic size and asymptotic p-value are $2\Phi(-t)$ and $2\Phi(-|\text{FACT}_{j|X_{-j}}|)$, respectively, for the testing procedure (12).

Let us gain some insights into the above idea of debiasing with conditioning. For each null feature $X_j$, the bias of the FACT test statistic with conditioning in (11) under the null hypothesis is given by

$$ \text{Bias}_2(N) := E \left\{ n^{-\frac{1}{2}} \sum_{i=1}^{n} [Y_i - \hat{Y}(X_{-ij})] [g(X_{ij}) - \hat{g}(X_{-ij})] \right\} $$

$$ = \sqrt{n} \left\{ E(Y|X_{-j}) - \hat{Y}(X_{-j}) \right\} \left\{ E(g(X_j)|X_{-j}) - \hat{g}(X_{-j}) \right\} $$

up to a bounded factor $(\hat{\sigma}_{j|X_{-j}})^{-1}$ in a probabilistic sense. Provided that Condition 1 holds and $\hat{g}(X_{-j})$ admits the same consistency rate as $\hat{Y}(X_{-j})$ in Condition 1, we have $\text{Bias}_2(N) \leq \sqrt{n} B_1$, which is obviously a smaller upper bound compared to (8). See the comments after Condition 4 in Section 4.1 for details. Such an intuition will also be justified empirically later in Section 6.

3.3 FACT test with ensemble

In view of the definitions for the basic FACT test statistic, the FACT test statistic with imbalancing, and the FACT test statistic with conditioning in (6), (9), and (11), respectively, we can potentially improve the selection power of these tests through multiple choices of
measurable feature transformation $g(\cdot)$. Specifically, denote by $g^{(l)}(\cdot)$ different measurable feature transformations with $l \in L := \{1, \ldots, m_1\}$ for some fixed positive integer $m_1$. Then we can define the FACT test statistic with ensemble for each feature $X_j$ as

$$\max_{l \in L} \left| \text{FACT}^{(l)}_j \right|,$$

where each $\text{FACT}^{(l)}_j$ for feature transformation $g^{(l)}(\cdot)$ with $l \in L$ is given as in (6) by

$$\text{FACT}^{(l)}_j := n^{-\frac{1}{2}} \sum_{i=1}^n \frac{Y_i - \hat{\Phi}(X_{-ij}) [g^{(l)}(X_{ij}) - n^{-1} \sum_{i=1}^n g^{(l)}(X_{ij})] \hat{\sigma}^{(l)}_j}{\sqrt{\sum_{i=1}^n (d_{i3} - n^{-1} \sum_{i=1}^n d_{i3})^2}},$$

$$\hat{\sigma}^{(l)}_j = n^{-1} \sum_{i=1}^n (d_{i3} - n^{-1} \sum_{i=1}^n d_{i3})^2, \quad d_{i3} = (Y_i - \hat{\Phi}(X_{-ij})) [g^{(l)}(X_{ij}) - n^{-1} \sum_{i=1}^n g^{(l)}(X_{ij})].$$

For the FACT test with ensemble in (13), with each given test threshold $t > 0$,

we reject the null hypothesis $H_0$ in (1) if

$$\max_{l \in L} \left| \text{FACT}^{(l)}_j \right| > t.$$  

(14)

Under the null hypothesis (1) and certain regularity conditions, Theorem 4 in Section 4 will establish that with threshold $t = -\Phi^{-1}(\alpha/(2|L|))$, the asymptotic size of the FACT test with ensemble in (14) is at most $\alpha$, and the asymptotic p-value for a given realization of the test statistic $\max_{l \in L} |\text{FACT}^{(l)}_j|$ can be conservatively estimated as $\min \{1, 2|L|\Phi(\max_{l \in L} |\text{FACT}^{(l)}_j|)\}$. In Section 4.2.2, the selection power enhancement of the FACT test with ensemble over the basic FACT test will be demonstrated formally under a nonparametric additive model; see Section 4.2 for details.

### 3.4 The general FACT test

We are now ready to introduce our general FACT test framework by incorporating the ideas of imbalancing and conditioning for debiasing and the idea of ensemble for enhanced power presented in Sections 3.2 and 3.3, respectively. Let $\{(X_i, Y_i)\}_{i=1}^n$ be an inference sample of i.i.d. observations and $X_0 = \{(U_i, V_i)\}_{i=1}^N$ with $N = n$ be its independent copy of the training sample. To simplify the technical presentation, we will focus on the set $L = \{1, 2\}$ of two simple feature transformations: the linear transformation $g^{(1)}(X_{ij}) = X_{ij}$ and the square transformation $g^{(2)}(X_{ij}) = X_{ij}^2$ or $(X_{ij} - n^{-1} \sum_{i=1}^n X_{ij})^2$, where the former form of the square transformation will be used for a more concise technical analysis and the latter one is commonly utilized for practical implementation. Denote by $\hat{\Phi}(X_{-j})$ and $\tilde{g}^{(l)}(X_{-j})$ the random forests estimates of the conditional means $\mathbb{E}(Y|X_{-j})$ and $\mathbb{E}(g^{(l)}(X_j)|X_{-j})$, respectively, that are constructed based on the independent training sample $X_0 = \{(U_i, V_i)\}_{i=1}^n$. Specifically, we apply random forests to the training data sets $\{(U_{-ij}, V_i)\}_{i=1}^n$ and $\{(U_{-ij}, g^{(l)}(U_{ij}))\}_{i=1}^n$ for the construction of estimates $\hat{\Phi}(\cdot)$ and $\tilde{g}^{(l)}(\cdot)$, respectively.

Let us define the general FACT test statistic for each feature $X_j$ as

$$\text{FACT}_j := \max_{l \in L, q \in Q} \left| \text{FACT}^{(l)}_{j,q} \right|,$$

(15)
where
\[
\text{FACT}_{j,q}^{(l)} := \sum_{i \in \mathcal{N}_q} \frac{[Y_i - \hat{Y}(X_{-ij})] [g^{(l)}(X_{ij}) - \hat{g}^{(l)}(X_{-ij})]}{|\mathcal{N}_q|^{1/2} \hat{\sigma}_{j,x}^{(l)}}
\]
for each \( l \in L, Q = \{1, \cdots, k_n\} \) with some slowly diverging \( k_n \). Here, \( \{\mathcal{N}_1, \cdots, \mathcal{N}_{k_n}\} \) is a random partition of set \( \{1, \cdots, n\} \) such that \( \sup_{k,l} ||\mathcal{N}_k| - |\mathcal{N}_l|| \leq 1, (\hat{\sigma}_{j,x}^{(l)})^2 = n^{-1} \sum_{i=1}^n (d_{ij} - n^{-1} \sum_{i=1}^n d_{ij}^2)^2 \), and \( d_{ij}^2 = [Y_i - \hat{Y}(X_{-ij})] [g^{(l)}(X_{ij}) - \hat{g}^{(l)}(X_{-ij})] \). Note that \((\hat{\sigma}_{j,x}^{(l)}))^2\) differs from \(\hat{\sigma}_{j,x}^2\) defined in (11) only in the use of \(\hat{g}^{(l)}()\) instead of \(\hat{g}()\). In light of (15), the imbalancing idea is exploited in the general FACT test statistic since each test statistic \(\text{FACT}_{j,q}^{(l)}\) above is constructed using the inference sample \(\mathcal{N}_q\) that satisfies \(|\mathcal{N}_q| = n/k_n = o(n)\) relative to the training sample size \(n\) (with a slight change of notation here) by assumption.

We see that the ideas of conditioning and ensemble are also exploited in the general FACT test statistic, as reflected in the use of \(\hat{g}^{(l)}()\) and \(g^{(l)}()\). As shown later in the simulation examples in Section 6, the choice of \(k_n = O(\log n)\) can be utilized for the practical implementation of the imbalancing idea, and the maximization over \(q \in Q\) in (15) can further boost the selection power of the test.

Formally, for each given test threshold \( t > 0 \), the testing procedure with the general FACT statistic (15) is that

we reject the null hypothesis \( H_0 \) in (1) if \( \text{FACT}_{j} > t \).  \hspace{1cm} (16)

Under the null hypothesis (1) and certain regularity conditions, we will establish in Theorem 5 in Section 4 that for large enough \( n \), if \( k_n = O(\log n) \) and test threshold \( t = \Phi^{-1}(\alpha/(4|Q|)) \), the asymptotic size of the general FACT test in (16) is at most \( \alpha \). For a given realization of the test statistic FACT, the associated p-value can estimated conservatively as \( \min \{1, 4|Q|\Phi(-\text{FACT}_{j})\} \) asymptotically. A formal power analysis for the general FACT test will be provided in Section 4.2.

**Remark 1.** We also explored the average version of the general FACT test, where we replace the maximum of \( |\text{FACT}_{j,q}^{(l)}| \) over \( q \) in (15) with the average. Our numerical results suggest that this approach is overly conservative with almost zero empirical sizes and very low powers in various settings.

### 3.5 Random forests out-of-bag estimation

Let us introduce the out-of-bag (OOB) prediction as a practical alternative to sample splitting. Suppose there are \( K \) trees in the random forests. For each \( k = 1, \cdots, K \), denote by \( a_k \subset \{1, \cdots, n\} \) the random subsamples used for training the \( k \)th decision tree. For each observation indexed by \( i = 1, \cdots, n \), let \( A(i) \subset \{1, \cdots, K\} \) be the set such that \( i \notin a_k \) for each \( k \in A(i) \). This means that for each \( 1 \leq i \leq n \), the set \( A(i) \) contains all the decision trees grown without using the \( i \)th observation. Naturally, the OOB prediction for the \( i \)th observation is the empirical average of predicted values given by all decision trees from set \( A(i) \). Thus, the OOB estimate is intended to disentangle the dependency between the training and the inference data points, making OOB an alternative to sample splitting. With sufficiently
many trees in the random forests models, the OOB estimates can provide more reproducible results by avoiding sample splitting.

All the test statistics in the FACT family can be implemented with the option of the OOB introduced above. To calculate the general FACT test statistic $\text{FACT}_j$ for each feature $X_j$ in (15) with the OOB, we can simply replace the corresponding random forests estimates with their OOB counterparts, which will make the independent training sample $X_0$ no longer needed for the resulting testing procedure. Specifically, we can apply random forests with the OOB to the data sets $\{(X_{-ij}, Y_i)\}_{i=1}^n$ and $\{(X_{-ij}, g^{(l)}(X_{ij}))\}_{i=1}^n$ for the construction of the OOB version of the random forests estimates $\hat{Y}(X_{-ij})$ and $\hat{g}^{(l)}(X_{-ij})$, respectively. We will demonstrate through simulation examples in Section 6 that each FACT test statistic $\text{FACT}_{j,q}$ in (15) with the OOB also enjoys asymptotic standard normality, the empirical size is close to the desired one, and the p-value is close to the theoretical p-value of the general FACT test with sample splitting, which is

$$\min \left\{ 1, \frac{4}{9} \right\} \mathbb{Q} \left( \Phi ( -\text{FACT}_j ) \right). \quad (17)$$

## 4 Nonasymptotic theory of FACT

In this section, we will establish a rigorous theoretical foundation for the basic and the general FACT tests for random forests inference in the high-dimensional nonparametric setting from both perspectives of the size and power through nonasymptotic analyses.

### 4.1 The FACT p-values and sizes

To facilitate our technical analysis, let us first introduce some necessary regularity conditions below. Recall that $g(\cdot)$ is a measurable function and $\hat{Y}(X_{-j})$ is the random forests estimate of $\mathbb{E}(Y|X_{-j})$; all notation is the same as in Sections 2–3.

**Condition 2.** Assume that $
\mathbb{E} \left\{ \left[ \mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j}) \right] \left[ g(X_j) - \mathbb{E}(g(X_j)) \right] \bigg| X_0 \right\} = 0 \quad \text{almost surely.} \n$

**Condition 3.** Assume that the measurable transformation $g(\cdot)$ is bounded between 0 and 1 on its domain. In addition, assume that $\text{Var}(g(X_j)|X_{-j}) \geq \varsigma_1$, $\text{Var}(Y|X) \geq \varsigma_2$, and $\text{Var}(Y|X_{-j}) \leq D$ almost surely, and that $\mathbb{E}Y^4 \leq D_2$ for some constants $\varsigma_1, \varsigma_2, D, D_2 > 0$.

In addition to Conditions 2–3, Theorem 1 below also requires Condition 1, which assumes a high-dimensional consistency rate $B_1$ for the random forests estimate. See Section 2 for how the consistency rate $B_1$ depends on the training sample size $N$, and how Condition 1 places some implicit constraints on the underlying distributions of the feature vector and the growth of feature dimensionality in the nonparametric model setting. The zero correlation assumption in Condition 2 is required to rule out the bias of the basic FACT test statistic; this assumption is unrealistic at the presence of correlated features, as discussed in Section 3.2. Hence, we introduce the techniques of imbalanced samples and conditioning as ways of debiasing for the FACT statistics in Section 3.2. We will see in Theorems 2–3 and
later that Condition 2 is not needed for a formal analysis of the debiased FACT tests and the general FACT test. Condition 3 is used to obtain the universal lower and upper bounds for the population variances of the proposed statistics; see Lemma 3 in Section B.7 of the Supplementary Material and each of the proofs for Theorems 1–5 for details. The assumption of upper and lower bounds for $g(\cdot)$ in Condition 3 is a basic assumption and these bounds can be replaced with some arbitrary constants $M_1 < M_2$, respectively.

**Theorem 1.** For all large $n$, each consistency rate $0 < B_1 < 1$, and any $1 \leq j \leq p$ such that 1) Conditions 1–3 hold, 2) the random forests estimate $\hat{Y}(X_{-j})$ is constructed based on the independent training sample $X_0$, and 3) $X_j$ is a null feature, it holds that for each $t \in \mathbb{R}$,

$$
\Pr(\text{FACT}_{j,0} \leq t) \leq \Phi(t) + \frac{4c}{5\sqrt{2}\varsigma_1} + (\log n)(B_1^{1/4} + n^{-1/4}),
$$

and for each $t > 0$,

$$
\Pr(|\text{FACT}_{j,0}| > t) \leq 2\Phi(-t) + \frac{8c}{5\sqrt{2}\varsigma_1} + 2(\log n)(B_1^{1/4} + n^{-1/4}),
$$

where $\text{FACT}_{j,0}$ is the basic FACT statistic defined in (6), $c = (\log n)(2B_1^{1/4} + n^{-1/4}\log n)(1 + |t|)$, and recall that $\varsigma_1$ and $\varsigma_2$ are given in Condition 3.

The results in Theorem 1 are nonasymptotic and hold for all large $n$. The value of $t$ is independent of $n$ and $p$, and $B_1$ is required to converge to zero as $n$ grows for the null distribution to be close to standard normal. We see from (18) of Theorem 1 that under the null hypothesis in (1), with the prespecified threshold $t = -\Phi^{-1}(\alpha/2)$, the asymptotic size of the basic FACT test defined in (7) is at most $\alpha$ if $B_1^{1/4} = o(1/\log n)$. Such a consistency rate is justified if, for example, we split the sample in half (i.e., $N = n$) and $B_1 = O(N^{-c})$ for some positive constant $c$. As discussed previously in Section 2, this polynomial consistency rate has been theoretically proved for high-dimensional random forests. Similarly, it can be seen that the asymptotic p-value for the basic FACT test in (7) can be conservatively estimated by $2\Phi(-|\text{FACT}_{j,0}|)$. Hereafter, we may omit the term “asymptotic” associated with the FACT p-values whenever there is no confusion.

Let us make some useful observations related to Theorem 1. First, in light of (18), both training sample size $N$ and feature dimensionality $p$ affect implicitly the probability bounds for the basic FACT test only through the asymptotically shrinking term $B_1$. Second, since the technical analysis for the basic FACT test with the OOB option can be rather involved, we will only empirically demonstrate the performance of the basic FACT test and the general FACT test implemented with the OOB later in Section 6. These results show that their finite-sample properties are similar to those of their non-OOB counterparts. Moreover, it is worth mentioning that the p-values and sizes in our paper are conservative (in the asymptotic sense) because our main theoretical results provide the probability upper bounds instead of exact probabilities.

**Remark 2.** In light of the results in Theorem 1, the nonasymptotic p-value and size of the basic FACT test given in (7) should involve both inference sample size $n$ and random forests.
consistency rate $B_1$. For practical implementation, we consider the asymptotic p-value and asymptotic size of the FACT test that are free of $n$ and $B_1$.

**Remark 3.** Theorem 1 requires that $j$ is prechosen and fixed in the high-dimensional setting where feature dimensionality $p$ can be much larger than the training and inference sample sizes. It does not provide a direct theoretical guarantee for large-scale multiple hypothesis tests where a diverging number of test statistics $\text{FACT}_{j,0}$’s are considered. The same remark applies to Theorems 2–7.

**Theorem 2.** For all large $n$, each consistency rate $0 < B_1 < 1$, each $t > 0$, and any $1 \leq j \leq p$ such that 1) Conditions 1 and 3 hold, 2) the random forests estimate $\hat{Y}(X_{-j})$ is constructed based on the independent training sample $X_0$, and 3) $X_j$ is a null feature, it holds that

$$
P\left( |\text{FACT}_{j,N/n}| > t \right) \leq 2\Phi(-t) + \frac{8c}{\sqrt{nB_1}} + (\log n) (B_1^{1/4} + n^{-1/4}) + (-\log B_1)^{-1},$$

where $\text{FACT}_{j,N/n}$ is the imbalancing form of the FACT statistic defined in (9) and $c = (\log n) (2B_1^{1/4} + n^{-1/4} \log n)(1 + t) + \sqrt{nB_1}(-\log B_1)$.

Theorem 2 above analyzes the FACT test with imbalancing defined in (10) under the null. In contrast to Theorem 1, Theorem 2 does not require Condition 2, an assumption that could be stringent for dependent features. Instead, for the test based on FACT$_{j,N/n}$ to be nontrivial we only need $\sqrt{nB_1}(-\log B_1) = o(1)$, which implicitly requires that $n = o(N)$ since $B_1$ generally converges to zero at a slower rate than the parametric rate of $O(N^{-1})$. See Remark 4 below for more details about the order of the inference sample size $n$ relative to the training sample size $N$. This demonstrates that the bias issue mentioned in Section 3.2 can be addressed asymptotically by the imbalancing idea without imposing the stringent assumption of Condition 2. This also improves upon MDA and MDI since both measures can be biased toward spurious features [48, 24, 42].

**Remark 4.** The theoretically grounded choice of the inference sample size $n$ can be restrictive according to Theorem 2. To understand this, let us assume, for example, that the random forests estimate $\hat{Y}$ is consistent with a rate of $B_1 = O(N^{-r})$ for some constant $0 < r \leq 1$. Then to ensure a nontrivial test, we need $n = o(N^r (\log N)^{-1})$ for achieving $\sqrt{nB_1}(-\log B_1) = o(1)$. However, our empirical experience suggests that a far less restrictive requirement on $N$ can perform reasonably well in practice. In fact, as illustrated in the simulation examples in Section 6, the empirical choice of $n = O\{(\log N)^{-1}N\}$ can already largely ease the bias issue.

Theorem 3 below analyzes the FACT test with conditioning defined in (12) under the null hypothesis. For the technical analysis of Theorem 3, we need Condition 4, which is similar to Condition 1 in Section 2. All notation is the same as in Section 3.2.2.

**Condition 4.** Assume that $E\{E(g(X_j)|X_{-j}) - \tilde{g}(X_{-j})\}^2 \leq B_2$ for some small $B_2 > 0$.

**Theorem 3.** For all large $n$, each $t > 0$, all consistency rates $0 < B_1, B_2 < 1$, and any $1 \leq j \leq p$ such that 1) Conditions 1 and 3–4 hold, 2) the random forests estimates $\hat{Y}(X_{-j})$
and \( \hat{g}(X_{-j}) \) are constructed based on the independent training sample \( X_0 \), and 3) \( X_j \) is a null feature, it holds that

\[
P \left( \left| \text{FACT}_{j|X_{-j}} \right| > t \right) \leq 2 \Phi(-t) + \frac{8c}{\sqrt{\log 5}} + (\log n)(n^{-1/4} + B_1^{1/4} + B_2^{1/4}) + (- \log (B_1 B_2))^{-1},
\]

where \( \text{FACT}_{j|X_{-j}} \) is the conditioning form of the FACT statistic defined in (11) and \( c = t n^{-1/4} \log n + (2t + 1)(2B_1^{1/4} + B_2^{1/4}) + \sqrt{nB_1 B_2}(- \log (B_1 B_2)). \)

According to Theorem 3, for the FACT test based on conditioning to have valid asymptotic normality, we need the conditions \( B_1 + B_2 = o(1) \) and \( \sqrt{nB_1 B_2}(- \log (B_1 B_2)) = o(1) \), where the latter condition is less restrictive compared to the condition \( \sqrt{nB_1}(- \log B_1) = o(1) \) required by Theorem 2.

**Remark 5.** In [47], by assuming sample versions of Conditions 1 and 4 with \( \sqrt{nB_1 B_2} + B_1 + B_2 = o_p(1) \) and regularity conditions, Theorems 6 and 8 therein indicate that for each \( j \in \{1, \ldots, p\} \),

\[
\sup_{t \in \mathbb{R}} \left| P\left( \text{FACT}_{j|X_{-j}} - \sqrt{n} \kappa_{j|X_{-j}}(\hat{\sigma}_{j|X_{-j}})^{-1} \leq t \right) - \Phi(t) \right| = o(1), \tag{19}
\]

where \( \kappa_{j|X_{-j}} := E\{[Y - E(Y|X_{-j})][g(X_j) - E(g(X_j)|X_{-j})]\} = 0 \) when \( X_j \) is a null feature. We see that the conditions required by our Theorem 3 for the smaller-order terms to vanish asymptotically is the same as those in [47], up to a logarithmic factor. It is worth mentioning that the finite-sample result in our Theorem 3 cannot be directly implied by (19) above, and vice versa. It is also unclear whether the sample versions of Conditions 1 and 4 required by [47] would hold for high-dimensional random forests, whereas our Conditions 1 and 4 have been justified in [17, 31, 49]. Moreover, note that different from (19), our result in Theorem 3 holds uniformly over \( j \in \{1, \ldots, p\} \).

Theorem 4 below establishes the nonasymptotic theory for \( \text{FACT}^{(l)}_j \) with \( l \in L \), which are the FACT statistics using the ensemble idea defined in (13). Recall that \( |\cdot| \) stands for the cardinality of a given set, and \(|L| \) is a fixed constant.

**Theorem 4.** For all large \( n \), each \( 0 < B_1 < 1 \), each \( t > 0 \), and any \( 1 \leq j \leq p \) such that 1) Condition 1 holds and Conditions 2–3 are satisfied for each transformation \( g^{(l)}(X_j) \), 2) the random forests estimate \( \hat{Y}(X_{-j}) \) is constructed based on the independent training sample \( X_0 \), and 3) \( X_j \) is a null feature, it holds that

\[
P \left( \bigcup_{l \in L} \left\{ \left| \text{FACT}^{(l)}_j \right| > t \right\} \right) \leq 2|L|\Phi(-t) + \frac{8|L|c}{\sqrt{\log 5}} + (\log n)(B_1^{1/4} + n^{-1/4}), \tag{20}
\]

where \( c = (\log n)(2B_1^{1/4} + n^{-1/4} \log n)(1 + t) \).

Theorem 4 shows that the asymptotic size and the asymptotic p-value for the FACT test with ensemble in (14) can be estimated conservatively as \( \min\{1, 2|L|\Phi(-t)\} \) and \( \min\{1, 2|L|\Phi(- \max_{l \in L} \left| \text{FACT}^{(l)}_j \right|)\} \), respectively. Finally, we present in Theorem 5 below the nonasymptotic theory for the null distribution of the general FACT test given in (16) with sample
splitting (instead of the OOB). To streamline the technical presentation, we will illustrate
the main idea by focusing on the square transformation \(g^{(2)}(x) = x^2\) due to its simplicity and
practical utility.

**Theorem 5.** For all large \(n\), each \(Q\) with \(1 \leq |Q| < n\), each \(t > 0\), all consistency rates
\(0 < B_1, B_2 < 1\), and any \(1 \leq j \leq p\) such that 1) Condition 1 holds and Conditions 3–4
are satisfied for \(g^{(l)}(X_j)\) and \(\hat{g}^{(l)}(X_{-j})\) for each \(l \in \{1, 2\}\) with \(g^{(1)}(x) = x\) and \(g^{(2)}(x) =
x^2\), 2) the random forests estimates \(\hat{Y}(X_{-j})\) and \(\hat{g}^{(l)}(X_{-j})\)'s are constructed based on the
independent training sample \(X_0\), and 3) \(X_j\) is a null feature, it holds that

\[
\mathbb{P}(\text{FACT}_j > t) \leq 4|Q|\Phi(-t) + \frac{16|Q|c}{5\sqrt{2}\varsigma_1} + 2(-\log(B_1B_2))^{-1} \\
+ |Q|(\log n) \left( \left( \frac{|Q|}{n - |Q|} \right)^{1/3} + n^{-1/4} + B_1^{1/4} + B_2^{1/4} \right)
\]

(21)

where \(\text{FACT}_j\) is the general FACT statistic defined in (15) and \(c = \frac{tn^{-1/4}\log n + (2t + 1)(2B_1^{1/4} + B_2^{1/4}) + \sqrt{nB_1B_2(-\log(B_1B_2))}}{nB_1B_2(-\log(B_1B_2))}\).

Theorem 5 holds even with fixed \(|Q|\). However, in Section 6, we will see that slowly
diverging \(|Q|\) such as \(|Q| = O\{\log n\}\) achieves better empirical performance than fixed \(|Q|\).

**Remark 6.** [47] introduced a test that is the maximum of a diverging number of GCM tests for
the purpose of testing (3) when \(Z_1\) and \(Z_2\) are high-dimensional. They derived the asymptotic
null distribution using the high-dimensional central limit theorem (CLT) developed in
[16]. In principle, their idea can be used to prove the asymptotic null distribution of our
FACT test (15). We choose not to proceed with such direction for two reasons. First, the
high-dimensional Gaussian approximation requires that the biases of the tests (before taking
maximum) are vanishing fast enough so that the mean-zero Gaussian can approximate the
joint distribution well enough; this assumption can be too stringent in finite-sample applica-
tions. Second, we consider fixed \(L\) and very slowly diverging \(|Q|\) so the powerful tool in [16]
is not really necessary in our application. In additional, our (21) is derived by ignoring the
correlations among statistics FACT\(_j^{(l)}\) and as a result, our critical value and p-value calculated
using (21) are more conservative than those from the high-dimensional CLT approach. This
conservative nature in fact helps counteract the effect of bias in finite samples.

### 4.2 Power analysis

We now investigate the selection power properties of the basic, ensemble, and general FACT
tests suggested in Section 3. To this end, let us define two useful population quantities

\[
k_{j}^{(l)} := \mathbb{E}\left\{ |Y - \mathbb{E}(Y|X_{-j})| |g^{(l)}(X_j) - \mathbb{E}(g^{(l)}(X_j))| \right\},
\]

\[
k_{j|X_{-j}}^{(l)} := \mathbb{E}\left\{ |Y - \mathbb{E}(Y|X_{-j})| |g^{(l)}(X_j) - \mathbb{E}(g^{(l)}(X_j)|X_{-j})| \right\}
\]

(22)

for each \(1 \leq j \leq p\) and \(l \in L = \{1, \cdots, m_1\}\), where \(m_1\) is a fixed integer.
4.2.1 Test power for general cases

**Theorem 6.** Let $C > 0$ be some sufficiently large constant. For all $n \geq 1$, each $B_1 > 0$, each $t > 0$, and any $1 \leq j \leq p$ such that 1) Condition 1 holds and Conditions 2–3 are satisfied for each measurable transformation $g^{(l)}(X_j)$, 2) the random forests estimate $\hat{Y}(X_{-j})$ is constructed based on the independent training sample $X_0$, and 3) $\sum_{l \in L} |\kappa^{(l)}_j| > 0$, it holds that

$$\Pr \left( \bigcap_{l \in L} \left\{ \left| \text{FACT}^{(l)}_j \right| \leq t \right\} \right) \leq \frac{(C + t) \left[ \sqrt{B_1} + \sqrt{\text{Var}(Y)} \right]}{\sqrt{n} \sum_{l \in L} |\kappa^{(l)}_j|},$$

(23)

where $\text{FACT}^{(l)}_j$ are the ensemble form of the FACT statistics defined in (13).

The nonasymptotic result in Theorem 6 complements the results of Theorem 4 by providing the power perspective for the ensemble FACT test (14). For the specific case of $|L| = 1$, Theorem 6 also complements the probability bound (18) in Theorem 1 for the basic FACT statistic. We see from Theorem 6 that when $X_j$ is relevant with signal strength $\sum_{l \in L} |\kappa^{(l)}_j| \gg n^{-1/2}$, the probability of not rejecting the null hypothesis (1) for the FACT test with ensemble in (14) is asymptotically shrinking under regularity conditions, which entails that the ensemble FACT test enjoys asymptotic power one. Specifically, in Section 4.2.2 later, we will assure the practical utility of the ensemble FACT test by deriving a nonzero lower bound on $\sum_{l \in L} |\kappa^{(l)}_j|$ for a class of additive regression functions, where feature $X_j$ has an additive effect on the response through a polynomial function of $X_j$.

Let us gain some insights into the regularity conditions assumed in Theorem 6. As mentioned in Section 4.1, Conditions 2–3 are imposed mainly to simplify the technical analysis. Condition 1 of Theorem 6 requires a consistent random forests estimate $\hat{Y}(X_{-j})$ for the conditional mean function $\mathbb{E}(Y|X_{-j})$ with a relevant feature $X_j$ left out when training the random forests model. Assume that the response is given by $Y = m(X) + \varepsilon$, where $m(\cdot)$ is some measurable function and $\varepsilon$ is the model error that is of zero mean and independent of the random feature vector $X$. Then for each $1 \leq j \leq p$, we can write

$$Y = \mathbb{E}(m(X)|X_{-j}) + \varepsilon + [m(X) - \mathbb{E}(m(X)|X_{-j})]$$

$$= \tilde{m}(X_{-j}) + \tilde{\varepsilon},$$

where $\tilde{m}(X_{-j}) = \mathbb{E}(m(X)|X_{-j})$ and $\tilde{\varepsilon} = \varepsilon + [m(X) - \mathbb{E}(m(X)|X_{-j})]$. Moreover, let us assume for simplicity that $\tilde{\varepsilon}$ is of zero mean and independent of $\tilde{m}(X_{-j})$, which can be satisfied when $m(x) = \sum_{j=1}^{p} m_j(x_j)$ is an additive function with $m_j(\cdot)$ some univariate functions, and $X_j$ and $X_{-j}$ are independent of each other. Then we can prove Condition 1 with feature dimensionality $p = O(N K_0)$ for some constant $K_0 > 0$ and random forests consistency rate $B_1 \to 0$ depending on the training sample size $N$. In particular, we can show that in such a case, if $m(X)$ satisfies Condition A1 introduced in Section 2, then $\tilde{m}(X_{-j})$ will satisfy the same condition. However, since high-dimensional random forests consistency is not the major focus of our current paper, we will leave the detailed consistency analysis for this and
more general cases to future work. We provide in Theorem 7 below a power analysis for the general FACT test with sample splitting (instead of the OOB) in (16).

**Theorem 7.** Let $C > 0$ be some sufficiently large constant. For all $n \geq 2$, each $|Q| < n$, each $B_1, B_2 > 0$, each $t > 0$, and any $1 \leq j \leq p$ such that 1) Condition 1 holds and Conditions 3–4 are satisfied for $g^{(l)}(X_j)$ and $\hat{g}^{(l)}(X_{-j})$ for each $l \in \{1, 2\}$ with $g^{(1)}(x) = x$, and $g^{(2)}(x) = x^2$, 2) the random forests estimates $\hat{Y}(X_{-j})$ and $\hat{g}^{(l)}(X_{-j})$’s are constructed based on the independent training sample $X_0$, and 3) $|\kappa_j^{(1)}| + |\kappa_j^{(2)}| > 0$, it holds that

$$P(\text{FACT}_j \leq t) \leq \frac{\sqrt{|Q|(C + t)(\text{Var}(Y) + \sqrt{B_1} + \sqrt{B_2} + \sqrt{nB_1B_2})}}{\sqrt{n} - |Q| \sum_{l=1}^{2} |\kappa_j^{(l)}|},$$

where FACT$_j$ is the general FACT test statistic defined in (15).

The nonasymptotic result in Theorem 7 for the general FACT test complement the results of Theorem 5 through the lens of power. As mentioned before, the use of a simple square transformation $g^{(2)}(x) = x^2$ is intended to simplify the technical analysis in the proof of Theorem 7. In implementations, prior knowledge (if available) can be incorporated in pre-choosing $g^{(l)}(\cdot)$’s. Similar discussions to Remark 5 can be made for the comparison between our Theorem 7 and the power results in [47] (where no ensemble was used); we omit the details here.

4.2.2 Test power for additive effects

Theorems 6–7 in Section 4.2.1 have shown that both the basic FACT test and the general FACT test can have power approaching one as sample size increases as long as the corresponding signal strength assumptions are satisfied for the general cases of high-dimensional nonparametric regression. In this section, we focus on the specific nonparametric case of additive effects and aim to build some concrete lower bounds on the key population quantities $\kappa_j^{(l)}$’s and $\kappa_j^{(l)}|X_{-j}|$’s. Specifically, we will analyze the power of the basic FACT test with the choice of $g(x) = x$ in Proposition 1 and then investigate the more powerful ensemble/general FACT test in Proposition 2 below. To this end, we will introduce an additional regularity condition.

**Condition 5.** Assume that the nonparametric regression model is given by $Y = h(X_j) + H(X_{-j}) + \varepsilon$, where $h(\cdot)$ and $H(\cdot)$ are some measurable functions and $\varepsilon$ is the model error that is of zero mean and independent of the random feature vector $X$. In addition, assume that the distribution of feature vector $X$ has a density function.

**Proposition 1.** Assume that Condition 5 holds, $g^{(1)}(x) = x$, $\mathbb{E}|H(X_{-j})| < \infty$, $h(\cdot)$ is monotonic, and the derivative of function $h(\cdot)$ is integrable and bounded in absolute value. Then we have

$$|\kappa_j^{(1)}| \geq \left( \inf_{x \in [0,1]} |h'(x)| \right) \mathbb{E}\{\text{Var}(X_j|X_{-j})\}.$$
Proposition 1 above gives an example that when \( \inf_{x \in [0,1]} |h'(x)\) \( \gg n^{-1/2} \), the basic FACT test in (7) with the choice of \( g(x) = x \) can enjoy asymptotic power one in light of Theorem 6 (for the specific choice of \( |L| = 1 \)). The above condition rules out the pathological case where \( X_j \) can be represented perfectly by a measurable function of \( X_{-j} \) almost surely.

To motivate the need of ensemble statistics, let us consider an example with a simple quadratic \( h(x) \) such that Condition 5 holds, \( X \) is uniformly distributed on \([0,1]^p\), \( g^{(1)}(x) = x \), and \( h(x) = (x - a)^2 \) for some \( a \in \mathbb{R} \). By (22) and some simple calculations, we can obtain

\[
\kappa_j^{(1)} = \kappa_j^{(1)}(X_{-j}) = \frac{1}{12} - \frac{a}{6},
\]

which implies that the relevance of the \( j \)th feature \( X_j \) can be measured in terms of \( |a - 0.5| \).

As a result, the basic FACT test and the FACT test with conditioning do not have nontrivial power when \( a \) is close to 0.5. To enhance the test power, we can exploit the FACT test with ensemble in (14) with transformations \( g^{(l)}(x) = x^l \) for \( l \in L \). The main intuition for the ensemble form of the FACT test is to use multiple feature transformations so that the population correlations \( \sum_{l \in L} |\kappa_j^{(l)}| \) are more likely to be nonzero and strengthened. Recall that \( m_1 = |L| \) is a fixed integer.

**Proposition 2.** Assume that Condition 5 holds for some \( 1 \leq j \leq p \), \( h(x) = a_0 + \sum_{l \in L} a_l x^l \) for some \( a_l \in \mathbb{R} \) with \( \sum_{l \in L} |a_l| > 0 \), \( \mathbb{E}|H(X_{-j})| < \infty \), \( X \) is uniformly distributed on \([0,1]^p\), and \( g^{(l)}(x) = x^l \) for \( l \in L \). Then, there exists some positive constant \( c_{|L|} \) depending on \( |L| \) such that

\[
\min \left\{ \sum_{l \in L} |\kappa_j^{(l)}|, \sum_{l \in L} |\kappa_j^{(l)}(X_{-j})| \right\} \geq \frac{\sum_{l \in L} |a_l|}{|L|} c_{|L|} > 0.
\]

**Particularly,** for \( 1 \leq |L| \leq 2 \), we have \( \min \left\{ \sum_{l \in L} |\kappa_j^{(l)}|, \sum_{l \in L} |\kappa_j^{(l)}(X_{-j})| \right\} \geq 0.001 \times \sum_{l \in L} |a_l| \).

Proposition 2 above reveals that the ensemble and general FACT test can indeed enjoy enhanced power compared to the FACT tests without ensemble in finite samples. Specifically, a combination of Proposition 2 and Theorem 6 assures that the FACT test with ensemble in (14) for each finite \( |L| \) can have asymptotic power one when feature \( X_j \) has an additive effect on the response through a polynomial function of \( X_j \). In particular, it follows from Proposition 2 and Theorem 7 that the general FACT test with the choices of \( g^{(1)}(x) = x \) and \( g^{(2)}(x) = x^2 \) (without the OOB) admits asymptotic power one in the above example (24) for each \( a \in \mathbb{R} \). On the other hand, it is worth mentioning that although our power analysis shows that additional measurable transformations \( g^{(l)}(\cdot) \)'s can potentially improve the test power at the population level, the use of too many transformations may have a negative (statistical) effect on the \( p \)-value and size, as shown in the upper bound in Theorem 4. Given a finite sample in practice, we often find that the general FACT test with linear and square transformations can lead to an appealing empirical performance as demonstrated in the simulation and real data examples later in Sections 6 and 7.
5 Comparisons with existing works

We have reviewed a closely related line of work on high-dimensional conditional independence testing in Sections 1.1. In this section, we will briefly review the main ideas of some existing random forests feature importance measures such as the MDI [12], MDA [11], CPI [48], permutation inference [1, 27], and prediction difference inference [41]. We will focus on their bias-resistance properties and their interpretability. In addition, we will discuss an identification problem of the MDA.

5.1 Related works on random forests feature importance

Mean decrease in impurity (MDI). For the decision tree, [12] measured the importance of a feature with respect to the response using the sum of impurity (i.e., sample variance) decreases resulting from all the splits on this feature. MDI of a feature in random forests is defined as the average of such importance measures of this feature over all trees. The intuition is that the larger the impurity decrease from all splits on a feature, the more important the feature in terms of explaining the variation of the response.

Mean decrease accuracy (MDA). For each feature \( X_j \), MDA measures its importance by the increase of the fitted loss (or the decrease of the prediction accuracy) after randomly permuting the \( j \)th feature. To assess its statistical properties, the theoretical version of the MDA measure [11, 26] is often defined as

\[
\text{MDA}(Y, X_j) := E(Y - m(X_{(j)}))^2 - E(Y - m(X))^2, \tag{25}
\]

where \( m(X) \) denotes a version of \( E(Y|X) \), and \( X_{(j)} := (X_1, \cdots, X_{j-1}, X_{(j)}, X_{j+1}, \cdots, X_p)^T \). Here, \( X_{(j)} \) is randomly permuted from \( X_j \), independent of \( Y \) and \( X \), and has the same distribution as the original feature \( X_j \). The intuition of the MDA measure is that an inactive feature tends to have a lower MDA value since it is less associated with response \( Y \) and the permutation has little effect on the model fitting accuracy.

Conditional permutation importance (CPI). For ease of presentation, we only present a simple version of CPI here. For each feature \( X_j \), the CPI measure [48] employs a similar MDA value as in (25) to quantify its importance but with a new permuted feature vector \( X_{(j)}^\dagger := (X_1, \cdots, X_{j-1}, X_{(j)}^\dagger, X_{j+1}, \cdots, X_p)^T \) in place of the simple marginally permuted feature vector \( X_{(j)} \), where given \( X_{-j} \), the new permuted feature \( X_{(j)}^\dagger \) has the same conditional distribution as the original feature \( X_j \) and is also conditionally independent of both response \( Y \) and feature \( X_j \). Specifically, the CPI measure for feature \( X_j \) is defined as

\[
\text{CPI}(Y, X_j) := E(Y - m(X_{(j)}^\dagger))^2 - E(Y - m(X))^2 \tag{26}
\]
at the population level. The intuition of the CPI measure is similar to that of the MDA measure mentioned above, and we will show that the CPI can improve over the MDA later in Section 5.2.

Permutation inference. For any given feature, the method in [1] permutes the response
and calculates the MDI value for this feature. Such an MDI value based on the randomly permuted response is understood as the null MDI. This step is repeated for a certain number of times and many null MDI values are obtained. The method proceeds with taking these null MDIs as the empirical null distribution and establishes the empirical test for assessing the significance of the MDI measure that is calculated with the original response. For such a procedure, the MDI can be replaced with any other random forests feature importance measures. The approach in [27] is similar to that in [1], but with the feature randomly permuted instead.

Prediction difference inference. The prediction at a test point tends to deviate from the ground truth when some relevant explanatory features are not used for prediction. By this intuition, [41] established a significance test for the $j$th feature based on the difference between predictions of two models trained respectively with all features and with all but the $j$th features (see Section 4.2 therein).

Many works have documented that both MDI and MDA measures can be biased [48, 24, 42] toward spurious features when there exists feature correlation. In general, permutation inference methods [1, 27] become biased when the underlying feature statistics are biased. In addition, the prediction difference inference [41] lacks formal theoretical analysis on its bias-resistance property. Meanwhile, CPI can improve over MDI and MDA to alleviate their bias issue [48], but how to efficiently and effectively generate conditional permutation in implementing CPI can be challenging.

From the perspective of interpretability, an easy-to-interpret inference method needs to be associated with a proper definition of null features. An example as we have seen in Section 4 is the FACT tests based on Definition 1. Here, we review two alternative null definitions that may not be best suited for our goal of statistical inference with random forests. First, marginal independence of $X_j$ with $Y$ is a popular definition of the null feature and has been used in random forests inference. This definition can be useful for dimensionality reduction but may not be appropriate for our goal, because we consider a joint regression model with random forests where the dependency structure of covariates needs to be taken into account. Second, it is also popular to define $X_j$ as a null feature if $m(X) = \tilde{m}(X_{-j})$ for some true underlying regression function $\tilde{m} : \mathbb{R}^{p-1} \mapsto \mathbb{R}$. This definition of null features is interpretable only when the model $\tilde{m}$ is uniquely identified. Yet, such model identification may require additional regularity assumptions. Indeed, model identifiability has always been a challenging issue for nonparametric inference. In Section 5.2, we illustrate this point with a specific example.

5.2 The identification issue of MDA

In this section, we give an example showing that the primitive construction of MDA can lead to indefinite values of importance measures for spurious features. In addition, we discuss that CPI and FACT are free of this issue.

Example 1. We consider random feature vector $X = (X_1, \cdots, X_p)^T$ such that 1) feature $X_1$ has a uniform distribution on interval $[0, 1]$; 2) $X$ has a uniform distribution over $[0, 0.7]^p$.
conditional on event \( \{X_1 \leq 0.7\} \); and 3) \( X_1 = \cdots = X_p \) conditional on event \( \{X_1 > 0.7\} \).

Let \( Y = 1_{0.3 \leq X_1 \leq 0.7} + \varepsilon \), where \( 1(.) \) represents the indicator function and \( \varepsilon \) is the model error that is of zero mean and independent of \( X \) with \( \mathbb{E}(\varepsilon^2) < \infty \).

Without loss of generality, Example 1 assumes constant coefficients 0.3 and 0.7 for simplicity. Given the model setting in Example 1 above, we establish in Proposition 3 below that the value of MDA\((Y, X_2)\) is indefinite in the presence of correlated null features \( X_2, \cdots, X_p \) in this example.

**Proposition 3.** There exist two versions of the conditional mean \( \mathbb{E}(Y|X) \) given by \( m(X) = 1_{0.3 \leq X_1 \leq 0.7} \) and \( \tilde{m}(X) = 1_{X_1 \geq 0.3} - 1_{X_2 > 0.7} \), respectively, such that MDA\((Y, X_2)\) > 0 if \( \tilde{m}(\cdot) \) is used in the MDA measure (25), whereas MDA\((Y, X_2)\) = 0 if \( m(\cdot) \) is used instead.

Proposition 3 above indicates that the sample version of MDA\((Y, X_2)\) may inherit the indefinite value issue if no further regularity conditions are imposed. This is because MDA\((Y, X_2)\) can take either zero or some positive values, which renders the MDA measure indecisive in such a model setting. To the best of our knowledge, our work is among the first to formally formulate the identification problem of the MDA. The existing theoretical results on the MDA, e.g., in [26], usually assume implicitly a uniquely identified conditional mean function \( m(\cdot) \), which can only hold under additional regularity conditions.

On the other hand, the following Proposition 4 shows that CPI is free of the above discussed problem, implying that CPI based on Definition 1 can be more interpretable.

**Proposition 4.** For any response \( Y \) and feature vector \( X = (X_1, \cdots, X_p)^T \) with a null feature \( X_j \) (characterized by Definition 1), it holds that CPI\((Y, X_j)\) = 0. Consequently, we have CPI\((Y, X_2) = \cdots = CPI(Y, X_p) = 0 \) in Example 1.

We note that the all versions of the FACT tests are free of the identifiablility issue since we have \( \kappa_{j|X_{-j}}^{(1)} = 0 \) and \( \kappa_{j}^{(1)} = 0 \) for any transform \( g^{(1)}(\cdot) \) and each \( j \in \{2, \cdots, p\} \) in Example 1.

## 6 Simulation studies

In this section, we verify the theoretical results of the FACT and demonstrate its finite-sample performance through several simulation examples.

### 6.1 Simulation settings

We first introduce the settings of our simulation examples. Denote by \( S^* := \{1, 11, 21, 31, 41\} \), \( S_{D,j} := \{j, j + 1, j + 2\} \) for each \( j \in S^* \), and \( S_I := \{1, \cdots, p\} \setminus \cup_{j \in S^*} S_{D,j} \), where \( p \) denotes the feature dimensionality. Set \( S^* \) contains all five relevant features in the nonparametric regression model (28) to be introduced below. Each feature \( X_j \) with \( j \in S^* \) has exactly two correlated features \( X_{j+1} \) and \( X_{j+2} \), while set \( S_I \) consists of independent noise features. Specifically, let us define

\[
X_i = (Z_{l,j} - 0.5)(1 - 2\lambda + 2\lambda^2)^{-1/2} + 0.5
\]  

\[
(27)
\]
for each $l \in S_{D,j}$ and $j \in S^*$, where $\lambda \in [0,1]$ is a tuning parameter, $Z_{l,j} = (1-\lambda)U_l + \lambda U_{p+j}$, and $(U_1, \cdots, U_p, U_{p+1}, U_{p+11}, U_{p+21}, U_{p+31}, U_{p+41})^T$ is uniformly distributed on the hypercube $[0,1]^{p+5}$. Moreover, we define $X_j = U_j$ for each $j \in S_l$. With such a setting, we see that the variance of each feature $X_j$ is $1/12$. The correlation between features in $S_{D,j}$ is

$$
\lambda^2(1 - 2\lambda + 2\lambda^2)^{-1}
$$

for each $j \in S^*$, whereas features in $S_{D,l}$ are independent of features in $S_{D,k}$ as long as $l \neq k$. We will work with such a distribution structure for covariate vector $\mathbf{X} = (X_1, \cdots, X_p)^T$ throughout our simulation studies.

Let us consider the nonparametric regression model

$$
Y = \underbrace{5X_1}_{\text{weak linear comp.}} + \underbrace{10X_{11}}_{\text{strong linear comp.}} + \underbrace{20(X_{21} - 0.5)^2}_{\text{quadratic comp.}} + \underbrace{10 \sin (\pi X_{31} X_{41})}_{\text{interactive comp.}} + \varepsilon,
$$

(28)

where $\varepsilon \sim N(0, \sigma^2)$ is the model error with standard deviation $\sigma > 0$ and is independent of random feature vector $\mathbf{X}$, and “comp.” is short for component. The nonparametric model given in (28) is popular for evaluating the performance of nonparametric learning and inference methods. This model is known as the Friedman function [23], which was designed to test the capability of a nonparametric method in learning the underlying true regression function in the presence of interaction, quadratic, and both weak and strong linear effects.

We present in Section C.1 of Supplementary Material a summary of some basic statistics for the data generating model (28), including the out-of-sample prediction accuracy of the random forests models in terms of the root mean-squared error (RMSE) as well as the signal-to-noise ratios (SNRs) for each additive component. Under the data generative model introduced above, we will demonstrate 1) the asymptotic normality of the basic FACT test statistics $\text{FACT}_{j,0}$ given in (6) and the general FACT test statistics given in (15) for the null features in Section 6.2, 2) the size and power of the general FACT test given in (16) in Section 6.3, and 3) the empirical comparisons of the general FACT test statistics given in (15) with the MDI, MDA, and CPI in Section 6.4 in terms of bias resistance. The square transformation of the general FACT statistics in this section is chosen as $g^{(2)}(X_{ij}) = (X_{ij} - n^{-1}\sum_{i=1}^n X_{ij})^2$, as mentioned previously in Section 3.4. For each simulation study, we will evaluate the finite-sample performance of random forests inference mainly in terms of the impact of correlated features and the selection power. We will drop the term “general” for the FACT hereafter whenever there is no confusion.

### 6.2 Asymptotic normality

We employ the quantile-quantile (Q-Q) plot to illustrate the asymptotic normality of the basic FACT test and the FACT test statistics for the null features. To this end, we generate 100 data sets, each with sample size $n = 200$ and feature dimensionality $p = 200$ from model (28) with the choices of $\sigma = 5$ and $\lambda \in \{0, 0.5, 0.6\}$. Features $X_j$’s are independent of each other when $\lambda = 0$, while the feature correlations at the population level are roughly 0.5 and 0.7 when $\lambda$ is 0.5 and 0.6, respectively. To examine the behavior of the null features, we consider the basic FACT test statistic $\text{FACT}_{12,0}$ given in (6) with $g(x) = x$ for null feature $X_{12}$, and the FACT test statistics $\text{FACT}_{12,1}^{(1)}$ and $\text{FACT}_{12,1}^{(2)}$ given in (15) with the OOB for null features.
The resulting Q-Q plots for the empirical distributions of these test statistics against the standard Gaussian distribution are contained in Figures 1–2 with the 45-degree red lines passing through the origin. Specifically, we present in Figure 1 the simulation results regarding test statistics $\text{FACT}_{12,0}$ and $\text{FACT}_{12,1}^{(1)}$ with $k_n = 1$ and $\lambda \in \{0, 0.6\}$. Observe that due to the choice of $k_n = 1$ in Figure 1, the difference between these two statistics comes from the use of the debiasing technique of conditioning introduced in Section 3.2.2. Further, we present in panels (a)–(c) of Figure 2 the simulation results for test statistic $\text{FACT}_{12,1}^{(1)}$, and in panels (d)–(f) of Figure 2 those for test statistic $\text{FACT}_{22,1}^{(2)}$. In particular, for the results in Figure 2, we allow the values of $k_n$ and $\lambda$ to vary from $\{3, 7\}$ and $\{0.5, 0.6\}$, respectively; see the panels of Figure 2 for their specific values.

We see from panel (a) of Figure 1 that for the case of independent features (i.e., $\lambda = 0$), the empirical distribution of the basic FACT test statistic $\text{FACT}_{12,0}$ for null feature $X_{12}$ is rather close to the standard Gaussian distribution, which is in line with our theoretical results obtained in Section 4. As shown in panel (b) of Figure 1, the basic FACT test statistic $\text{FACT}_{12,0}$ becomes biased when $\lambda = 0.6$ due to the high correlation level among the features. Comparing panels (b)–(c) of Figure 1 demonstrates clearly the usefulness of the debiasing technique of conditioning, which alleviates substantially the bias issue of the basic FACT test statistic $\text{FACT}_{12,0}$ at the presence of highly correlated features.

We now turn our attention to the simulation results shown in Figure 2. Since all tests exhibit the standard asymptotic normality when $\lambda = 0$, we omit those results to save space. As an illustrative example, we focus on the FACT statistics $\text{FACT}_{12,1}^{(1)}$ and $\text{FACT}_{22,1}^{(2)}$ for null features $X_{12}$ and $X_{22}$, which showcase the performances of FACT tests applied to spurious features that are correlated with the strong linear and quadratic components in model (28), respectively. From panels (a) and (d) of Figure 2, we can see that when both debiasing techniques of imbalancing (with $k_n = 3$) and conditioning introduced in Section 3.2 are
advantages of the general FACT test over the GCM test \cite{47} in terms of bias-resistance. In technique of imbalancing introduced in Section 3.2.1; such results also illustrate the practical of Supplementary Material. Despite the challenges of the high-dimensional nonparametric starting point for practical implementation of the FACT test. We also would like to mention to (b) and panels (d) to (e) in Figure 2 reveals that higher feature correlations enlarge slightly \( p \)-correlated (the feature correlation level is around 0.5 when \( \lambda = 0.5 \)). Comparing panels (a) to (b) and panels (d) to (e) in Figure 2 reveals that higher feature correlations enlarge slightly the bias of the FACT test statistics.

Further, we can see from panel (c) of Figure 1 and panels (b)–(c) and (e)–(f) of Figure 2 that a higher \( k_n \) tends to reduce the bias more, indicating the usefulness of the debiasing technique of imbalancing introduced in Section 3.2.1; such results also illustrate the practical advantages of the general FACT test over the GCM test \cite{47} in terms of bias-resistance. In particular, our simulation results suggest that the choice of \( k_n = O\{\log n\} \) can serve as a good starting point for practical implementation of the FACT test. We also would like to mention that due to the high dimensionality of \( p = n = 200 \), it is expected that nonparametric learning can be generally challenging including the use of random forests. More details on the prediction accuracy of random forests in model (28) are contained in Section C.1 of Supplementary Material. Despite the challenges of the high-dimensional nonparametric settings, we can observe that the general FACT test indeed admits the asymptotic standard
normality for null features as ensured by our theoretical results, and is rather robust to the feature dependency for random forests inference.

6.3 The size and power

We now investigate the empirical performance of the general FACT test introduced in (16) in terms of the size and power across different model settings, where we allow the significance level $\alpha$ to vary among $\{0.1, 0.05, 0.025\}$. We set $k_n = \lfloor \log_e n \rfloor / 2$, where $\lfloor \cdot \rfloor$ denotes the closest integer ($k_n = 3$ if $n \in \{300, 500\}$), and recall that $|L| = 2$ in the test (16). In view of (17), the corresponding values of the rejection threshold $t_\alpha$ at significance level $\alpha$ for the FACT test are $t_{0.1} = 2.40$, $t_{0.05} = 2.66$, and $t_{0.025} = 2.87$, respectively. For each feature $X_j$ with $j \in \{1, 11, 21, 31, 2, 12, 22, 32\}$, the empirical rejection rates over 100 simulation repetitions are reported in Table 2, where the data is generated from the nonparametric model (28) with $\sigma = 5$ and dependent features. Specifically, we consider six cases of $(n, p, \lambda)$: I) $(n, p, \lambda) = (300, 200, 0.3)$, II) $(n, p, \lambda) = (300, 200, 0.6)$, III) $(n, p, \lambda) = (500, 200, 0.6)$, IV) $(n, p, \lambda) = (500, 1000, 0.6)$, V) $(n, p, \lambda) = (500, 1000, 0.3)$, and VI) $(n, p, \lambda) = (500, 10, 0.6)$, where the feature correlations at the population level are roughly 0.15 and 0.7 for the choices of $\lambda = 0.3$ and 0.6, respectively. In case VI, the ten explanatory features are $\{X_1, X_2, X_{11}, X_{12}, X_{21}, X_{22}, X_{31}, X_{32}, X_{41}, X_{42}\}$, while we use $X_1, \cdots, X_p$ in the

| $(n, p, \lambda)$ | $\alpha$ | Relevant features | Null features |
|-------------------|----------|------------------|--------------|
|                   | $X_1$    | $X_{11}$ | $X_{21}$ | $X_{31}$ | $X_2$ | $X_{12}$ | $X_{22}$ | $X_{32}$ |
| I $(300, 200, 0.3)$ | 0.1      | 0.85    | 1.00    | 0.93    | 1.00 | 0.08    | 0.09    | 0.08    | 0.09 |
|                   | 0.05     | 0.75    | 1.00    | 0.89    | 0.98 | 0.06    | 0.06    | 0.07    | 0.04 |
|                   | 0.025    | 0.67    | 1.00    | 0.79    | 0.93 | 0.02    | 0.03    | 0.03    | 0.00 |
| II $(300, 200, 0.6)$ | 0.1      | 0.68    | 1.00    | 0.96    | 0.94 | 0.18    | 0.13    | 0.15    | 0.10 |
|                   | 0.05     | 0.53    | 0.98    | 0.93    | 0.89 | 0.13    | 0.09    | 0.07    | 0.04 |
|                   | 0.025    | 0.42    | 0.96    | 0.87    | 0.74 | 0.08    | 0.05    | 0.04    | 0.01 |
| III $(500, 200, 0.6)$ | 0.1      | 0.89    | 1.00    | 1.00    | 1.00 | 0.15    | 0.11    | 0.17    | 0.11 |
|                   | 0.05     | 0.82    | 1.00    | 1.00    | 1.00 | 0.08    | 0.04    | 0.12    | 0.05 |
|                   | 0.025    | 0.71    | 1.00    | 1.00    | 0.95 | 0.06    | 0.02    | 0.06    | 0.02 |
| IV $(500, 1000, 0.6)$ | 0.1      | 0.84    | 1.00    | 1.00    | 1.00 | 0.19    | 0.10    | 0.21    | 0.12 |
|                   | 0.05     | 0.77    | 1.00    | 1.00    | 0.99 | 0.05    | 0.02    | 0.09    | 0.07 |
|                   | 0.025    | 0.63    | 1.00    | 1.00    | 0.95 | 0.02    | 0.02    | 0.06    | 0.03 |
| V $(500, 1000, 0.3)$ | 0.1      | 0.98    | 1.00    | 1.00    | 1.00 | 0.12    | 0.10    | 0.11    | 0.11 |
|                   | 0.05     | 0.93    | 1.00    | 0.99    | 1.00 | 0.08    | 0.04    | 0.05    | 0.09 |
|                   | 0.025    | 0.88    | 1.00    | 0.98    | 0.99 | 0.03    | 0.04    | 0.01    | 0.03 |
| VI $(500, 10, 0.6)$   | 0.1      | 0.88    | 1.00    | 1.00    | 1.00 | 0.06    | 0.06    | 0.11    | 0.13 |
|                   | 0.05     | 0.78    | 1.00    | 1.00    | 1.00 | 0.01    | 0.06    | 0.06    | 0.07 |
|                   | 0.025    | 0.69    | 1.00    | 1.00    | 0.97 | 0.00    | 0.04    | 0.02    | 0.05 |

Table 2: The empirical size and power of the FACT test with $\sigma = 5$ across different model settings from Section 6.3 at each significance level $\alpha \in \{0.1, 0.05, 0.025\}$ over 100 simulation repetitions.
other cases.

From Table 2, we see that the empirical sizes of the FACT test for null features are generally close to the target ones in cases I, V, and VI with mild correlation or few noise features. Comparing case I with case II, higher spurious correlation causes larger size distortion. Comparing case II with case III, the size distortion only slightly gets better as sample size increases, but the power gets much higher. Moving from case III to case IV, the size distortion becomes slightly more severe because of increased number of noise features. The size distortion may come from the fact that consistency rates of random forests are not fast enough due to nonlinear model (28), high dimensionality, strong feature dependency, and high noise level. To verify this conjecture, we further explored cases V and VI, where the former has lower feature dependence level and the latter has fewer noise features. When compared with case IV, the size distortion issue is much alleviated in cases V and VI, showing evidence supporting our conjecture. Random forests is known to be biased toward correlated features, and the simulation results in Table 2 show that FACT has largely improved the bias issue. Such an improvement is even more apparent when compared with standard random forests feature importance measures in Table 1 from Section 6.4.

From the power perspective, Table 2 reveals that the selection performance of the FACT test is generally satisfactory across cases I–IV for the relevant features except for feature $X_{12}$, which is the weak linear component in model (28). Moreover, we see that the selection power of the FACT test increases with the sample size and is robust to both high dimensionality and feature dependency. These simulation results support our asymptotic theory of the FACT test presented in Section 4 on both perspectives of the size and power. Overall, we see that FACT provides a powerful tool to infer the relevance of random forests features in the high-dimensional nonparametric regression.

6.4 Comparisons with MDI, MDA, and CPI

We now provide details on how we obtain results in Table 1 presented earlier in the Introduction. To this end, we consider the first four settings of nonparametric model (28) as in Section 6.3; that is, the data is generated from model (28) with $\sigma = 5$ for four cases of $(n, p, \lambda)$: I) $(n, p, \lambda) = (300, 200, 0.3)$, II) $(n, p, \lambda) = (300, 200, 0.6)$, III) $(n, p, \lambda) = (500, 200, 0.6)$, and IV) $(n, p, \lambda) = (500, 1000, 0.6)$. Recall that the population feature correlation levels are around $0.15$ and $0.7$ when $\lambda = 0.3$ and $0.6$, respectively. To calculate the MDI and MDA measures, we employ the R package randomForest [34], while for the calculation of the CPI measure [20, 48], we use the R package permimp [19]. The computation is done with the default configurations of those R packages. We provide in Table 1 the simulation results for examining the spurious effects of different random forests feature importance measures and the FACT statistics with respect to the null feature $X_{12}$, which is correlated with the strong linear component $X_{11}$ in model (28). Specifically, each entry of Table 1 stands for the fraction of times (out of 100 simulation repetitions) when the feature importance measure of the null spurious feature $X_{12}$ exceeds that of relevant feature $X_1$ or $X_{21}$. A larger entry in Table 1 suggests a stronger spurious effect.
Table 1 unveils several interesting phenomena on the spurious effects of different random forests feature importance measures. First, we see from Table 1 that the importance of the null spurious feature $X_{12}$ dominates frequently that of both relevant features $X_1$ and $X_{21}$ for all three feature importance measures of the MDI, MDA, and CPI across cases II-IV, which is due to the high correlation between the null feature $X_{12}$ and the relevant feature $X_{11}$. In particular, the use of the CPI measure alleviates the spurious effects to certain extent compared to the MDI and MDA measures. In sharp contrast, the feature significance measure of the FACT statistic suppresses the spurious effects satisfactorily across all cases I–IV. Second, comparing case IV with case III suggests that including more noise features causes more difficulties to the MDI, MDA, and CPI measures in terms of assessing the relative feature relevance. In contrast, the results for FACT in Table 1 demonstrate that the FACT statistic is robust to high feature dimensionality for evaluating the relative feature importance.

7 Real data application

In this section, we examine the practical performance of FACT on an economic forecasting application in terms of evaluating the feature significance for random forests.

7.1 Economic forecasting with FRED-MD

We now demonstrate how to apply the general FACT test introduced in (16) to assess the significance of features with respect to different monthly macroeconomic responses across time. Specifically, we are interested in forecasting the one-month ahead interest rate, inflation, and unemployment rate with 81 macroeconomic features. These monthly time series are contained in the FRED-MD data set [39] from the Federal Reserve Economic Data (FRED) database. Since many of these features resemble each other in their roles in economy, there could be an issue of collinearity which can lead to much lower selection power. To address such a power loss issue due to highly correlated features, we divide all 81 features into a total of 12 groups following [39], each of which represents a major aspect of the U.S. economy. We then select one specific feature from each of the 12 groups and remove the effects of this feature on all the remaining features from the same group through random forests. More specifically, for each group, we first obtain the residual for each non-selected feature by regressing it on the selected feature in the same group using random forests, and then we replace all but the selected feature in the group with their respective residuals. The processed 81 features are then used for evaluating their feature importance. Each selected feature in Table 3 is representative of its corresponding group, and the list of the 12 selected features is in Table 3. As mentioned before, we focus our attention on three one-month ahead responses: the interest rate (FEDFUNDS), inflation (CPIAUCSL), and unemployment rate (UNRATE). More details about these 12 groups of features and the preprocessing of the data set are provided in Section C.2 of Supplementary Material.

To quantify the feature importance, we implement both the FACT with the choices of $k_n = 1$ and OOB, and the MDI for random forests. The empirical results of the MDA and CPI
Table 3: The list of selected representative features from the 12 groups. Details of these features are included in Section C.2 of Supplementary Material.

| FRED Code   | Description                                      | Remark                          |
|-------------|--------------------------------------------------|---------------------------------|
| RPI         | Real Personal Income                             | Output and income               |
| INDPRO      | IP Index                                         | Output and income               |
| UNRATE      | Civilian Unemployment Rate                       | Labor market                    |
| PAYEMS      | All Employees: Total nonfarm                     | Labor market                    |
| HOUST       | Housing Starts: Total New Privately Owned        | Housing                         |
| PERMIT      | New Private Housing Permits                       | Housing                         |
| M1SL        | M1 Money Stock                                   | Money and credit                |
| S&P 500     | S&P’s Common Stock Price Index: Composite        | Stock market                    |
| FEDFUNDS    | Effective Federal Funds Rate                     | Interest rates                  |
| TB3MS       | 3-Month Treasury Bill Interest Rate              | Interest rates                  |
| WPSFD49207  | PPI: Finished Goods                              | Prices                          |
| CPIAUCSL    | CPI: All Items                                   | Prices (inflation)              |

in this real data application are similar to those of the MDI and thus we omit those details here for simplicity. The choice of \( k_n = 1 \) for FACT is for improving the inference stability due to the relatively small sample size in this application. In Figure 3, we present the feature importance results with respect to the aforementioned three responses. In particular, the sample of observations consists of monthly data over a five-year period of January 2015 to December 2019, giving rise to a sample of size 60 with feature dimensionality \( p = 81 \). The choice of the ending period is specifically for avoiding the onset of the COVID-19 pandemic for a clean analysis of the feature importance at this stage. The one-month ahead responses (i.e., from February 2015 to January 2020 in this case) are indicated at the top of each column in Figure 3. The top panel in each column displays the feature significance results by the FACT, while the bottom panel depicts the feature importance results by the MDI for random forests. The \( x \)-axis of each plot represents the index of each of the 81 features. For the FACT test, the rejection thresholds \( t_\alpha \) at significance levels (i.e., sizes) \( \alpha = 0.1, 0.05, \) and \( 0.025 \) are 1.96, 2.25, and 2.50, respectively, in view of (17). These rejection thresholds are also marked in Figure 3 for evaluating the feature significance.

To examine the effects of time on the feature significance, we expand the time period to July 2000 to December 2020 for calculating the random forests feature p-values over time. More specifically, we consider a total of 63 five-year rolling windows ending every three months from June 2005 to December 2020. As a result, each time window contains a sample of monthly observations over the previous five years. The ends of those 63 time windows are 06/2005, 09/2005, \( \cdots \), 12/2020, respectively. For each time window, we calculate the corresponding p-values for features of interest with respect to the one-month ahead responses of FEDFUNDS and UNRATE, and report the time-varying p-values in Figure 4. With such a rolling-window analysis, we are now able to unveil the impacts of the COVID-19 pandemic on the random forests feature significance.
Figure 3: The top panel presents the feature significance results given by the FACT, while the bottom panel shows the feature importance results given by the MDI for random forests. The x-axis denotes the indices of features. The solid dots represent the relevant features selected with the false discovery rate (FDR) controlled at the 0.2 level. The values of 1.96, 2.25, and 2.50 are the rejection thresholds $t_\alpha$ for the FACT test statistic at significance levels $\alpha = 0.1, 0.05, \text{and} 0.025$, respectively.

7.2 The empirical results

Let us gain some insights into the feature significance and feature importance results for random forests shown in Figures 3 and 4. The feature p-values by the FACT are calculated using (17). To correct for the issue of multiple comparisons, we apply the widely used Benjamini–Hochberg procedure (BH) procedure [5] to select significant features with the target false discovery rate (FDR) level of 0.2. The features TB3MS and M1SL are relevant with respect to responses FEDFUNDS and UNRATE, respectively, when the FDR is taken into account; these two features are highlighted in respective left and right panels of Figure 3. In contrast, all the features are irrelevant with respect to response CPIAUCSL (i.e., inflation) after the FDR correction at the 0.2 level. It is interesting to observe that the most active feature with respect to response CPIAUCSL is S&P 500 in terms of both FACT statistic and MDI measure; S&P 500 is highlighted in the middle panel of Figure 3. We also see from Figure 3 that many features with relatively high MDI measures are inactive in terms of the FACT statistics, suggesting that the associations of these features with the responses may be spurious.

We now turn to the rolling-window random forests feature p-value curves obtained by the FACT across the 20-year period shown in Figure 4. To aid the visualization, we focus our attention on the three most active features with respect to responses FEDFUNDS and UNRATE, respectively, in terms of the FACT statistics as reported in Figure 3. The details of these features are given in the description of Figure 4. In particular, from the left panel of Figure 4, we see that only feature TB3MS remains active with respect to response FEDFUNDS across time. Indeed, both FEDFUNDS and TB3MS are crucial interest rates in the U.S. economy and thus it is natural to expect their strong relationship. In contrast, we are not aware of any obvious economic intuition for the relationship between UNRATE.
Figure 4: The two responses for random forests inference with FACT are given at the top of each panel. The left panel (for FEDFUNDS) displays the five-year rolling window p-values for features TB3MSL (black solid curve), WPSID61 (blue solid curve), and USGOVT (red dashed curve). The right panel (for UNRATE) depicts the five-year rolling window p-values for features M1SL (black solid curve), WPSID62 (blue solid curve), and S&P 500 (red dashed curve). The x-axis represents the month and year (the last two digits) of the ending time point for each five-year rolling window. The solid dots denote the random forests feature p-values that are less than 0.01, while the dashed horizontal line marks the 0.05 significance level.

and M1SL. The right panel of Figure 4 suggests that the relevance of feature M1SL with respect to response UNRATE becomes trendy toward the end of 2019 (right before the onset of the COVID-19 pandemic). However, such a trend is interrupted by the COVID-19 pandemic right after December 2019, making it unclear whether the trend would have continued if there had not been the COVID-19 pandemic. A further study on whether the trend during that time period is meaningful to the U.S. economy would be an interesting topic.

Moreover, the rolling-window p-value analysis by the FACT provides a way to unveil the effects of the COVID-19 pandemic. Many important time series have large variations during the period of the pandemic and many economic patterns, including the relevance of features, may weaken or even disappear consequently. Such a phenomenon can be observed clearly in Figure 4 after December 2019, when all the features become inactive suddenly. Such behavior of the rolling-window random forests feature p-values is interesting and not observed during the earlier financial crisis back in 2008. In summary, we have seen that the newly suggested FACT method provides a powerful tool for assessing the feature significance for random forests and testing economic intuitions. We have also demonstrated how the basic economic knowledge can be used for grouping features for improved selection power and how to exploit the rolling-window p-values for examining the feature significance across time.

8 Discussions

We have investigated in this paper the problem of feature significance testing for high-dimensional random forests. Such a high-dimensional nonparametric inference task is key to enabling interpretable machine learning inference, particularly given the rapidly growing popularity and success of random forests in various empirical applications. Among the
first attempts, we have suggested a new framework of the self-normalized feature-residual correlation test (FACT), which is grounded on the latest developments on high-dimensional random forests consistency, for providing justified random forests feature p-values under the null hypothesis that an individual feature is conditionally independent of the response given all remaining features. The general FACT test statistic incorporates both techniques of im-balancing and conditioning for debiasing, and the ensemble idea for power enhancement. Through nonasymptotic analysis, we have shown that the size of FACT is controlled at or below the desired level as sample size increases for general high-dimensional nonparametric models; such a result is robust to feature dependency. We have also established a formal nonasymptotic power analysis for FACT. The advantages of FACT compared to the existing random forests feature importance measures have been well demonstrated through simulation and real data examples in terms of bias-resistance.

Our current inference framework has focused on the case of an individual feature. In real applications, it is often of great importance to evaluate the significance of a given group of features, e.g., features that share similar economic interpretations, genetic pathways, or brain functionalities. It would be interesting to extend FACT to test the significance of a group of features for random forests. Such an extension could help address the selection power issue mentioned in Section 7, where features in the same group play a similar role in the underlying data generating process, resulting in a much weakened test power for each individual feature. In many applications such as bioinformatics [44, 21], one may probe tens of thousands of genetic features simultaneously, which gives rise to the important problem of multiple comparisons. We have shown in Section 7 that FACT coupled with the BH procedure can be employed as an empirical tool for the FDR control in the multiple testing problem. It would be interesting to formally establish the theory for such a procedure in terms of both FDR control and power.

Finally, the computational cost of FACT can become expensive when the number of features and the sample size become very large. It is thus of practical importance to develop a more scalable procedure for random forests inference in the high-dimensional big data setting. It would also be interesting to extend the suggested FACT framework to other popular machine learning methods such as deep neural networks (DNN) for interpretable deep learning inference and establish the corresponding theoretical properties. These problems are beyond the scope of the current paper and will be interesting topics for future research.

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Supplementary Material to “FACT: High-Dimensional Random Forests Inference”

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This Supplementary Material contains the proofs of Theorems 1–7, Propositions 1–4, and some technical lemmas, as well as some additional simulation and real data results. All the notation is the same as defined in the main body of the paper. Throughout the proofs, we use the generic constants such as $C$ and $K$; unless specified otherwise, these constants are independent of the sample size.

A Proofs of Theorems 1–7

A.1 Proof of Theorem 1

We will decompose the test statistic FACT$_{j,0}$ into a sum of four terms of summations and argue that the first summation is the leading term, while the other summations are asymptotically negligible. In particular, we will show that the first summation has the asymptotic normality by resorting to the central limit theorem [32, 43]. Let us begin with defining four terms $A_{li,l}=1,\cdots,4$, as

$$FACT_{j,0} = \frac{1}{\sigma_{j0}\sqrt{n}} \sum_{i=1}^{n} \left[ (Y_i - \mathbb{E}(Y_i|X_{-ij}))(g(X_{ij}) - \mathbb{E}g(X_j)) ight.$$

$$\left. + (\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}))(g(X_{ij}) - \mathbb{E}g(X_j)) ight. $$

$$\left. + (Y_i - \mathbb{E}(Y_i|X_{-ij}))(\mathbb{E}g(X_j) - n^{-1}\sum_{i=1}^{n} g(X_{ij})) ight. $$

$$\left. + (\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}) - \mu)(\mathbb{E}g(X_j) - n^{-1}\sum_{i=1}^{n} g(X_{ij})) \right)$$

$$A_{li}_i,$$

$$+ \mu(\mathbb{E}g(X_j) - n^{-1}\sum_{i=1}^{n} g(X_{ij}))\right]$$

$$= \frac{1}{\sigma_{j0}\sqrt{n}} \sum_{i=1}^{n} \left( A_{1i} + A_{2i} + A_{3i} + A_{4i} + \mu(\mathbb{E}g(X_j) - n^{-1}\sum_{i=1}^{n} g(X_{ij})))\right),$$

where $\mu = \mathbb{E}(\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j})|X_0)$.

In view of (A.1), we can write $\hat{\sigma}^2_{j0}$ as

$$\hat{\sigma}^2_{j0} = \frac{1}{n} \sum_{i=1}^{n} \left( A_{1i} + A_{2i} + A_{3i} + A_{4i} - \frac{1}{n} \sum_{i=1}^{n} (A_{1i} + A_{2i} + A_{3i} + A_{4i}) \right)^2.$$

Recall that $\sigma^2_{j0} = \text{Var}\left\{ [Y - \mathbb{E}(Y|X_{-j})] [g(X_j) - \mathbb{E}g(X_j)] \right\}$, which is bounded from above and away from zero due to Lemma 3 in Section B.7 and Condition 3.
Let us assume that $\hat{\sigma}_{j0} > 0$ for simplicity. Then by Lemma 1 in Section B.5, we can deduce that for all large $n$, each $0 < B_1 < 1$, and each $t \in \mathbb{R},$

$$\mathbb{P}(\text{FACT}_{j,0} \leq t) = \mathbb{P}(n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_{j0}t + c + (\hat{\sigma}_{j0} - \sigma_{j0})t) - n^{-1/2} \sum_{i=1}^{n} (A_{2i} + A_{3i} + A_{4i} + \mu(\mathbb{E}g(X_j) - n^{-1} \sum_{i=1}^{n} g(X_{ij}))) - c) \leq \mathbb{P}(\{n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_{j0}t + c + |\hat{\sigma}_{j0} - \sigma_{j0}|t\} \cap \mathbb{E}_{n,B_1}) + \mathbb{P}(\mathbb{E}_{n,B_1}^c) \leq \mathbb{P}(\{n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_{j0}t + c\} \cap \mathbb{E}_{n,B_1}) + \mathbb{P}(\mathbb{E}_{n,B_1}^c) \leq \mathbb{P}(n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_{j0}t + c) + \mathbb{P}(\mathbb{E}_{n,B_1}^c),$$

(A.2)

where events $\mathbb{E}_{n,B_1}$ are as given in Lemma 1 and with a slight abuse of the notation, the superscript $c$ denotes the complement of a given subset.

Next, due to the property of Gaussian distribution, it holds that for any $\sigma > 0$ and $t, x \in \mathbb{R},$

$$\left| \Phi(t + \frac{x}{\sigma}) - \Phi(t) \right| \leq 0.4 \times \frac{|x|}{\sigma}. \quad \text{(A.3)}$$

In addition, due to Condition 3 and Lemma 3, we have

$$0.4 \times \frac{c}{\sigma_{j0}} \leq \frac{4c}{5\sqrt{2} \varsigma_1}. \quad \text{(A.4)}$$

By Lemma 2 in Section B.6, the assumption of $\mathbb{E}(Y^4) < D_2$ (Condition 3), and (A.2)–(A.4), there exists some constant $C > 0$ such that for each $n \geq 1,$

$$\left| \mathbb{P}(n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_{j0}t + c) - \Phi(t) \right| \leq \left| \mathbb{P}(n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_{j0}t + c) - \Phi(t + \frac{c}{\sigma_{j0}}) \right| + \left| \Phi(t + \frac{c}{\sigma_{j0}}) - \Phi(t) \right| \leq Cn^{-1/3} + \frac{4c}{5\sqrt{2} \varsigma_1}. \quad \text{(A.5)}$$

With (A.2), Lemma 1, (A.5), and the fact that $n^{-1/3} = o(n^{-1/4}),$ we conclude the first inequality of Theorem 1.
It remains to prove the second inequality of Theorem 1. A similar probability bound can be established for the other case as well. It follows from Lemma 1 that for all large \( n \), each \( 0 < B_1 < 1 \), and each \( t \in \mathbb{R} \), we have

\[
P(\text{FACT}_{j,0} \leq t) = \mathbb{P}(n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_j t - c + (\tilde{\sigma}_j t - \sigma_j t))
- n^{-1/2} \sum_{i=1}^{n} (A_{2i} + A_{3i} + A_{4i} + \mu(Eg(X_j) - n^{-1} \sum_{i=1}^{n} g(X_{ij}))) + c
\]
\[
\geq \mathbb{P}(\{n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_j t - c\} \cap E_{n,B_1})
\]
\[
= \mathbb{P}((\{n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_j t - c\} \cap E_{n,B_1}) \cup (\{n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_j t - c\} \cap E^{c}_{n,B_1}))
- \mathbb{P}(\{n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_j t - c\} \cap E^{c}_{n,B_1})
\geq \mathbb{P}(n^{-1/2} \sum_{i=1}^{n} A_{1i} \leq \sigma_j t - c) - \mathbb{P}(E^{c}_{n,B_1}),
\]  

where the second equality above holds because a probability measure is countably additive given disjoint events. With (A.2)–(A.6) and the previous arguments, we can show that

\[
P(\{|\text{FACT}_{j,0}| > t\} = \left(1 - \mathbb{P}(\text{FACT}_{j,0} \leq t)\right) + \mathbb{P}(\text{FACT}_{j,0} < -t)
\leq 2\Phi(-t) + 2(\log n)(B_1^{1/4} + n^{-1/4}) + \frac{8c}{5\sqrt{2\varsigma_1}},
\]

which yields the desired conclusion. This completes the proof of Theorem 1.

A.2 Proof of Theorem 2

The main ideas for the proof of Theorem 2 are similar to those for the proof of Theorem 1 in Section A.1. Since we do not assume Condition 2 now, the decomposition of the feature importance statistic FACT\(_{jN/n}\) will involve two additional terms, \( \mu_1 \) and \( \mu_2 \) to be introduced.
below, for centering. Specifically, we decompose the test statistic $\text{FACT}_{jN/n}$ as

$$
\text{FACT}_{jN/n} = \frac{1}{\sigma_{jN/n} \sqrt{n}} \sum_{i=1}^{n} \left[ (Y_i - \mathbb{E}(Y_i|X_{-ij}))(g(X_{ij}) - \mathbb{E}g(X_j)) 
+ \frac{\left( (\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}))(g(X_{ij}) - \mathbb{E}g(X_j)) - \mu_1 \right)}{A_{2i}} + \mu_1 
+ (Y_i - \mathbb{E}(Y_i|X_{-ij}))(\mathbb{E}g(X_j) - n^{-1} \sum_{i=1}^{n} g(X_{ij})) 
+ \mu_2(\mathbb{E}g(X_j) - n^{-1} \sum_{i=1}^{n} g(X_{ij})) \right] 
=: \frac{1}{\sigma_{jN/n} \sqrt{n}} \sum_{i=1}^{n} \left[ A_{1i} + A_{2i} + \mu_1 + A_{3i} + A_{4i} + \mu_2(\mathbb{E}g(X_j) - n^{-1} \sum_{i=1}^{n} g(X_{ij})) \right],
$$

(A.8)

where the two additional terms $\mu_1$ and $\mu_2$ are given by

$$
\mu_1 := \mathbb{E}\left( (\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j}))(g(X_j) - \mathbb{E}g(X_j)) \middle| \lambda_0 \right),
\mu_2 := \mathbb{E}(\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j})|\lambda_0).
$$

By considering $\mu_1$ and $\mu_2$, we have that $\mathbb{E}(A_{2i}|\lambda_0) = 0$ and $\mathbb{E}(\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}) - \mu_2|\lambda_0) = 0$.

Next, in light of (A.8), we can deduce that

$$
\mathbb{P}\left( \left| \text{FACT}_{jN/n} \right| > t \right) 
\leq \mathbb{P}\left( \left| n^{-1/2} \sum_{i=1}^{n} A_{1i} \right| > \sigma_{jN/n} t - c - |\sigma_{jN/n} - \sigma_{jN/n}|t - Q_1 - Q_2 - \sqrt{n} |\mu_1| + c \right),
$$

(A.9)

where $Q_1 := \sqrt{n} \sum_{i=1}^{n} (A_{2i} + A_{3i} + A_{4i})$, $Q_2 := \sqrt{n} |\mu_2| \left\{ \mathbb{E}g(X_j) - n^{-1} \sum_{i=1}^{n} g(X_{ij}) \right\}$, and

$$
\sigma_{jN/n}^2 := \text{Var}\left\{ (Y - \mathbb{E}(Y|X_{-j}))(g(X_j) - \mathbb{E}g(X_j)) \right\},
$$

which is bounded from above and away from zero due to Lemma 3 in Section B.7 and Condition 3. Notice that $(\sigma_{jN/n})^2 = (\sigma_0)^2$. We will resort to Lemma 4 in Section B.8 to analyze the right-hand side (RHS) of (A.9). Specifically, an application of Lemma 4 shows
that for all large $n$, each $0 < B_1 < 1$, and each $t > 0$,

$$\text{RHS of (A.9)} \leq P\left(\left\{n^{-1/2} \sum_{i=1}^{n} A_{1i} > \sigma_{jN/n} t - c \right\} \cap E_{n,B_1} \right) + P(E_{n,B_1}^c),$$

$$\leq P(E_{n,B_1}^c) + P\left(n^{-1/2} \sum_{i=1}^{n} A_{1i} > \sigma_{jN/n} t - c \right),$$

(A.10)

where event $E_{n,B_1}$ is given in Lemma 4.

Moreover, it follows from Lemma 2 and the assumption of $E(Y^4) < D_2$ (Condition 3) that for each $n, B_1 > 0$, we have

$$\sup_{t>0} \left| P\left(n^{-1/2} \sum_{i=1}^{n} \frac{A_{1i}}{\sigma_{jN/n}} > t - \frac{c}{\sigma_{jN/n}} \right) - 2\Phi\left(-t + \frac{c}{\sigma_{jN/n}}\right) \right| \leq Cn^{-1/3},$$

(A.11)

where $C > 0$ is some constant. Therefore, by (A.11), Lemma 4, and (A.3)–(A.4), it holds that for all large $n$, each $0 < B_1 < 1$, and each $t > 0$,

$$\text{RHS of (A.10)} \leq 2\Phi(-t) + \frac{8c}{5\sqrt{2}\xi_1} + (\log n)(B_1^{1/4} + n^{-1/4}) + (-\log B_1)^{-1},$$

which concludes the proof of Theorem 2.

### A.3 Proof of Theorem 3

The main ingredients of the proof for Theorem 3 are similar to those of the proof for Theorem 1 in Section A.1. We would like to mention that although the FACT test with conditioning is a GCM test [47], their proof techniques and results for the analysis of GCM in their Theorem 6 mostly do not apply here, because we aim to establish nonasymptotic results and our conditions are different from theirs (population versus sample versions).

Let us decompose the test statistic $\text{FACT}_{j|iX_{-j}}$ defined in (11) as

$$\text{FACT}_{j|iX_{-j}} = \frac{1}{\hat{\sigma}_{j|iX_{-j}}/\sqrt{n}} \sum_{i=1}^{n} \left[ (Y_i - \mathbb{E}(Y_i|X_{-ij}))(g(X_{ij}) - \mathbb{E}(g(X_{ij})|X_{-ij})) \right.\right.

$$

$$\left. + \left(\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}_i(X_{-ij})\right) \left(\mathbb{E}(g(X_{ij})|X_{-ij}) - \hat{g}(X_{-ij})\right) \right.\left.\right.

$$

$$\left. + \left(Y_i - \mathbb{E}(Y_i|X_{-ij})\right) \left(\mathbb{E}(g(X_{ij})|X_{-ij}) - \hat{g}(X_{-ij})\right) \right.\left.\right.

$$

$$\left. + \left(\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}_i(X_{-ij})\right) \left(\mathbb{E}(g(X_{ij})|X_{-ij}) - \hat{g}(X_{-ij})\right) - \mu\right]_{\text{A}4i} + \mu, (A.12)$$

$$= \frac{1}{\hat{\sigma}_{j|iX_{-j}}/\sqrt{n}} \sum_{i=1}^{n} \left( A_{1i} + A_{2i} + A_{3i} + A_{4i} + \mu \right),$$

where $\mu = \mathbb{E}\left[\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}_i(X_{-ij})\right] \mathbb{E}(g(X_{ij})|X_{-ij}) - \hat{g}(X_{-ij})]\mathbb{X}_0]$. Observe that random variables $A_{1i}, A_{2i}, A_{3i}, A_{4i}$ given in (A.12) all have zero mean conditional on $X_0$ by construc-
tion. For a null feature $X_j$, it holds that

$$(\sigma_j | X_{-j})^2 := \text{Var}\{ [Y - \mathbb{E}(Y|X_{-j})] [g(X_j) - \mathbb{E}(g(X_j)|X_{-j})] \}$$

$$= \mathbb{E}\{ [Y - \mathbb{E}(Y|X_{-j})] [g(X_j) - \mathbb{E}(g(X_j)|X_{-j})] \}^2,$$

which is bounded from above and away from zero due to Lemma 3 in Section B.7 and Condition 3. In view of (A.12), some simple calculations lead to

$$\left\{ \frac{\sum_{i=1}^n A_{1i}}{\sqrt{n}} > t \right\} \subset \left\{ \left| \sum_{i=1}^n A_{1i} \right| > \sigma_j | X_{-j} | t - c + c - |\hat{\sigma}_j | X_{-j} | - \sigma_j | X_{-j} | t - \sqrt{n} |\mu| - n^{-1/2} \sum_{i=1}^n \sum_{l=2,3,4} A_{li} \right\}. \quad \text{(A.13)}$$

Next, we apply similar arguments to those in the proof of Theorem 1 to deal with the RHS of (A.13). In particular, the arguments below are similar to those for the proof of Lemma 1 in Section B.5, and hence we will omit some of the technical details here for simplicity. First, we establish upper bounds on $|\hat{\sigma}_j | X_{-j} | - \sigma_j | X_{-j} |$, $\sqrt{n} |\mu|$, and $n^{-1/2} \sum_{i=1}^n \sum_{l=2,3,4} A_{li}$, respectively. To this end, let us define eight events below

$$E_1^\mathbb{C} := \{ |n^{-1/2} \sum_{i=1}^n A_{1i}| \geq n^{1/4} \}, \quad E_2^\mathbb{C} := \{ |n^{-1/2} \sum_{i=1}^n A_{2i}| \geq B_1^{1/4} \},$$

$$E_3^\mathbb{C} := \{ |n^{-1/2} \sum_{i=1}^n A_{3i}| \geq B_2^{1/4} \}, \quad E_4^\mathbb{C} := \{ |n^{-1/2} \sum_{i=1}^n A_{4i}| \geq B_1^{1/4} \},$$

$$E_5^\mathbb{C} := \{ |n^{-1} \sum_{i=1}^n A_{2i}| \geq B_1^{1/2} \}, \quad E_6^\mathbb{C} := \{ |n^{-1} \sum_{i=1}^n A_{3i}| \geq B_2^{1/2} \},$$

$$E_7^\mathbb{C} := \{ |n^{-1} \sum_{i=1}^n A_{4i}| \geq B_1^{1/2} \}, \quad E_8^\mathbb{C} := \{ |n^{-1/2} \sum_{i=1}^n (A_{1i}^2 - \sigma_j^2 | X_{-j} |) \geq n^{1/4} \},$$

$$E_9^\mathbb{C} := \{ |\mu| \geq \sqrt{nB_1B_2 (-\log (B_1B_2))} \}$$

without specifying the dependence on $n$ and the convergence rates $B_1$ and $B_2$. Next, to deal with the term $|\hat{\sigma}_j | X_{-j} | - \sigma_j | X_{-j} |$, we use the following upper bound, which is similar to (A.75). From the definition of $\hat{\sigma}_j | X_{-j} |$ and (A.72)–(A.74), we can show that if $\sigma_j^2 | X_{-j} | \geq n^{-1} \sum_{i=1}^n (A_{1i}^2 - \sigma_j^2 | X_{-j} |)$,

$$|\hat{\sigma}_j | X_{-j} | - \sigma_j | X_{-j} | \leq \frac{1}{\theta_1} \sum_{i=1}^n (A_{1i}^2 - \sigma_j^2 | X_{-j} |)$$

$$+ \sum_{l=2}^4 \sqrt{n^{-1} \sum_{i=1}^n A_{li}^2 + n^{-1} \sum_{i=1}^n (A_{1i} + A_{2i} + A_{3i} + A_{4i})}.$$ 

By (A.14), it holds on event $\bigcap_{i=1}^9 E_i$ that for all large $n$,

$$|\hat{\sigma}_j | X_{-j} | - \sigma_j | X_{-j} | \leq n^{-1/4} \log n + 4B_1^{1/4} + 2B_2^{1/4}. \quad \text{(6)}$$
In addition, on event $\cap_{l=1}^4 E_l$, we can show that for all large $n$,

$$n^{-1/2} \left| \sum_{i=1}^n \sum_{l=2,3,4} A_{li} \right| \leq 2B_1^{1/4} + B_2^{1/4}.$$ 

Moreover, on event $E_9$, it holds that

$$\sqrt{n}|\mu| \leq \sqrt{nB_1B_2(-\log (B_1B_2))}.$$ 

From these upper bounds, the definition of $c$, and (A.13), it holds on event $\cap_{l=1}^9 E_l$ that for all large $n$, each $t > 0$, and each $B_1, B_2 > 0$,

$$\left\{ \left| \text{FACT}_{j|X_{-j}} \right| > t \right\} \leq \left\{ \left| \frac{\sum_{l=1}^n A_{lj}}{\sqrt{n}} \right| > \sigma_{j|X_{-j}} t - c \right\},$$

where we recall that

$$c = tn^{-1/4} \log n + (2t + 1)(2B_1^{1/4} + B_2^{1/4}) + \sqrt{nB_1B_2(-\log (B_1B_2))}.$$ 

Thus, an application of Lemma 2 along with the regularity assumptions (see (A.7) for details), (A.15), and arguments for (A.3)–(A.5) yields that for some $C > 0$, all large $n$, each $t > 0$, and each $B_1, B_2 > 0$, we have

$$\mathbb{P}(\left| \text{FACT}_{j|X_{-j}} \right| > t) \leq 2\Phi(-t) + \frac{8c}{5\sqrt{2}\varsigma_1} + Cn^{-1/3} + \sum_{l=1}^9 \mathbb{P}(E_l^c).$$

(A.16)

It remains to upper bound the probabilities $\mathbb{P}(E_1^c), \ldots, \mathbb{P}(E_9^c)$ that appear in (A.16) above. Let us begin with the bound for term $\mathbb{P}(E_3^c)$. Note that we have $\mathbb{E}(A_{3i}|X_0) = 0$. Then using Markov’s inequality, the Burkholder–Davis–Gundy inequality [13], and Jensen’s inequality, we can show that there exists some $K > 0$ such that for all large $n$ and each $B_2 > 0$,

$$\mathbb{P}(E_3^c) \leq B_2^{-1/4} \mathbb{E}|n^{-1/2} \sum_{i=1}^n A_{3i}|$$

$$\leq B_2^{-1/4} K \left( n^{-1} \sum_{i=1}^n \mathbb{E}(A_{3i})^2 \right)^{1/2}$$

$$= B_2^{-1/4} K \left\{ \mathbb{E} \left[ (Y - \mathbb{E}(Y|X_{-j}))^2 [\mathbb{E}(g(X_j)|X_{-j}) - \hat{g}(X_{-j})]^2 \right] \right\}^{1/2}$$

$$= B_2^{-1/4} K \left\{ \mathbb{E} \left[ (Y - \mathbb{E}(Y|X_{-j}))^2 |X_0, X_{-j}| [\mathbb{E}(g(X_j)|X_{-j}) - \hat{g}(X_{-j})]^2 \right] \right\}^{1/2}$$

$$\leq B_2^{-1/4} D^{1/2} K \left\{ \mathbb{E} \left[ (Y - \mathbb{E}(Y|X_{-j}))^2 |X_{-j}| \right] \right\}^{1/2}$$

$$\leq B_2^{1/4} D^{1/2} K,$$

where the first equality above is due to the fact that $(X,Y)$ and $(X_i, Y_i)$ have the same distribution for each $i$, the second equality is because $\mathbb{E}(g(X_j)|X_{-j})$ and $\hat{g}(X_{-j})$ are $\sigma(X_0, X_{-j})$-measurable, the third inequality is entailed by the assumptions that $\mathbb{E}\{ (Y - \mathbb{E}(Y|X_{-j}))^2 |X_{-j}\}$
\[ \text{Var}(Y|X_{-j}) \leq D \text{ (see Condition 3)} \] and \( X_0 \) is an independent sample, and the last inequality utilizes Condition 4. For more details about the application of the Burkholder–Davis–Gundy inequality, see (A.76) in the proof of Lemma 1 in Section B.5.

The arguments for the rest of the upper bounds are similar to those for (A.17). Hence, we will omit the technical details here for simplicity and stress only which consistency condition among Condition 1, Condition 4, and (A.18) below will be needed for each upper bound. Because random forests makes predictions via conditional sample averages and we have assumed \( 0 \leq g(X_j) \leq 1 \), it holds that \( 0 \leq \hat{g}(X_{-j}) \leq 1 \). By \( 0 \leq \hat{g}(X_{-j}) \leq 1 \), Condition 1, and the assumption that \( 0 \leq g(x) \leq 1 \), we can deduce that

\[
\begin{align*}
\mathbb{E}\{(\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j})) &\mathbb{E}(g(X_j)|X_{-j}) - \hat{g}(X_{-j})) - \mu\}^2 \\
&\leq \mathbb{E}\{(\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j}))|\mathbb{E}(g(X_j)|X_{-j}) - \hat{g}(X_{-j})\}^2 \\
&\leq \mathbb{E}[\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j})]^2
\end{align*}
\]

(A.18)

It follows from (A.18) and other regularity conditions that there exists some \( K > 0 \) such that for all large \( n \) and each \( B > 0 \),

\[ \mathbb{P}(E_4^c) \leq KB_1^{1/4}. \] (A.19)

By Condition 1 and other regularity conditions, there exists some \( K > 0 \) such that for all large \( n \) and each \( B > 0 \),

\[ \mathbb{P}(E_2^c) \leq KB_1^{1/4}. \] (A.20)

From Condition 4 and other regularity conditions, we can show that for all large \( n \) and \( B_2 > 0 \),

\[ \mathbb{P}(E_6^c) \leq DB_2^{1/2}. \] (A.21)

Furthermore, by Condition 1 and other regularity conditions, we can deduce that for all large \( n \) and \( B_1 > 0 \),

\[ \mathbb{P}(E_5^c) \leq B_1^{1/2}. \] (A.22)

An application of (A.18) and other regularity conditions yields that for all large \( n \) and \( B_1 > 0 \),

\[ \mathbb{P}(E_7^c) \leq 4B_1^{1/2}. \] (A.23)

In addition, by the assumptions, we can show that there exists some \( C > 0 \) such that for all large \( n \),

\[ \mathbb{P}(E_5^c) \leq Cn^{-1/4}, \]
\[ \mathbb{P}(E_7^c) \leq Cn^{-1/4}. \] (A.24)

By Markov’s inequality, Jensen’s inequality, the Cauchy–Schwartz inequality, and Condi-
tions 1 and 4, it holds that for all $n \geq 1$, each $B_1, B_2 > 0$, and each $t > 0$,
\[
\mathbb{P}(E_0^c) \leq \mathbb{E}\left[\mathbb{E}\left(\left[\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j})\right]\left[\mathbb{E}(g(X_j)|X_{-j}) - \hat{g}(X_{-j})\right]\right)\right] (-\log(B_1B_2))^{-1} \leq (-\log(B_1B_2))^{-1}.
\]

This completes the proof of Theorem 3.

A.4 Proof of Theorem 4

The main ideas for the proof of Theorem 4 are similar to those for the proof of Theorem 1 in Section A.1. The major differences are that 1) the transformation $g^{(f)}$ has a superscript which makes no difference in terms of the technical analysis and 2) we now consider a union of multiple events. For completeness, we still provide a formal proof but omit some of the technical details. Let us decompose the test statistic $FACT^{(f)}_j$ as
\[
FACT^{(f)}_j = \frac{1}{\tilde{\sigma}_j^{(f)}} \sum_{i=1}^{n} \left[ \left( Y_i - \mathbb{E}(Y_i|X_{-ij}) \right) (g^{(f)}(X_{ij}) - \mathbb{E}g^{(f)}(X_j)) + \left( \mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}) \right) (g^{(f)}(X_{ij}) - \mathbb{E}g^{(f)}(X_j)) + \left( Y_i - \mathbb{E}(Y_i|X_{-ij}) \right) (\mathbb{E}g^{(f)}(X_j) - n^{-1} \sum_{i=1}^{n} g^{(f)}(X_{ij})) + \left( \mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}) - \mu \right) (\mathbb{E}g^{(f)}(X_j) - n^{-1} \sum_{i=1}^{n} g^{(f)}(X_{ij})) + \mu (\mathbb{E}g^{(f)}(X_j) - n^{-1} \sum_{i=1}^{n} g^{(f)}(X_{ij})) \right] = \frac{1}{\tilde{\sigma}_j^{(f)}} \sum_{i=1}^{n} \left[ A^{(f)}_{1i} + A^{(f)}_{2i} + A^{(f)}_{3i} + A^{(f)}_{4i} + \mu \right],
\]
where $\mu = \mathbb{E}(\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j})|\mathbf{X}_0)$. In light of (A.26), we can deduce that
\[
\mathbb{P}\left( \bigcup_{i \in L} \left\{ \left| FACT^{(f)}_j \right| > t \right\} \right) \leq \mathbb{P}\left( \bigcup_{i \in L} \left\{ \left| n^{-1/2} \sum_{i=1}^{n} A^{(f)}_{ki} \right| > |\sigma_j^{(f)}| t - c \right\} \right) \leq \mathbb{P}\left( \bigcup_{i \in L} \left\{ \left| n^{-1/2} \sum_{i=1}^{n} A^{(f)}_{ki} \right| > |\sigma_j^{(f)}| t - c \right\} \right)
\]
\[
\leq \mathbb{P}\left( \bigcup_{i \in L} \left\{ \left| n^{-1/2} \sum_{i=1}^{n} A^{(f)}_{ki} \right| > |\sigma_j^{(f)}| t - c \right\} \right) \leq \mathbb{P}\left( \bigcup_{i \in L} \left\{ \left| n^{-1/2} \sum_{i=1}^{n} A^{(f)}_{ki} \right| > |\sigma_j^{(f)}| t - c \right\} \right) \leq \mathbb{P}\left( \bigcup_{i \in L} \left\{ \left| n^{-1/2} \sum_{i=1}^{n} A^{(f)}_{ki} \right| > |\sigma_j^{(f)}| t - c \right\} \right).
\]
where we define $(\sigma_j^{(l)})^2 := \text{Var}\{[Y - \mathbb{E}(Y|X_{-j})][g^{(l)}(X_j) - \mathbb{E}(g^{(l)}(X_j))]\}$. Note that $(\sigma_j^{(l)})^2$ is bounded from above and away from zero due to Lemma 3 in Section B.7 and Condition 3.

Since the set cardinality $|L|$ is a constant and all the conditions of Lemma 1 are satisfied, an application of Lemma 1 yields that for some constant $C > 0$, all large $n$, each $0 < B_1 < 1$, and each $t > 0$, there exist some events $\{E_{n,B_1}\}$ such that 1) $\mathbb{P}(E_{n,B_1}^c) \leq C(B_1^{1/4} + n^{-1/4})$ and 2) on event $E_{n,B_1}$, it holds that

$$c \geq |\hat{\sigma}_j^{(l)} - \sigma_j^{(l)}| t + |n^{-1/2} \sum_{i=1}^{n} \sum_{k=2}^{4} A_{ki}^{(l)}| + \sqrt{n}|\mu||E_j^{(l)}(X_{ij}) - n^{-1} \sum_{i=1}^{n} g^{(l)}(X_{ij})|$$

for each $l \in L$.

Then it follows from the definition of event $E_{n,B_1}$ that for all large $n$, each $0 < B_1 < 1$, and each $t > 0$,

$$\text{RHS of (A.27)} \leq \mathbb{P} \left( \left( \bigcup_{l \in L} \left\{ n^{-1/2} \sum_{i=1}^{n} A_{ii}^{(l)} > \sigma_j^{(l)} t - c \right\} \right) \cap E_{n,B_1} \right) + \mathbb{P}(E_{n,B_1}^c) \leq \sum_{l \in L} \mathbb{P} \left( n^{-1/2} \sum_{i=1}^{n} A_{ii}^{(l)} > \sigma_j^{(l)} t - c \right) + \mathbb{P}(E_{n,B_1}^c). \quad (A.28)$$

Moreover, we can apply Lemma 2 to show that there exists some $C > 0$ such that for each $n > 0$ and $l \in L$,

$$\sup_{t \geq 0} \mathbb{P}(n^{-1/2} \sum_{i=1}^{n} A_{ii}^{(l)} > (\sigma_j^{(l)}) t - c) - 2\Phi(-t + \frac{c}{\sigma_j^{(l)}}) \leq Cn^{-1/3}. \quad (A.29)$$

Therefore, from the definition of event $E_{n,B_1}$, (A.29), the arguments for (A.3)–(A.5), and that $|L|$ is a constant, it holds that for all large $n$, each $0 < B_1 < 1$, and each $t > 0$,

$$\text{RHS of (A.28)} \leq 2|L|\Phi(-t) + \frac{8|L|c}{5\sqrt{2\pi}1} + (\log n)(B_1^{1/4} + n^{-1/4}),$$

which concludes the proof of Theorem 4.

### A.5 Proof of Theorem 5

The main ingredients of the proof for Theorem 5 are similar to those of the proofs for Theorems 1 and 3 in Sections A.1 and A.3, respectively. By the definition of the test statistic $\text{FACT}_j$, it holds that

$$\mathbb{P}(\text{FACT}_j > t) \leq \mathbb{P} \left( \bigcup_{1 \leq l \leq 2, q \in Q} \left\{ \left| \text{FACT}_{j,q}^{(l)} \right| > t \right\} \right). \quad (A.30)$$

To upper bound the left-hand side of (A.30), it suffices to bound each term on the RHS of (A.30) above. Without loss of generality, let us consider the case when $l = 1$ and $q = 1$. We
define terms $A_{1i}, \ldots, A_{4i}$ with $i \in \mathcal{N}_1$ as given by the following decomposition

$$\text{FACT}^{(1)}_{j,1} = \frac{1}{\hat{\sigma}^{(1)}_{j|\mathbf{X}_{-j}} \sqrt{|\mathcal{N}_1|}} \sum_{i \in \mathcal{N}_1} \left[ (Y_i - \mathbb{E}(Y_i|\mathbf{X}_{-ij}))(g^{(1)}(X_{ij}) - \mathbb{E}(g^{(1)}(X_{ij})|\mathbf{X}_{-ij})) ight. $$

$$+ \left. (\mathbb{E}(Y_i|\mathbf{X}_{-ij}) - \hat{Y}(\mathbf{X}_{-ij}))(g^{(1)}(X_{ij}) - \mathbb{E}(g^{(1)}(X_{ij})|\mathbf{X}_{-ij})) + \mathbb{E}(Y_i|\mathbf{X}_{-ij}) - \hat{Y}(\mathbf{X}_{-ij})) \right] $$

$$(A.31)$$

$$+ \left( \mathbb{E}(Y_i|\mathbf{X}_{-ij}) - \hat{Y}(\mathbf{X}_{-ij})) (g^{(1)}(X_{ij}) - \mathbb{E}(g^{(1)}(X_{ij})|\mathbf{X}_{-ij})) - \mu^{(1)} \right) + \mu^{(1)} \right]$$

where $\mu^{(1)} = \mathbb{E}\left\{ \left[ \mathbb{E}(Y|\mathbf{X}_{-j}) - \hat{Y}(\mathbf{X}_{-j}) \right] \left[ \mathbb{E}(g^{(1)}(X_j)|\mathbf{X}_{-j}) - \hat{g}^{(1)}(\mathbf{X}_{-j}) \right] \right\} |\mathcal{X}_0}$. Further, we define terms $A_{1i}, \ldots, A_{4i}$ with $i \in \{1, \ldots, n\} \setminus \mathcal{N}_1$ similarly. From (A.31), we can see that each of random variables $A_{1i}, A_{2i}, A_{3i}, A_{4i}$ has zero mean conditional on $\mathcal{X}_0$ by construction.

For each null feature $X_j$, it holds that

$$(\sigma^{(1)}_{j|\mathbf{X}_{-j}})^2 := \text{Var}\left\{ \left[ Y - \mathbb{E}(Y|\mathbf{X}_{-j}) \right] \left[ g^{(1)}(X_j) - \mathbb{E}(g^{(1)}(X_j)|\mathbf{X}_{-j}) \right] \right\}$$

$$= \mathbb{E}\left\{ \left[ Y - \mathbb{E}(Y|\mathbf{X}_{-j}) \right] \left[ g^{(1)}(X_j) - \mathbb{E}(g^{(1)}(X_j)|\mathbf{X}_{-j}) \right] \right\}^2,$$

which is bounded from above and away from zero due to Lemma 3 in Section B.7 and Condition 3.

Then from (A.31), we can deduce that

$$\left\{ \text{FACT}^{(1)}_{j,1} > \ell \right\} \subset \left\{ \left| \sum_{i \in \mathcal{N}_1} A_{1i} \right| > \sigma^{(1)}_{j|\mathbf{X}_{-j}} t - c + c - |\hat{\sigma}^{(1)}_{j|\mathbf{X}_{-j}} - \sigma^{(1)}_{j|\mathbf{X}_{-j}}| t - |\mu^{(1)}| \sqrt{|\mathcal{N}_1|} \right. $$

$$- \left. |\mathcal{N}_1|^{-1/2} \left| \sum_{i \in \mathcal{N}_1} \sum_{l=2,3,4} A_{li} \right| \right\}. $$

(A.32)

We can resort to the similar arguments to those in the proof of Theorem 1 in Section A.1 to deal with the RHS of (A.32). In particular, the technical arguments are similar to those for the proof of Lemma 1 in Section B.5, and thus the full details are omitted here for simplicity. It follows from the definition of $(\hat{\sigma}^{(1)}_{j|\mathbf{X}_{-j}})^2$ and (A.72)–(A.74) that if $(\sigma^{(1)}_{j|\mathbf{X}_{-j}})^2 \geq \left| n^{-1} \sum_{i=1}^{n} (A_{1i}^2 - (\sigma^{(1)}_{j|\mathbf{X}_{-j}})^2) \right|$, we have

$$|\hat{\sigma}^{(1)}_{j|\mathbf{X}_{-j}} - \sigma^{(1)}_{j|\mathbf{X}_{-j}}| \leq \left| \frac{1}{n \sigma^{(1)}_{j|\mathbf{X}_{-j}}} \sum_{i=1}^{n} (A_{1i}^2 - (\sigma^{(1)}_{j|\mathbf{X}_{-j}})^2) \right| $$

$$+ 4 \sqrt{n^{-1} \sum_{i=1}^{n} A_{1i}^2 + n^{-1} \sum_{i=1}^{n} (A_{1i} + A_{2i} + A_{3i} + A_{4i})}, $$

(A.33)
It remains to upper bound terms $|\sigma_{ij}^{(1)} - \sigma_{ij}^{(1)}|, |\mu(1)| \sqrt{|N_1|}$, and $|N_1|^{-1/2} \sum_{i \in N_1} \sum_{t=2,3,4} A_{it}$ separately. We define some key events below

\[
E_1 := \{|n^{-1/2} \sum_{i=1}^n A_{i1}| \geq n^{1/4}\}, \quad E_2 := \{|n^{-1/2} \sum_{i=1}^n A_{i2}| \geq B_1^{1/4}\},
\]

\[
E_3 := \{|n^{-1/2} \sum_{i=1}^n A_{i3}| \geq B_2^{1/4}\}, \quad E_4 := \{|n^{-1/2} \sum_{i=1}^n A_{i4}| \geq B_1^{1/4}\},
\]

\[
E_5 := \{|n^{-1} \sum_{i=1}^n A_{i2}^2| \geq B_1^{1/2}\}, \quad E_6 := \{|n^{-1} \sum_{i=1}^n A_{i3}^2| \geq B_2^{1/2}\},
\]

\[
E_7 := \{|n^{-1} \sum_{i=1}^n A_{i4}^2| \geq B_1^{1/2}\}, \quad E_8 := \{|n^{-1/2} \sum_{i=1}^n (A_{i1}^2 - (\sigma_{ij}^{(1)}|X_{-j})^2)| \geq n^{1/4}\},
\]

\[
E_9 := \{||N_1|^{-1/2} \sum_{i \in N_1} A_{i1}| \geq B_1^{1/4}\}, \quad E_{10} := \{||N_1|^{-1/2} \sum_{i \in N_1} A_{i2}| \geq B_2^{1/4}\},
\]

\[
E_{11} := \{||N_1|^{-1/2} \sum_{i \in N_1} A_{i3}| \geq B_1^{1/4}\}, \quad E_{12} := \{\max\{\mu(1), |\mu(2)|\} \geq \sqrt{B_1 B_2 (- \log (B_1 B_2))}\},
\]

where $\mu(2) = \mathbb{E}\left[\mathbb{E}(Y|X_{-j}) - \hat{\sigma}_{ij}^{(1)}(X_{-j})|X_{-j}) - \hat{\sigma}_{ij}^{(2)}(X_{-j})|X_{-j}\right]|\mathcal{X}_0$, and we do not specify the dependence on $n$ and the convergence rates $B_1$ and $B_2$. Then in view of (A.33), there exists some $N_1 > 0$ such that on event $\cap_{i=1}^8 E_i$, for all $n \geq N_1$ and $B_1, B_2 > 0$, we have

\[
|\hat{\sigma}_{ij}^{(1)}(X_{-j}) - \sigma_{ij}^{(1)}(X_{-j})| \leq n^{-1/4} \log n + 4B_1^{1/4} + 2B_2^{1/4}.
\]

(A.34)

In addition, there exists some $N_2 > 0$ such that on event $\cap_{i=9}^{11} E_i$, it holds that for all $n \geq N_2$ and $B_1, B_2 > 0$,

\[
|N_1|^{-1/2} \sum_{i \in N_1} \sum_{t=2,3,4} A_{it}| \leq 2B_1^{1/4} + B_2^{1/4}.
\]

Moreover, on event $E_{12}$, we have

\[
\sqrt{|N_1|} \mu(1) \leq \sqrt{nB_1 B_2 (- \log (B_1 B_2))}.
\]

From the above upper bounds, the definition of $c$, and (A.32), we can deduce that on event $\cap_{i=1}^{12} E_i$, for all $n \geq \max\{N_1, N_2\}$ and $B_1, B_2 > 0$ we have

\[
\left\{|\text{FACT}_{j,1}^{(1)}| > t\right\} \subset \left\{|\sum_{i \in N_1} A_{i1}| > \sigma_{ij}^{(1)}(X_{-j}) t - c\right\},
\]

(A.35)

where we recall that

\[
c = tn^{-1/4} \log n + (2t + 1)(2B_1^{1/4} + B_2^{1/4}) + \sqrt{nB_1 B_2 (- \log (B_1 B_2))}.
\]

Then an application of Lemma 2, (A.35), and arguments for (A.3)–(A.5) yields that there
exist some $N_3, C > 0$ such that for all $n \geq N_3$, each $B_1, B_2 > 0$, and each $t > 0$,

$$
P(|\text{FACT}_{j,q}^{(i)}| > t) \leq 2\Phi(-t) + \frac{8c}{5\sqrt{2}\pi} + C|N_q|^{-1/3} + \sum_{i=1}^{12} P(E^c_{i,q}). \quad (A.36)
$$

To establish similar results for the cases with $l \in \{1, 2\}$ and $q \in Q$, let us respectively define events $E_{1,l}^c, \ldots, E_{9,q,l}^c, E_{10,q,l}^c, E_{11,q,l}^c$ as $E_1^c, \ldots, E_{11}^c$, but with $N_q$ and $g^{(l)}$ instead for each $l \in \{1, 2\}$ and $q \in \{2, \ldots, |Q|\}$. Note that only events $E_{9,q,l}, E_{10,q,l}, E_{11,q,l}$ depend on $q \in Q$. Define $E^* := (\cap_{1 \leq k \leq 8, 1 \leq l \leq 2} E_{k,l}) \cap (\cap_{9 \leq k \leq 11, 1 \leq l \leq 2} q \in Q E_{k,q,l}) \cap E_{12}$. It holds that

$$
P\left(\bigcup_{1 \leq l \leq 2, q \in Q} \left\{|\text{FACT}_{j,q}^{(l)}| > t\right\}\right) \leq P\left(\bigcup_{1 \leq l \leq 2, q \in Q} \left\{|\text{FACT}_{j,q}^{(l)}| > t\right\} \cap E^*\right) + P(E^*) \\
\leq \sum_{1 \leq l \leq 2, q \in Q} P\left(|\text{FACT}_{j,q}^{(l)}| > t\right) + P(E_{12}^c) + \sum_{9 \leq i \leq 11, 1 \leq l \leq 2, q \in Q} P(E_{i,q,l}^c) + \sum_{1 \leq l \leq 8, 1 \leq l \leq 2} P(E_{i,q,l}^c). \quad (A.37)
$$

Then a similar probability bound as in (A.36) can be obtained for the first term on the RHS of (A.37) for each $l$ and $q$. Specifically, for all $n \geq N_3$, each $B_1, B_2 > 0$, and each $t > 0$,

$$
\text{RHS of (A.37)} \\
\leq 4|Q|\Phi(-t) + \frac{16|Q|c}{5\sqrt{2}\pi} + 2C \sum_{q \in Q} |N_q|^{-1/3} + P(E_{12}^c) \\
\quad + \sum_{9 \leq i \leq 11, 1 \leq l \leq 2, q \in Q} P(E_{i,q,l}^c) + \sum_{1 \leq l \leq 8, 1 \leq l \leq 2} P(E_{i,q,l}^c), \quad (A.38)
$$

where constant $C > 0$ is given in (A.36).

To deal with term $|N_q|$, recall that $|N_q| \geq \frac{n}{|Q|} - 1$ by the definition of $N_q$. Hence, it holds that

$$
|N_q|^{-1/3} \leq \left(\frac{|Q|}{n - |Q|}\right)^{1/3}. \quad (A.39)
$$

Furthermore, to bound the probabilities of events $E_{i,q,l}^c$’s, we can apply similar arguments as in (A.17) in the proof of Theorem 3 in Section A.3 to obtain that there exist some $C, N_0 > 0$ such that for all $n \geq N_0$, all $0 < B_1, B_2 < 1$ (see Section A.3 for details of the requirements on $B_1, B_2 < 1$),

$$
\sum_{9 \leq i \leq 11, 1 \leq l \leq 2, q \in Q} P(E_{i,q,l}^c) + \sum_{1 \leq l \leq 8, 1 \leq l \leq 2} P(E_{i,q,l}^c) \leq 2|Q|(n^{-1/4} + B_1^{1/4} + B_2^{1/4}). \quad (A.40)
$$

By Conditions 1 and 4 and an argument similar to that for (A.25), it holds that for each $0 < B_1, B_2 < 1$, $t > 0$, and all $n \geq 1$,

$$
P(E_{12}^c) \leq 2(-\log (B_1 B_2))^{-1}. \quad (A.41)$$
Note that constants $N_0, N_1, N_2, N_3, C$ above are independent of the feature index $1 \leq j \leq p$. Therefore, a combination of (A.30) and (A.37)–(A.41) completes the proof of Theorem 5.

A.6 Proof of Theorem 6

The main idea of the proof for this theorem is to use the fact that $|\kappa_j^{(l)}| > 0$ for some $l \in L$ and that $\text{FACT}_j^{(l)} - \sqrt{n} \frac{\kappa_j^{(l)}}{\hat{\sigma}_j^{(l)}}$ is centered at zero asymptotically to establish the desired probability upper bound.

In light of the assumption $\sum_{s \in L} |\kappa_j^{(s)}| > 0$, let some $l \in L$ with $|\kappa_j^{(l)}| > 0$ be fixed. We deduce that

$$
\mathbb{P} \left( \cap_{s \in L} \left\{ \left| \text{FACT}_j^{(s)} \right| \leq t \right\} \right)
= \mathbb{P} \left( \cap_{s \in L} \left\{ \left| \text{FACT}_j^{(s)} - \sqrt{n} \frac{\kappa_j^{(s)}}{\hat{\sigma}_j^{(s)}} + \sqrt{n} \frac{\kappa_j^{(s)}}{\hat{\sigma}_j^{(s)}} \right| \leq t \right\} \right)
\leq \mathbb{P} \left( \cap_{s \in L} \left\{ - \left| \text{FACT}_j^{(s)} - \sqrt{n} \frac{\kappa_j^{(s)}}{\hat{\sigma}_j^{(s)}} \right| + \sqrt{n} \frac{\kappa_j^{(s)}}{\hat{\sigma}_j^{(s)}} \leq t \right\} \right) \quad (A.42)
\leq \mathbb{P} \left( - \left| \text{FACT}_j^{(l)} - \sqrt{n} \frac{\kappa_j^{(l)}}{\hat{\sigma}_j^{(l)}} \right| + \sqrt{n} \frac{\kappa_j^{(l)}}{\hat{\sigma}_j^{(l)}} \leq t \right)
= \mathbb{P} \left( \sqrt{n} \frac{\kappa_j^{(l)}}{\hat{\sigma}_j^{(l)}} \leq \left| \text{FACT}_j^{(l)} - \sqrt{n} \frac{\kappa_j^{(l)}}{\hat{\sigma}_j^{(l)}} \right| + t \right).
$$

It remains to establish the probability upper bound for the RHS of (A.42) above. As in the proof of Theorem 1 in Section A.1, let us define random variables $A_5i, \ldots, A_8i$ as

$$
\text{FACT}_j^{(l)} - \sqrt{n} \frac{\kappa_j^{(l)}}{\hat{\sigma}_j^{(l)}}
= \frac{1}{\hat{\sigma}_j^{(l)} \sqrt{n}} \sum_{i=1}^{n} \left[ (Y_i - \mathbb{E}(Y_i|X_{-ij}))(g^{(l)}(X_{ij}) - \hat{g}^{(l)}(X_j)) - \kappa_j^{(l)} \right]
+ (\mathbb{E}(Y_i|X_{-ij}) - \hat{g}(X_{-ij}))(g^{(l)}(X_{ij}) - \hat{g}^{(l)}(X_j))
+ (Y_i - \mathbb{E}(Y_i|X_{-ij}))(\hat{g}^{(l)}(X_j) - n^{-1} \sum_{i=1}^{n} g^{(l)}(X_{ij}))
+ (\mathbb{E}(Y_i|X_{-ij}) - \hat{g}(X_{-ij}))(\hat{g}^{(l)}(X_j) - n^{-1} \sum_{i=1}^{n} g^{(l)}(X_{ij}))
=: \frac{1}{\hat{\sigma}_j^{(l)} \sqrt{n}} \sum_{i=1}^{n} (A_5i + A_6i + A_7i + A_8i).
$$
By (A.42)–(A.43) and Markov’s inequality, we can deduce that

\[
\mathbb{P}\left( \sqrt{n} \frac{\hat{\sigma}_j(l)}{\tilde{\sigma}_j(l)} \leq t + \left| \text{FACT}_j(l) - \sqrt{n} \frac{\hat{\sigma}_j(l)}{\tilde{\sigma}_j(l)} \right| \right)
\]

\[
\leq \mathbb{P}\left( \sqrt{n} \hat{\sigma}_j(l) \leq t \tilde{\sigma}_j(l) + \left| n^{-\frac{1}{2}} \sum_{i=1}^{n} A_{5i} \right| + \left| n^{-\frac{1}{2}} \sum_{i=1}^{n} A_{6i} \right| \right)
\]

\[
+ \left| n^{-\frac{1}{2}} \sum_{i=1}^{n} A_{7i} \right| + \left| n^{-\frac{1}{2}} \sum_{i=1}^{n} A_{8i} \right| \right)
\]

\[
\leq \frac{1}{\sqrt{n} \kappa_j(l)} \left( t \mathbb{E}(\tilde{\sigma}_j(l)) + \mathbb{E} \left( \sum_{i=1}^{n} A_{5i} \sqrt{n} \right) + \mathbb{E} \left( \sum_{i=1}^{n} A_{6i} \sqrt{n} \right) + \mathbb{E} \left( \sum_{i=1}^{n} A_{7i} \sqrt{n} \right) + \mathbb{E} \left( \sum_{i=1}^{n} A_{8i} \sqrt{n} \right) \right). \quad (A.44)
\]

In what follows, we bound the expected values above. By Jensen’s inequality, Condition 1, the assumptions of i.i.d. observations and that \(0 \leq g(l)(X_j) \leq 1\), it holds that for each \(B_1 > 0\) and all \(n \geq 1\),

\[
\mathbb{E}(\tilde{\sigma}_j(l)) \leq \sqrt{\mathbb{E}(\tilde{\sigma}_j(l))^2}
\]

\[
\leq \sqrt{\mathbb{E}\left( \frac{1}{n} \sum_{i=1}^{n} [Y_i - \hat{Y}(\mathbf{X}_{-ij})]^2[g(l)(X_{ij}) - n^{-1} \sum_{i=1}^{n} g(l)(X_{ij})]^2 \right)}
\]

\[
\leq \sqrt{\mathbb{E}[\left( Y - \hat{Y}(\mathbf{X}_{-j}) \right)^2]}
\]

\[
= \sqrt{\mathbb{E}[\left( Y - \mathbb{E}(Y|\mathbf{X}_{-j}) \right)^2 + \mathbb{E}(Y|\mathbf{X}_{-j}) - \hat{Y}(\mathbf{X}_{-j})]^2]}
\]

\[
\leq \sqrt{\mathbb{E}(Y - \mathbb{E}(Y|\mathbf{X}_{-j})]^2 + \mathbb{E}(\mathbb{E}(Y|\mathbf{X}_{-j}) - \hat{Y}(\mathbf{X}_{-j})]^2]}
\]

\[
\leq \sqrt{\text{Var}(Y) + B_1}. \quad (A.45)
\]

By the Burkholder–Davis–Gundy inequality, Jensen’s inequality, the assumptions of i.i.d. observations and that \(0 \leq g(l)(X_j) \leq 1\), there exists some constant \(K > 0\) such that for each \(t > 0, B_1 > 0\), and all \(n \geq 1\),

\[
\mathbb{E} \left| \sum_{i=1}^{n} \frac{A_{5i}}{\sqrt{n}} \right| \leq K \sqrt{\mathbb{E} \left( (Y - \mathbb{E}(Y|\mathbf{X}_{-j}))g(l)(X_j) - \mathbb{E}g(l)(X_j) \right)^2}
\]

\[
\leq K \sqrt{\text{Var}(Y)}. \quad (A.46)
\]

By Condition 2, the Burkholder–Davis–Gundy inequality, Jensen’s inequality, the assumptions of i.i.d. observations and that \(0 \leq g(l)(X_j) \leq 1\), we can show that there exists some constant \(K > 0\) such that for each \(t > 0, B_1 > 0\), and all \(n \geq 1\),

\[
\mathbb{E} \left| \sum_{i=1}^{n} \frac{A_{6i}}{\sqrt{n}} \right| \leq K \sqrt{B_1}. \quad (A.47)
\]

Moreover, by Jensen’s inequality, the Cauchy–Schwartz inequality, the assumptions of
i.i.d. observations and that $0 \leq g^{(l)}(X_j) \leq 1$, and an application of the Burkholder–Davis–Gundy inequality, there exists some constant $K > 0$ such that for each $t > 0$, $B_1 > 0$, and all $n \geq 1$,

$$
\mathbb{E} \left| \sum_{i=1}^{n} \frac{A_{ni}}{\sqrt{n}} \right| \leq \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left| (Y_i - \mathbb{E}(Y_i|X_{-ij})) \left( \frac{\sum_{i=1}^{n} [g^{(l)}(X_{ij}) - \mathbb{E}g^{(l)}(X_{j})]}{\sqrt{n}} \right) \right| \\
\leq \sqrt{\mathbb{E}[Y - \mathbb{E}(Y|X_{-j})]^2} \sqrt{\mathbb{E} \left( \frac{\sum_{i=1}^{n} [g^{(l)}(X_{ij}) - \mathbb{E}g^{(l)}(X_{j})]}{\sqrt{n}} \right)^2} \leq \sqrt{K \text{Var}(Y)}. \quad (A.48)
$$

By Jensen’s inequality, the Cauchy–Schwartz inequality, the assumptions of i.i.d. observations and that $0 \leq g^{(l)}(X_j) \leq 1$, Condition 1, and an application of the Burkholder–Davis–Gundy inequality, we can show that there exists some constant $K > 0$ such that for each $t > 0$, $B_1 > 0$, and all $n \geq 1$,

$$
\mathbb{E} \left| \sum_{i=1}^{n} \frac{A_{8i}}{\sqrt{n}} \right| \leq \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left| \mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}) \right| \left( \frac{\sum_{i=1}^{n} [g^{(l)}(X_{ij}) - \mathbb{E}g^{(l)}(X_{j})]}{\sqrt{n}} \right) \\
\leq \sqrt{\mathbb{E}[Y|X_{-j}] - \hat{Y}(X_{-j})]^2} \sqrt{\mathbb{E} \left( \frac{\sum_{i=1}^{n} [g^{(l)}(X_{ij}) - \mathbb{E}g^{(l)}(X_{j})]}{\sqrt{n}} \right)^2} \leq \sqrt{KB_1}. \quad (A.49)
$$

Therefore, by (A.42)–(A.49) and the property of the subadditivity inequality, there exists some $C > 0$ such that for each $t > 0$, $B_1 > 0$, and all $n \geq 1$,

$$
\mathbb{P} \left( \bigcap_{s \in L} \left\{ \left| \text{FACT}_j^{(s)} \right| \leq t \right\} \right) \leq \frac{(C + t) \left[ \sqrt{B_1} + \sqrt{\text{Var}(Y)} \right]}{\sqrt{n} |\kappa_j^{(l)}|} \leq \frac{(C + t) \left[ \sqrt{B_1} + \sqrt{\text{Var}(Y)} \right]}{\sqrt{n} \sum_{l \in L} |\kappa_j^{(l)}|},
$$

which concludes the proof of Theorem 6.

**A.7  Proof of Theorem 7**

The main ideas for the proof of Theorem 7 are similar to those for the proof of Theorem 6 in Section A.6. We spell out some necessary technical details for completeness. As in the proof of Theorem 6, we note that the arguments in this proof apply to any feature index $1 \leq j \leq p$ provided that the required conditions hold.

In light of the assumption $\sum_{s=1}^{2} |\kappa_j^{(s)}|X_{-j}| > 0$, let us fix some $l \in L = \{1, 2\}$ with $|\kappa_j^{(l)}|X_{-j}| >$
0 and fix any \( \eta \in Q \). Then we can deduce that

\[
\Pr(\text{FACT}_j \leq t)
\leq \Pr\left( \bigcap_{s \in L, \alpha \in Q} \left\{ \text{FACT}_{j,\alpha}^{(s)} - \sqrt{\frac{\kappa_j^{(s)} X_{-j}}{\sigma_j^{(s)} X_{-j}}} + \sqrt{\frac{\kappa_j^{(s)} X_{-j}}{\sigma_j^{(s)} X_{-j}}} \leq t \right\} \right)
\leq \Pr\left( \bigcap_{s \in L, \alpha \in Q} \left\{ - \text{FACT}_{j,\alpha}^{(s)} - \sqrt{\frac{\kappa_j^{(s)} X_{-j}}{\sigma_j^{(s)} X_{-j}}} + \sqrt{\frac{\kappa_j^{(s)} X_{-j}}{\sigma_j^{(s)} X_{-j}}} \leq t \right\} \right)
\leq \Pr\left( - \text{FACT}_{j,\alpha}^{(l)} - \sqrt{\frac{\kappa_j^{(l)} X_{-j}}{\sigma_j^{(l)} X_{-j}}} + \sqrt{\frac{\kappa_j^{(l)} X_{-j}}{\sigma_j^{(l)} X_{-j}}} \leq t \right)
\leq \Pr\left( \sqrt{\frac{\kappa_j^{(l)} X_{-j}}{\sigma_j^{(l)} X_{-j}}} \leq t + \text{FACT}_{j,\alpha}^{(l)} - \sqrt{\frac{\kappa_j^{(l)} X_{-j}}{\sigma_j^{(l)} X_{-j}}} \right) \tag{A.50}
\]

We next bound the RHS of (A.50). As we have done in the proof of Theorem 6, we define terms \( A_{5i}, \cdots, A_{8i} \) for \( i \in N_q \) as

\[
\text{FACT}_{j,\alpha}^{(l)} - \sqrt{\frac{\kappa_j^{(l)} X_{-j}}{\sigma_j^{(l)} X_{-j}}} = \frac{1}{\sigma_j^{(l)} X_{-j} \sqrt{\kappa_j^{(l)} X_{-j}}} \sum_{i \in N_q} \left[ \left( Y_i - \mathbb{E}(Y_i|X_{-ij}) \right) \left( g^{(l)}(X_{ij}) - \mathbb{E}(g^{(l)}(X_{ij})|X_{-ij}) \right) - \kappa_j^{(l)} X_{-j} \right]
+ \left( \mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}) \right) \left( g^{(l)}(X_{ij}) - \mathbb{E}(g^{(l)}(X_{ij})|X_{-ij}) \right)
+ \left( Y_i - \mathbb{E}(Y_i|X_{-ij}) \right) \left( \mathbb{E}(g^{(l)}(X_{ij})|X_{-ij}) - \hat{g}^{(l)}(X_{-ij}) \right)
+ \left( \mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}) \right) \left( \mathbb{E}(g^{(l)}(X_{ij})|X_{-ij}) - \hat{g}^{(l)}(X_{-ij}) \right)
\]

By (A.51) and Markov’s inequality, we can show that

\[
\Pr\left( \sqrt{\frac{\kappa_j^{(l)} X_{-j}}{\sigma_j^{(l)} X_{-j}}} \leq t + \text{FACT}_{j,\alpha}^{(l)} - \sqrt{\frac{\kappa_j^{(l)} X_{-j}}{\sigma_j^{(l)} X_{-j}}} \right)
\leq \Pr\left( \sqrt{\frac{\kappa_j^{(l)} X_{-j}}{\sigma_j^{(l)} X_{-j}}} \leq t\sigma_j^{(l)} X_{-j} + \sum_{k=5}^{8} \frac{\sum_{i \in N_q} A_{ki}}{\sqrt{\kappa_j^{(l)} X_{-j}}} \right) \tag{A.52}
\leq \frac{t\mathbb{E}(\sigma_j^{(l)} X_{-j}) + \sum_{k=5}^{8} \mathbb{E} \left[ \sum_{i \in N_q} A_{ki} \sqrt{\frac{\kappa_j^{(l)} X_{-j}}{\sqrt{\kappa_j^{(l)} X_{-j}}}} \right]}{\sqrt{\kappa_j^{(l)} X_{-j}}}
\]

Recall that a random forests estimate is some average of the training sample. Since \( \hat{g}^{(l)}(X_{-j}) \) is a random forests estimate of \( \mathbb{E}(g^{(l)}(X_{j})|X_{-j}) \) and that \( 0 \leq g^{(l)}(X_j) \leq 1 \) by assumption, it holds that \( 0 \leq \hat{g}^{(l)}(X_{-j}) \leq 1 \). By this, the assumptions of i.i.d. observations,
and Condition 1, it holds that for each \( t > 0 \), \( B_1, B_2 > 0 \), and all \( n \geq 1 \),

\[
\mathbb{E}(\hat{\sigma}^{(l)}_{ji}(X_{-j})) \leq \sqrt{\mathbb{E}(\hat{\sigma}^{(l)}_{ji}(X_{-j}))^2} \\
\leq \sqrt{\mathbb{E}\left( \left[ Y - \hat{Y}(X_{-j}) \right] \left[ g^{(l)}(X_j) - \hat{g}^{(l)}(X_{-j}) \right] \right)^2} \\
\leq \sqrt{\mathbb{E}(Y - \hat{Y}(X_{-j}))^2} \\
\leq \sqrt{\mathbb{E}(Y - \mathbb{E}(Y|X_{-j})) + \mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j}))^2} \\
\leq \sqrt{\text{Var}(Y) + B_1}.
\]

By the Burkholder–Davis–Gundy inequality, Jensen’s inequality, the assumptions of i.i.d. observations and that \( 0 \leq g^{(l)}(X_j) \leq 1 \), there exists some constant \( K > 0 \) such that for each \( t > 0 \), \( B_1, B_2 > 0 \), and all \( n \geq 1 \),

\[
\mathbb{E} \left| \sum_{i \in \mathcal{N}_q} A_{6i} \right| \leq K \sqrt{\mathbb{E}\left( (Y - \mathbb{E}(Y|X_{-j}))(g^{(l)}(X_j) - \mathbb{E}(g^{(l)}(X_j)|X_{-j} - \hat{g}^{(l)}(X_{-j})) \right)^2} \\
\leq K \sqrt{\text{Var}(Y)}.
\]

By the Burkholder–Davis–Gundy inequality, Jensen’s inequality, the assumptions of i.i.d. observations and that \( 0 \leq g^{(l)}(X_j) \leq 1 \), and Condition 2, we can show that there exists some constant \( K > 0 \) such that for each \( t > 0 \), \( B_1, B_2 > 0 \), and all \( n \geq 1 \),

\[
\mathbb{E} \left| \sum_{i \in \mathcal{N}_q} A_{6i} \right| \leq K \sqrt{B_1}.
\]

Furthermore, by the Burkholder–Davis–Gundy inequality, Jensen’s inequality, the assumptions of i.i.d. observations and \( \text{Var}(Y|X_{-j}) \leq D \) almost surely (see Condition 3), the assumption that the training sample is an independent sample, and Condition 4, there exists some constant \( K > 0 \) such that for each \( t > 0 \), \( B_1, B_2 > 0 \), and all \( n \geq 1 \),

\[
\mathbb{E} \left| \sum_{i \in \mathcal{N}_q} A_{7i} \right| \leq K \sqrt{\mathbb{E}\left( (Y - \mathbb{E}(Y|X_{-j}))(g^{(l)}(X_j)|X_{-j} - \hat{g}^{(l)}(X_{-j}) \right)^2} \\
\leq K \sqrt{D \mathbb{E}(g^{(l)}(X_j)|X_{-j} - \hat{g}^{(l)}(X_{-j})))^2} \\
\leq K \sqrt{DB_2},
\]

where the second inequality uses an argument similar to that for (A.17). By Conditions 1 and 4, the assumptions of i.i.d. observations, and the Cauchy–Schwartz inequality, it holds that for each \( t > 0 \), \( B_1, B_2 > 0 \), and all \( n \geq 1 \),

\[
\mathbb{E} \left| \sum_{i \in \mathcal{N}_q} A_{8i} \right| \leq \sqrt{|\mathcal{N}_q|B_1B_2}.
\]

Therefore, by (A.50)–(A.57) and the property of the subadditivity inequality, there exists
some $C > 0$ such that for each $t > 0$, $B_1, B_2 > 0$, $|Q| < n$, and all $n \geq 2$,

$$
P(\text{FACT}_j \leq t) \leq \frac{(C + t)(\text{Var}(Y) + \sqrt{B_1} + \sqrt{B_2} + \sqrt{nB_1B_2})}{\sqrt{|N_q|} \kappa_j^{(1)}(X_{-j})} \leq \frac{\sqrt{|Q|(C + t)(\text{Var}(Y) + \sqrt{B_1} + \sqrt{B_2} + \sqrt{nB_1B_2})}}{\sqrt{n - |Q|} \sum_{l=1}^{\sqrt{n}} \kappa_j^{(l)}(X_{-j})},$$

(A.58)

where we use the fact that $|N_q| \geq \frac{n}{|Q|} - 1$ in the last inequality. This result concludes the proof of Theorem 7.

**B Proofs of Propositions 1–4 and some key lemmas**

**B.1 Proof of Proposition 1**

To show that $\kappa_j^{(1)}$ is lower bounded in this specific setting, let us write

$$\kappa_j^{(1)} = \mathbb{E}\left( \mathbb{E}\left( (Y - \mathbb{E}(Y|X_{-j}))(X_j - \mathbb{E}X_j)|X_{-j} \right) \right),$$

where by the assumptions, these expectations and conditional expectations are well-defined, and the equality is due to the law of the total expectation. For the inner conditional expectation of $\kappa_j^{(1)}$, we can deduce that

$$\mathbb{E}\left( (Y - \mathbb{E}(Y|X_{-j}))(X_j - \mathbb{E}X_j)|X_{-j} \right)$$

$$= \mathbb{E}\left( (h(X_j) - \mathbb{E}(h(X_j)|X_{-j}))(X_j - \mathbb{E}X_j)|X_{-j} \right)$$

$$= \mathbb{E}\left( (h(X_j) - \mathbb{E}(h(X_j)|X_{-j}))(X_j - \mathbb{E}(X_j|X_{-j}))|X_{-j} \right)$$

$$= \mathbb{E}\left( (h(X_j) - h(\mathbb{E}(X_j|X_{-j}))) \left( X_j - \mathbb{E}(X_j|X_{-j}) \right) \right),$$

where the first equality is due to Condition 5 and the last one is because $h(\mathbb{E}(X_j|X_{-j}))$ is $\sigma(X_{-j})$-measurable. Our proof relies on the techniques in [14], where a lower bound of covariance between $h(X_j)$ and $X_j$ is obtained in terms of the first-order derivative of $h$. Since our technical analysis further takes the conditional expectation into account, we provide a self-contained proof here for completeness.

In light of Condition 5, let us define the conditional density of $X_j$ given $X_{-j} = z$ as $f_{X_j|z}(x)$ such that

$$f_{X_j|z}(x) \times f_{X_{-j}}(z) = f_{X_j}(x),$$

where $f_{X_j}$ and $f_{X_{-j}}$ denote the density functions of the distributions of $X_j$ and $X_{-j}$, respectively. In addition, we denote the versions of $\mathbb{E}(X_j|X_{-j})$ and the RHS of (A.59) as $\mu(X_{-j})$ and $\nu(X_{-j})$, respectively, for some measurable $\mu$ and $\nu$. We will derive an expression for the RHS of (A.59) in terms of $\partial h(x)/\partial x$. By the change of variable formula, for each $z \in [0, 1]^{p-1}$ we have

$$\nu(z) = \int_{-\infty}^{\infty} (h(x) - h(\mu(z)))(x - \mu(z))f_{X_j|z}(x)dx.$$
Thus, it holds almost surely that

\[
\text{RHS of (A.59)} = \nu(X-)
= \int_{-\infty}^{\infty} (h(x) - h(\mu(X-))) (x - \mu(X-)) f_{X_j|X-} (x) dx.
\] (A.60)

Recall the assumption that the derivative of \( h \) is integrable and denote by \( 1 \) the indicator function. Then we can resort to the fundamental theorem of calculus [10] to deduce that for \( x \in \mathbb{R} \),

\[
h(x) - h(\mu(X-)) = \left( \int_{\mu(X-)}^{x} \frac{\partial h(t)}{\partial t} dt \right) 1_{x \geq \mu(X-)} + \left( \int_{x}^{\mu(X-)} \frac{\partial h(t)}{\partial t} dt \right) 1_{x \leq \mu(X-)},
\]

which is equal to zero at \( x = \mu(X-) \). It follows from such a representation that

\[
\text{RHS of (A.60)}
= \int_{-\infty}^{\infty} \left( \int_{\mu(X-)}^{x} \frac{\partial h(t)}{\partial t} dt \right) 1_{x \geq \mu(X-)} (x - \mu(X-)) f_{X_j|X-} (x) dx
+ \int_{-\infty}^{\infty} \left( \int_{x}^{\mu(X-)} \frac{\partial h(t)}{\partial t} dt \right) 1_{x \leq \mu(X-)} (\mu(X-) - x) f_{X_j|X-} (x) dx
\]

(A.61)

Since the derivative is bounded in absolute value and \( 0 \leq X_j \leq 1 \), we can show that the two integrations on the RHS of (A.61) are absolutely integrable. Hence, an application of Fubini’s theorem and the facts that \( 1_{t \in [\mu(X-), x]} = 1_{x \geq t \geq \mu(X-)} \) and \( 1_{t \in [x, \mu(X-)]} = 1_{x \leq t \leq \mu(X-)} \) yields that

\[
\text{RHS of (A.61)}
= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} 1_{t \in [\mu(X-), x]} \left( \frac{\partial h(t)}{\partial t} \right) (x - \mu(X-)) f_{X_j|X-} (x) dx dt
+ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} 1_{t \in [x, \mu(X-)]} \left( \frac{\partial h(t)}{\partial t} \right) (\mu(X-) - x) f_{X_j|X-} (x) dx dt
\]

(A.62)
Furthermore, since

$$\int_t^\infty (x - \mu(X_{-j}))f_{X_j|X_{-j}}(x)dx = \int_{-\infty}^t (\mu(X_{-j}) - x)f_{X_j|X_{-j}}(x)dx,$$

we see that the RHS of (A.62) becomes

$$\text{RHS of (A.62)} = \int_{-\infty}^\infty \frac{\partial h(t)}{\partial t} \left( \int_{-\infty}^t (\mu(X_{-j}) - x)f_{X_j|X_{-j}}(x)dx \right) dt. \quad (A.63)$$

Let us set $h(x) = x$ in (A.63). Then from (A.59), we have

$$\mathbb{E}(\text{Var}(X_j|X_{-j})) = \mathbb{E} \left[ \int_{-\infty}^\infty \left( \int_{-\infty}^t (\mu(X_{-j}) - x)f_{X_j|X_{-j}}(x)dx \right) dt \right]. \quad (A.64)$$

Therefore, it follows from the assumption that $h$ is monotonic and (A.59)–(A.64) that

$$|\kappa_j^{(1)}| = \mathbb{E} \left[ \int_{-\infty}^\infty \left| \frac{\partial h(t)}{\partial t} \right| \left( \int_{-\infty}^t (\mu(X_{-j}) - x)f_{X_j|X_{-j}}(x)dx \right) dt \right]$$

$$\geq \left( \inf_{x \in [0,1]} \left| \frac{\partial h(x)}{\partial x} \right| \right) \mathbb{E}(\text{Var}(X_j|X_{-j})), \quad$$

which concludes the proof of Proposition 1.

### B.2 Proof of Proposition 2

From Condition 5, $g^{(l)}(x) = x^l$, and the distributional assumption of $X$, it holds that

$$\kappa_j^{(l)} = \kappa_j^{(l)} = \mathbb{E}((Y - \mathbb{E}(Y|X_{-j}))(X_j^l - \mathbb{E}X_j^l))$$

$$= \mathbb{E}(H(X_j)(X_j^l - \mathbb{E}X_j^l)), \quad (A.65)$$

where the conditional expectation $\mathbb{E}(H(X_{-j}) + \varepsilon|X_{-j})$ is well-defined since we assume that the first moments of $H(X_{-j})$ and $\varepsilon$ exist. In view of this, we consider only the case of $\kappa_j^{(l)}$'s and a similar result holds for $\sum_{l \in L} |\kappa_j^{(l)}X_{-j}|$ as well. By (A.65), the distributional assumption of $X$, and the form of $h$, we can deduce that for $l \in L$,

$$\kappa_j^{(l)} = (a_1, \cdots, a_{m_1})(\mathbb{E}X_j^{1+l} - (\mathbb{E}X_j)(\mathbb{E}X_j^l), \cdots, \mathbb{E}X_j^{m_1+l} - (\mathbb{E}X_j^{m_1})(\mathbb{E}X_j^l))^T$$

$$= (a_1, \cdots, a_{m_1})$$

$$\times \left( \frac{1}{l+2} - \frac{1}{l+1}, \cdots, \frac{1}{m_1+l+1} - \frac{1}{m_1+1} \right)^T, \quad (A.66)$$

where we have used the fact that $\mathbb{E}X_j^k = (k + 1)^{-1}$ due to the distributional assumption.

Let us define an $m_1 \times m_1$ matrix

$$D := [(i + j + 1)^{-1}]_{i,j=1,\cdots,m_1}$$

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and $m_1$-dimensional vectors $B = C := (\frac{1}{2}, \cdots, \frac{1}{m_1+1})^T$. Then by (A.66), we have

$$(\kappa_j^{(1)}, \cdots, \kappa_j^{(m_1)}) = (a_1, \cdots, a_m)(D - CB^T).$$

(A.67)

We will show that $D - CB^T$ is positive definite. To this end, let us introduce a Hilbert matrix of order $m_1 + 1$

$$[(i + j - 1)^{-1}]_{i,j=1,\cdots,m_1+1} = \begin{pmatrix} 1 & B^T \\ C & D \end{pmatrix}.$$

Since a Hilbert matrix is positive definite [18], its inverse exists and is also positive definite. With the aid of the block matrix inversion formula, we see that $(D - CB^T)^{-1}$ is the bottom-right block of the inverse of the Hilbert matrix and hence is positive definite. This entails that $D - CB^T$ is positive definite. Therefore, it follows from this result and (A.67) that if $\sum |a_l| > 0$, we have

$$\sum_{l=1}^{m_1} |\kappa_j^{(l)}| \geq \left( \sum_{l=1}^{m_1} |a_l| \right)^{-1} \left( \sum_{l=1}^{m_1} \kappa_j^{(l)} a_l \right) \geq \frac{\sum_{l=1}^{m_1} |a_l|}{m_1} \lambda_{\min}(D - CB^T) > 0,$$

where in the second inequality we have used the fact that $\sum_{l=1}^{m_1} |a_l| \leq \sqrt{m_1 \sum_{l=1}^{m_1} |a_l|^2}$. By this result, we conclude the first assertion of Proposition 2.

Next, a direct calculation shows that the minimum eigenvalues of $D - CB^T$ is larger than 0.002 for $1 \leq m_1 \leq 2$, and hence for $1 \leq m_1 \leq 2$, we have

$$\sum_{l=1}^{m_1} |\kappa_j^{(l)}| \geq 0.001 \times \sum_{l=1}^{m_1} |a_l|,$$

which completes the proof of Proposition 2.

B.3 Proof of Proposition 3

Let us first observe that $m(X) = \tilde{m}(X)$ almost surely since

$$1_{X_2 > 0.7} = 1_{X_1 > 0.7}$$

almost surely by the definition of $X$. Thus, both $m(X)$ and $\tilde{m}(X)$ are versions of $E(Y|X)$.

We will establish the main assertion of Proposition 3. By $EY^2 < \infty$, we can see that if $m$ is used in (25),

$$\text{MDA}(Y, X_2) = 0.$$  

(A.68)

On the other hand, we can deduce that

$$E(Y - \tilde{m}(X_{(2)}))^2 = E(Y - E(Y|X)) + 1_{X_1 > 0.7} - 1_{X_{(2)} > 0.7})^2$$

$$= E(Y - E(Y|X))^2 + E(1_{X_1 > 0.7} - 1_{X_{(2)} > 0.7})^2,$$

(A.69)
where \( X_{(2)} \) is given in (25) and the second equality holds because \( X_{(2)} \) is independent of \((X,Y)\). Then it follows from (A.69) that if \( \tilde{m} \) is used in (25), we have

\[
\text{MDA}(Y, X_2) = \mathbb{E}(1_{X_1 > 0.7} - 1_{X_{(2)} > 0.7})^2 > 0
\]

since \( X_{(2)} \) is independent of \( X_1 \). Therefore, combining this result and (A.68) concludes the proof of Proposition 3.

### B.4 Proof of Proposition 4

Let \( X_j \) be a null feature and \( m(X) \) a version of \( \mathbb{E}(Y|X) \). We will establish that \( m(X^{\dagger}_{(j)}) = m(X) \), which along with the definition of CPI leads to the first assertion of Proposition 4; recall that \( X^{\dagger}_{(j)} \) has been defined in (26). Observe that the second assertion of Proposition 4 is a direct consequence of the first assertion since \( X_2, \ldots, X_p \) are null features in Example 1.

It remains to show that \( m(X^{\dagger}_{(j)}) = m(X) \). We begin with proving that \( \mathbb{E}(Y|X_{-j}) = \mathbb{E}(Y|X) \). Let \( \mathcal{R}^p \) be the \( \sigma \)-algebra generated by all the open sets in \( \mathbb{R}^p \) and define

\[
\sigma(X) := \{X^{-1}(A) : A \in \mathcal{R}^p\}.
\]

Since \( \mathbb{E}(Y|X_{-j}) \) is \( \sigma(X) \)-measurable, it suffices (by the definition of the conditional expectation) to show that for each \( A \in \sigma(X) \),

\[
\mathbb{E}(1_A \mathbb{E}(Y|X_{-j})) = \mathbb{E}(1_A Y).
\]

For any two events \( A_1 \in \sigma(X_{-j}) \) and \( A_2 \in \sigma(X_j) \), we can deduce that

\[
\begin{align*}
\mathbb{E}(1_{A_1} 1_{A_2} \mathbb{E}(Y|X_{-j})) &= \mathbb{E}(\mathbb{E}(1_{A_1} 1_{A_2} \mathbb{E}(Y|X_{-j})|X_{-j})) \\
&= \mathbb{E}(1_{A_1} \mathbb{E}(Y|X_{-j}) \mathbb{E}(1_{A_2}|X_{-j})) \\
&= \mathbb{E}(1_{A_1} \mathbb{E}(1_{A_2} Y|X_{-j})) = \mathbb{E}(1_{A_1} 1_{A_2} Y),
\end{align*}
\]

where the first equality is due to the law of the total expectation, the second one follows from the fact that both \( \mathbb{E}(Y|X_{-j}) \) and \( 1_{A_1} \) are \( \sigma(X_{-j}) \)-measurable, the third one is by the definition of the null feature, and the last one is entailed by the definition of \( A_1 \) and the law of the total expectation. With the aid of (A.70), we can resort to the \( \pi – \lambda \) theorem [22] to show that

\[
\mathbb{E}(Y|X_{-j}) = \mathbb{E}(Y|X),
\]

which is formally established in Lemma 5 in Section B.9.

Further, let \( \tilde{m}(X_{-j}) \) be a version of \( \mathbb{E}(Y|X_{-j}) \). Then it holds that

\[
m(X) = \tilde{m}(X_{-j})
\]

as we have shown previously. By this result, it suffices to show that \( m(X^{\dagger}_{(j)}) = \tilde{m}(X_{-j}) \) for concluding the desired result. Since \( m(X^{\dagger}_{(j)}) \) and \( \tilde{m}(X_{-j}) \) are both \( \sigma(X^{\dagger}_{(j)}) \)-measurable, it
remains to establish that for any $A \in \sigma(X^{\dagger}_{(j)})$,
\[ \mathbb{E}(1_A \times m(X^{\dagger}_{(j)})) = \mathbb{E}(1_A \times \tilde{m}(X_{-j})). \]
Let us define $A_2 := \{X^{\dagger}_{(j)} \in B\}$ and $A_3 := \{X_j \in B\}$ for each $B \in \mathcal{R}$. Then for each $A_1 \in \sigma(X_{-j})$ and $B \in \mathcal{R}$, we have
\[
\mathbb{E}(1_{A_1}1_{A_2}(m(X^{\dagger}_{(j)}) - \tilde{m}(X_{-j}))) = \mathbb{E}(1_{A_1}\mathbb{E}(1_{A_2}(m(X^{\dagger}_{(j)}) - \tilde{m}(X_{-j}))|X_{-j}))
= \mathbb{E}(1_{A_1}\mathbb{E}(1_{A_2}(m(X) - \tilde{m}(X_{-j}))|X_{-j})) \quad (A.71)
= 0,
\]
where the first equality is due to the law of the total expectation, the second one is from the assumption that given $X_{-j}$, $X^{\dagger}_{(j)}$ has the same conditional distribution as $X$, and the last one is because $m(X) = \tilde{m}(X_{-j})$.

It is worth mentioning that given $X_{-j}$, $X^{\dagger}_{(j)}$ (for MDA) and $X$ are not conditionally identically distributed. This is where CPI improves over MDA. By (A.71), we can again apply the $\pi - \lambda$ theorem and similar arguments to those for the proof of Lemma 5 in Section B.9 to obtain that
\[ m(X^{\dagger}_{(j)}) = \tilde{m}(X_{-j}) \]
almost surely. We omit these technical details for simplicity. Therefore, combining $m(X^{\dagger}_{(j)}) = \tilde{m}(X_{-j})$ with the previous results can yield the desired conclusion in the first assertion. This completes the proof of Proposition 4.

**B.5 Lemma 1 and its proof**

All the notation, including $A_{11}, \cdots, A_{4i}, \mu, \tilde{\sigma}_0,$ and $\sigma_0$, is the same as in the proof of Theorem 1.

**Lemma 1.** Assume that all the conditions of Theorem 1 are satisfied. Then for some constant $C > 0$, all large $n$, each $0 < B_1 < 1$, and each $t \in \mathbb{R}$, there exist some events $\{E^e_{n,B_1}\}$ such that 1) $\mathbb{P}(E^e_{n,B_1}) \leq C(B_1^{1/4} + n^{-1/4})$ with $E^e$ standing for the complement of an event $E$ and 2) on event $E_{n,B_1}$, it holds that $c \geq |\tilde{\sigma}_0 - \sigma_0| |t| + |n^{-1/2} \sum_{i=1}^{n} (A_{2i} + A_{3i} + A_{4i})| + \sqrt{n}|\mu||\mathbb{E}g(X_j) - n^{-1} \sum_{i=1}^{n} g(X_{ij})|$. Particularly, constant $C$ is independent of $1 \leq j \leq p$.

**Proof.** The proof of this lemma mainly consists of three steps. First, we will build an upper bound of $|\tilde{\sigma}_0 - \sigma_0|$ in terms of $A_{li}$’s. Second, we will construct events $E^e_{n,B_1}$’s such that on these events, $c$ is indeed an upper bound of $|\tilde{\sigma}_0 - \sigma_0| |t| + |n^{-1/2} \sum_{i=1}^{n} (A_{2i} + A_{3i} + A_{4i})| + \sqrt{n}|\mu||\mathbb{E}g(X_j) - n^{-1} \sum_{i=1}^{n} g(X_{ij})|$. Third, we will establish the probability upper bounds for the complement events $E^c_{n,B_1}$’s. Let us begin with providing an upper bound for $|\tilde{\sigma}_0 - \sigma_0|$. 

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Note that for any $a, \varepsilon > 0$ and $a^2 \geq \varepsilon$, it holds that

$$
\sqrt{a^2 - \varepsilon} \geq \sqrt{(a - \frac{\varepsilon}{a})^2} = a - \frac{\varepsilon}{a},
$$
\hspace{1cm} (A.72)

$$
\sqrt{a^2 + \varepsilon} \leq \sqrt{(a + \frac{\varepsilon}{a})^2} = a + \frac{\varepsilon}{a}.
$$

Define event $E_8 := \{|n^{-1/2}\sum_{i=1}^{n}(A_{1i}^2 - \sigma_{j0}^2)| < n^{1/4}\}$. On event $E_8$, for large enough $n$, we have $\sigma_{j0}^2 > \left| n^{-1}\sum_{i=1}^{n}(A_{1i}^2 - \sigma_{j0}^2) \right|$. Using Minkowski’s inequality, we can deduce that

$$
|\hat{\sigma}_{j0}| \geq \sqrt{n^{-1}\sum_{i=1}^{n}A_{1i}^2} - \sqrt{n^{-1}\sum_{i=1}^{n}\left(-A_{2i} - A_{3i} - A_{4i} + n^{-1}\sum_{i=1}^{n}(A_{1i} + A_{2i} + A_{3i} + A_{4i})\right)^2}
$$
$$
\geq \sqrt{n^{-1}\sum_{i=1}^{n}A_{1i}^2 - \frac{4}{n}\sum_{i=1}^{n}A_{1i}^2 - \sqrt{n^{-1}\sum_{i=1}^{n}\left(n^{-1}\sum_{i=1}^{n}(A_{1i} + A_{2i} + A_{3i} + A_{4i})\right)^2}}
$$
$$
\geq \sqrt{\sigma_{j0}^2 - n^{-1}\sum_{i=1}^{n}(A_{1i}^2 - \sigma_{j0}^2)} - \frac{4}{n}\sum_{i=1}^{n}A_{1i}^2 - \left| n^{-1}\sum_{i=1}^{n}(A_{1i} + A_{2i} + A_{3i} + A_{4i}) \right|.
$$
\hspace{1cm} (A.73)

Similarly, we can show that

$$
|\hat{\sigma}_{j0}| \leq \sqrt{\sigma_{j0}^2 + n^{-1}\sum_{i=1}^{n}(A_{1i}^2 - \sigma_{j0}^2)} + \frac{4}{n}\sum_{i=1}^{n}A_{1i}^2 + \left| n^{-1}\sum_{i=1}^{n}(A_{1i} + A_{2i} + A_{3i} + A_{4i}) \right|.
$$
\hspace{1cm} (A.74)

From (A.72)–(A.74), we can see that on event $E_8$, it holds that for all large $n$,

$$
|\hat{\sigma}_{j0} - \sigma_{j0}| \leq \frac{1}{n\sigma_{j0}}\sum_{i=1}^{n}(A_{1i}^2 - \sigma_{j0}^2) + \frac{4}{n}\sum_{i=1}^{n}A_{1i}^2 + \left| n^{-1}\sum_{i=1}^{n}(A_{1i} + A_{2i} + A_{3i} + A_{4i}) \right|,
$$
\hspace{1cm} (A.75)

which establishes the desired upper bound of $|\hat{\sigma}_{j0} - \sigma_{j0}|$.

To further bound the RHS of (A.75), $|n^{-1/2}\sum_{i=1}^{n}(A_{2i} + A_{3i} + A_{4i})|$, and $\sqrt{n}\mu\|\mathbb{E}g(X_j) -
\[ n^{-1} \sum_{i=1}^{n} g(X_{ij}) \] in terms of \( B_1 \) and \( n \), we introduce nine events below

\begin{align*}
E_1^c := \{ |n^{-1/2} \sum_{i=1}^{n} A_2 | \geq B_1^{1/4} \}, \\
E_2^c := \{ |n^{-1/2} \sum_{i=1}^{n} (Y_i - \mathbb{E}(Y_i | X_{-ij})) | \geq n^{1/4} \}, \\
E_3^c := \{ |n^{-1/2} \sum_{i=1}^{n} (\mathbb{E}(Y_i | X_{-ij}) - \hat{Y}(X_{-ij}) - \mu) | \geq 1 \}, \\
E_4^c := \{ |n^{-1} \sum_{i=1}^{n} g(X_{ij}) - \mathbb{E}g(X_j) | \geq n^{-1/2} \log n \}, \\
E_5^c := \{ |n^{-1/2} \sum_{i=1}^{n} A_{1i} | \geq n^{1/4} \}, \\
E_6^c := \{ |n^{-1} \sum_{i=1}^{n} (\mathbb{E}(Y_i | X_{-ij}) - \hat{Y}(X_{-ij}))^2 \geq B_1^{1/2} \}, \\
E_7^c := \{ |n^{-1} \sum_{i=1}^{n} (Y_i - \mathbb{E}(Y_i | X_{-ij}))^2 \geq n^{1/2} \}, \\
E_8^c := \{ |n^{-1/2} \sum_{i=1}^{n} (A_{2i}^2 - \sigma_j^2) | \geq n^{1/4} \}, \\
E_9^c := \{ |\mu| \geq B_1^{1/4} \},
\end{align*}

where \( E_8 \) is the same as defined previously and the dependence on \( n \) and \( B_1 \) is suppressed here for the notational simplicity.

By the definitions of the events introduced above, we can establish the following facts. On event \( E_4 \cap E_9 \), it holds that

\[ \sqrt{n}|\mu||\mathbb{E}g(X_j) - n^{-1} \sum_{i=1}^{n} g(X_{ij})| \leq B_1^{1/4} \log n. \]

On event \( \bigcap_{l=1}^{2} E_l \), it holds that

\[ |n^{-1/2} \sum_{i=1}^{n} (A_{2i} + A_{3i} + A_{4i})| \leq B_1^{1/4} + n^{-1/4} \log n + n^{-1/2} \log n. \]

On event \( E_4 \cap E_7 \), we have

\[ n^{-1} \sum_{i=1}^{n} A_{3i}^2 \leq n^{-1/2} (\log n)^2. \]

By \( 0 \leq g(X_j) \leq 1 \), it holds on event \( E_6 \) that

\[ n^{-1} \sum_{i=1}^{n} A_{li}^2 \leq B_1^{1/2} \]

for \( l = 2, 4 \).
Furthermore, on event $\cap_{i=1}^5 E_i$, we have

$$|n^{-1} \sum_{i=1}^n (A_{1i} + A_{2i} + A_{3i} + A_{4i})| \leq n^{-1/4} + B_{1/4}^{1/4} n^{-1/2} + n^{-3/4} \log n + n^{-1} \log n.$$ 

On event $E_8$, it holds that

$$|\frac{1}{n\sigma_{j0}} \sum_{i=1}^n (A_{1i}^2 - \sigma_{j0}^2)| \leq \sigma_{j0}^{-1} n^{-1/4}.$$ 

Recall that $c = (\log n)(2B_1^{1/4} + n^{-1/4} \log n)(1 + |t|)$. Then from (A.75), we can see that for all large $n$, each $B_1 > 0$, and each $t \in \mathbb{R}$, it holds on event $\cap_{i=1}^9 E_i$ that

$$c \geq |\hat{\sigma}_{j0} - \sigma_{j0}| |t| + n^{-1/2} \sum_{i=1}^n (A_{2i} + A_{3i} + A_{4i})| + \sqrt{n} |\mu| E g(X_j) - n^{-1} \sum_{i=1}^n g(X_{ij}).$$

Thus, setting $E_{n,B_1} = \cap_{i=1}^9 E_i$ leads to the second assertion of Lemma 1.

Let us proceed with the last step of the proof. Specifically, we will show that for all large $n$, each $B_1 > 0$, and each $t \in \mathbb{R}$,

$$\sum_{i=1}^9 P(E_i^c) \leq C(B_1^{1/4} + n^{-1/4})$$

for some $C > 0$. The probability bounds rely mostly on Markov’s inequality and the Burkholder–Davis–Gundy inequality [13]. In what follows, we demonstrate in details how to apply the Burkholder–Davis–Gundy inequality to obtain an upper bound for $P(E_i^c)$. The applications of these inequalities to other cases are similar and thus the remaining technical details are omitted for simplicity. Let us begin with specifying the underlying martingale. It follows from Condition 2, the definition of $\hat{Y}$, and the assumption of i.i.d. observations that $\{\sum_{i=1}^k n^{-1/2} A_{2i}\}_{k \geq 1}$ is a martingale sequence with respect to $\{F_k\}$, where $F_k := \sigma(\mathcal{X}_0, A_{21}, \cdots, A_{2k})$ and $\sigma(\cdot)$ denotes the $\sigma$-algebra generated by the given random mappings. Here, we also define $\sum_{i=1}^0 (\cdot) = 0$ and $F_0 := \sigma(\mathcal{X}_0)$.

Since the Burkholder–Davis–Gundy inequality deals with a martingale sequence of infinitely many elements, let us consider a martingale sequence $\{\sum_{i=1}^k n^{-1/2} A_{2i}'\}$, where $A_{2i}' = A_{2i}$ for $k \leq n$ and $A_{2i}' = 0$ for $k > n$. Then it follows that for some $C > 0$,

$$E|n^{-1/2} \sum_{i=1}^n A_{2i}| = E|n^{-1/2} \sum_{i \geq 1} A_{2i}'|$$

$$\leq C E\left(n^{-1} \sum_{i \geq 1} (A_{2i}')^2\right)^{1/2}$$

(A.76)

$$= C E\left(n^{-1} \sum_{i=1}^n (A_{2i})^2\right)^{1/2},$$

where the inequality with constant $C$ is due to the Burkholder–Davis–Gundy inequality. We
are now ready to establish the probability bounds.

We start with the probability bound for event $E_1^t$. Specifically, there exists some $K_1 > 0$ such that for each positive integer $n$, $B_1 > 0$, and $t \in \mathbb{R}$,

$$\mathbb{P}(E_1^t) \leq B_1^{-1/4} \mathbb{E}|n^{-1/2} \sum_{i=1}^{n} A_{2i}|$$

$$\leq B_1^{-1/4} K_1 \mathbb{E}(n^{-1} \sum_{i=1}^{n} A_{2i}^2)^{1/2}$$

$$\leq B_1^{-1/4} \mathbb{E}(n^{-1} \sum_{i=1}^{n} A_{2i}^2)^{1/2}$$

$$\leq B_1^{-1/4} K_1 \mathbb{E}(\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j}))^2)^{1/2}$$

$$\leq K_1 B_1^{1/4},$$

(A.77)

where the first inequality is due to Markov’s inequality, the second one is an application of the Burkholder–Davis–Gundy inequality (see (A.76) above for details), and the third one is entailed by Jensen’s inequality. Here, the fourth inequality above is because of the facts that $0 \leq g(X_j) \leq 1$, $\hat{Y}$ is trained on an independent sample, and $(Y_i, X_i)$ and $(Y, X)$ have the same distribution for each $i$, while the last inequality in (A.77) is a consequence of Condition 1.

For event $E_2^t$, we can deduce that there exists some constant $K_2 > 0$ such that for each positive integer $n$, $B_1 > 0$, and $t \in \mathbb{R}$,

$$\mathbb{P}(E_2^t) \leq n^{-1/4} \mathbb{E}(|n^{-1/2} \sum_{i=1}^{n} (Y_i - \mathbb{E}(Y_i|X_{-ij}))|)$$

$$\leq n^{-1/4} K_2 [\mathbb{E}(n^{-1} \sum_{i=1}^{n} (Y_i - \mathbb{E}(Y_i|X_{-ij}))^2)]^{1/2}$$

$$\leq n^{-1/4} K_2 \{\text{Var}(Y)\}^{1/2},$$

(A.78)

where the first inequality is from Markov’s inequality, the second one is entailed by the Burkholder–Davis–Gundy inequality and Jensen’s inequality, and the last one is due to the assumption of i.i.d. observations and the fact that $\mathbb{E}(Y - \mathbb{E}(Y|X_{-j}))^2 \leq \text{Var}(Y)$. Moreover, we can show that there exists some $K_3 > 0$ such that for each positive integer $n$, $B_1 > 0$, and $t \in \mathbb{R}$,

$$\mathbb{P}(E_3^t) \leq K_3 \mathbb{E}(\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j}))^2)^{1/2}$$

$$\leq K_3 B_1^{1/2},$$

(A.79)

where the second inequality is due to Condition 1 and the first one is entailed by Markov’s inequality, the Burkholder–Davis–Gundy inequality (note that $\mathbb{E}(\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}) - \mu_i|X_0) = 0$), and Jensen’s inequality along with the fact that $\hat{Y}$ is trained on an independent sample and the assumption that $(Y_i, X_i)$ and $(Y, X)$ have the same distribution for each $i$.

Since $0 \leq g(X_j) \leq 1$, an application of Hoeffding’s inequality yields that for each positive
integer \( n \), \( B_1 > 0 \), and \( t \in \mathbb{R} \),

\[
\mathbb{P}(E^c_5) \leq 2 \exp \left(-2(\log n)^2\right). \tag{A.80}
\]

For event \( E^c_6 \), it follows from the assumptions of \( \text{Var}(Y) < \infty \), \( 0 \leq g(X_j) \leq 1 \), and i.i.d. observations that there exists some \( K_4 > 0 \) such that for each positive integer \( n \), \( B_1 > 0 \), and \( t \in \mathbb{R} \),

\[
\mathbb{P}(E^c_6) \leq n^{-1/4} \mathbb{E}[n^{-1/2} \sum_{i=1}^{n} A_{1i}] \\
\leq n^{-1/4} K_4 \{\mathbb{E}(n^{-1} \sum_{i=1}^{n} A_{1i}^2)\}^{1/2} \\
\leq n^{-1/4} K_4 \{\text{Var}(Y)\}^{1/2},
\]

where the first inequality uses Markov’s inequality, the second one is an application of the Burkholder–Davis–Gundy inequality and Jensen’s inequality along with the assumption that \( X_j \) is a null feature, and the last one is due to the facts that \( 0 \leq g(X_j) \leq 1 \), \((Y, X_i)\) and \((Y, X)\) have the same distribution for each \( i \), and \( \mathbb{E}(Y - \mathbb{E}(Y|X_{-j}))^2 \leq \text{Var}(Y) \). Furthermore, using Condition 1 and Markov’s inequality, we can deduce that for each positive integer \( n \), \( B_1 > 0 \), and \( t \in \mathbb{R} \),

\[
\mathbb{P}(E^c_6) \leq B_1^{1/2}, \\
\mathbb{P}(E^c_7) \leq n^{-1/2} \text{Var}(Y), \tag{A.82}
\]

where we have used the facts that \((Y, X_i)\) and \((Y, X)\) have the same distribution for each \( i \), and that \( \mathbb{E}(Y - \mathbb{E}(Y|X_{-j}))^2 \leq \text{Var}(Y) \).

It remains to deal with term \( \mathbb{P}(E^c_8) \). Using Minkowski’s and Jensen’s inequalities, we can bound \( \mathbb{E}(Y - \mathbb{E}(Y|X_{-j}))^4 \) as

\[
\mathbb{E}(Y - \mathbb{E}(Y|X_{-j}))^4 \leq 2^4 \mathbb{E}Y^4. \tag{A.83}
\]

Then it follows that there exists some \( K_5 > 0 \) such that for each positive integer \( n \), \( B_1 > 0 \), and \( t \in \mathbb{R} \),

\[
\mathbb{P}(E^c_8) \leq n^{-1/4} \mathbb{E}[n^{-1/2} \sum_{i=1}^{n} (A_{1i}^2 - \sigma_{j0}^2)] \\
\leq n^{-1/4} K_5 \{\mathbb{E}(n^{-1} \sum_{i=1}^{n} (A_{1i}^2 - \sigma_{j0}^2)^2)\}^{1/2} \\
\leq n^{-1/4} K_5 (\mathbb{E} A_{1i}^4)^{1/2} \\
\leq n^{-1/4} 4 K_5 (\mathbb{E}Y^4)^{1/2},
\]

where the first and second inequalities are due to Markov’s inequality, the Burkholder–Davis–Gundy inequality, and Jensen’s inequality, the third one follows from the i.i.d. assumption
and the fact of \( \sigma_{j0}^2 = \mathbb{E}A_{i1}^2 \) due to the assumption that \( X_j \) is a null feature, and the last one is entailed by (A.83) and the facts that \( 0 \leq g(x) \leq 1 \) and that \( (X_1, Y_1) \) and \( (X, Y) \) have the same distribution. By Markov’s inequality, Jensen’s inequality, and Condition 2, it holds that for each positive integer \( n \), \( B_1 > 0 \), and \( t \in \mathbb{R} \),

\[
\mathbb{P}(E^c_0) \leq B_1^{-1/4} \mathbb{E}|\mathbb{E}(E(Y|X_{-j}) - \hat{Y}(X_{-j}),Y)| \leq B_1^{1/4}.
\] (A.85)

Therefore, combining (A.77)–(A.85) and the assumption of \( \mathbb{E}Y^4 < D_2 \) (Condition 3) yields that there exists some \( C > 0 \) such that for all large \( n \), each \( 0 < B_1 < 1 \) \( (B_1^{1/2} \leq B_1^{1/4} \) since \( B_1 < 1 \)), and each \( t \in \mathbb{R} \),

\[
\mathbb{P}(E^c_{n,B_1}) \leq \sum_{l=1}^{9} \mathbb{P}(E^c_l) \leq C(B_1^{1/4} + n^{-1/4}),
\]

which concludes the proof of Lemma 1.

B.6 Lemma 2 and its proof

All the notation is the same as in the proof of Theorem 1. In particular, recall that \( A_{i1} = (Y_i - \mathbb{E}(Y_i|X_{-i}))(g(X_{ij}) - \mathbb{E}g(X_j)) \) and \( \sigma_{j0}^2 = \text{Var}(A_{i1}) \).

**Lemma 2.** Let \( X_j \) be a null feature and assume that \( \mathbb{E}Y^4 < \infty \), \( 0 < \sigma_{j0}^2 < \infty \), and \( 0 \leq g(X_j) \leq 1 \). Then there exists some \( C > 0 \) such that for each positive integer \( n \),

\[
\sup_{t \in \mathbb{R}} |\mathbb{P}(n^{-1/2} \sum_{i=1}^{n} \frac{A_{i1}}{\sigma_{j0}} \leq t) - \Phi(t)| \leq C(16\mathbb{E}Y^4)^{1/3} \sigma_{j0}^{-4/3} n^{-1/3},
\]

where \( \Phi(\cdot) \) stands for the cumulative distribution function of the standard Gaussian distribution. Note that constant \( C \) does not depend on \( \mathbb{E}Y^4 \), \( \sigma_{j0}^2 \), or index \( 1 \leq j \leq p \).

**Proof.** The proof of this lemma involves an application of the central limit theorem [32, 43]. To do so, we will verify the required conditions. Since \( X_j \) is a null feature and the observations are i.i.d., we have that \( \mathbb{E}A_{i1} = 0 \) and \( \sigma_{j0}^2 = \mathbb{E}(A_{i1}^2) \) for each \( i \). Let \( s := \sqrt{n} \sigma_{j0} \) and \( \varepsilon = 16^{1/3}(\mathbb{E}Y^4)^{1/3} \sigma_{j0}^{-4/3} n^{-1/3} \). Then we can deduce that

\[
\sum_{i=1}^{n} \mathbb{E} \left( \frac{A_{i1}}{s} \right)^2 1_{|A_{i1}| > s \varepsilon} = \frac{1}{n \sigma_{j0}^2} \sum_{i=1}^{n} \mathbb{E} (A_{i1}^2 1_{|A_{i1}| > s \varepsilon}) = \sigma_{j0}^{-2} \mathbb{E}(A_{i1}^2 1_{|A_{i1}| > s \varepsilon}) \leq \sigma_{j0}^{-2} (\mathbb{E}A_{i1}^4)^{1/2} \{\mathbb{P}(|A_{i1}| > s \varepsilon)\}^{1/2} \leq \sigma_{j0}^{-2} (\mathbb{E}A_{i1}^4)^{1/2} \left( \frac{\mathbb{E}A_{i1}^4}{s \varepsilon^4} \right)^{1/2} \leq \varepsilon,
\]

where \( 1 \) represents the indicator function, the second equality is due to the assumption of i.i.d. observations, the first inequality is due to the Cauchy–Schwartz inequality, the second
Lemma 3. Assume that all the notation is the same as in the main text.

This completes the proof of Lemma 2.

B.7 Lemma 3 and its proof

All the notation is the same as in the main text.

**Lemma 3.** Assume that $\text{Var}(g(X_j)|X_{-j}) \geq \varsigma_1$ and $\text{Var}(Y|X) \geq \varsigma_2$ almost surely for some $0 \leq g(X_j) \leq 1$ and $\varsigma_1, \varsigma_2 > 0$. Then we have

$$\text{Var} \{ (Y - \mathbb{E}(Y|X_{-j})) | g(X_j) - \mathbb{E}(g(X_j)) \} \geq \frac{1}{4} \varsigma_2 \varsigma_1^2,$$

$$\text{Var} \{ (Y - \mathbb{E}(Y|X_{-j})) | g(X_j) - \mathbb{E}(g(X_j|X_j)) \} \geq \frac{1}{4} \varsigma_2 \varsigma_1^2,$$

$$\text{Var} \{ (Y - \mathbb{E}(Y|X_{-j})) | g(X_j) - \mathbb{E}(g(X_j)) \} \leq \mathbb{E} Y^2,$$

$$\text{Var} \{ (Y - \mathbb{E}(Y|X_{-j})) | g(X_j) - \mathbb{E}(g(X_j|X_j)) \} \leq \mathbb{E} Y^2.$$

**Proof** For any $G(X)$ with $\mathbb{P}(|G(X)| > d) > \delta$ for some $d, \delta > 0$, it holds that

$$\text{Var} \{ (Y - \mathbb{E}(Y|X_{-j}))G(X) \} \geq \mathbb{E} \{ \text{Var} \{ (Y - \mathbb{E}(Y|X_{-j}))G(X) | X \} \} = \mathbb{E} \{ \text{Var} \{ (Y - \mathbb{E}(Y|X) + \mathbb{E}(Y|X) - \mathbb{E}(Y|X_{-j}))G(X) | X \} \} = \mathbb{E} \{ \left[ (Y - \mathbb{E}(Y|X) + \mathbb{E}(Y|X) - \mathbb{E}(Y|X_{-j}))G(X) \right] \} \geq \mathbb{E} \{ (Y - \mathbb{E}(Y|X))d \}^2 1_{|G(X)| > d} \geq \varsigma_2 d^2 \delta,$$

where the third equality follows from the facts that $\mathbb{E} \{ \left[ \mathbb{E}(Y|X) - \mathbb{E}(Y|X_{-j}) \right] G(X) | X \} = \mathbb{E} \{ \left[ \mathbb{E}(Y|X) - \mathbb{E}(Y|X_{-j}) \right] G(X) \}$ almost surely and that $\mathbb{E} \{ (Y - \mathbb{E}(Y|X)) G(X) | X \} = 0$, and the last inequality is due to the assumption of $\text{Var}(Y|X) \geq \varsigma_2$.

Next, for each Borel set $\mathcal{A} \in \mathcal{R}$ and $G(X)$ such that $-1 \leq G(X) \leq 1$ and $\mathbb{E}(G(X)) = 0$, we have

$$\text{Var}(G(X)) = \mathbb{E} \{ [G(X) - \mathbb{E}(G(X))]^2 1_{G(X) \in \mathcal{A}} + [G(X) - \mathbb{E}(G(X))]^2 1_{G(X) \in \mathcal{A}^c} \} \leq (\sup \mathcal{A} - \inf \mathcal{A})^2 \mathbb{P}(G(X) \in \mathcal{A}) + \mathbb{P}(G(X) \in \mathcal{A}^c).$$
and thus
\[ \mathbb{P}(G(X) \in \mathcal{A}) \leq \frac{1 - \text{Var}(G(X))}{1 - (\sup \mathcal{A} - \inf \mathcal{A})^2}. \]
This in combination with setting \( \mathcal{A} = [-\sqrt{\frac{3}{8}}, \sqrt{\frac{3}{8}}] \) and an additional assumption that \( \text{Var}(G(X)) \geq \varsigma_1 \) leads to
\[ \mathbb{P}(\|G(X)\| > \sqrt{\frac{\varsigma_1}{2}}) > \frac{1}{2}\varsigma_1. \] \hspace{1cm} (A.87)

By (A.86)–(A.87), the assumption of \( \text{Var}(g(X_j)|X_{-j}) \geq \varsigma_1 \), and letting \( G(X) = g(X_j) - \mathbb{E}(g(X_j)) \) or \( G(X) = g(X_j) - \mathbb{E}(g(X_j)|X_{-j}) \), we conclude the proof for the lower bounds.

For the variance upper bounds, it follows that
\[
\text{Var}([Y - \mathbb{E}(Y|X_{-j})][g(X_j) - \mathbb{E}(g(X_j))]) \leq \mathbb{E}\left\{ [Y - \mathbb{E}(Y|X_{-j})][g(X_j) - \mathbb{E}(g(X_j))] \right\}^2 \\
\leq \mathbb{E}(Y - \mathbb{E}(Y|X_{-j}))^2 \\
\leq \mathbb{E}Y^2,
\]
where the second inequality is because \( 0 \leq g(X_j) \leq 1 \). The other upper bound can be established similarly, and hence we omit the details. With these upper bounds, we can complete the proof of Lemma 3.

B.8 Lemma 4 and its proof

All notation is the same as in the proof of Theorem 2. For the reader’s convenience, some key terms are recalled below
\[
A_{1i} = (Y_i - \mathbb{E}(Y_i|X_{-ij}))(g(X_{ij}) - \mathbb{E}g(X_{ij})), \\
A_{2i} = (\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}))(g(X_{ij}) - \mathbb{E}g(X_{ij})) - \mu_1, \\
A_{3i} = (Y_i - \mathbb{E}(Y_i|X_{-ij}))(\mathbb{E}g(X_{ij}) - n^{-1}\sum_{i=1}^{n} g(X_{ij})), \\
A_{4i} = (\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij})) - \mu_2)(\mathbb{E}g(X_{ij}) - n^{-1}\sum_{i=1}^{n} g(X_{ij})) - \mu_1, \\
\mu_1 = \mathbb{E}\left( (\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j}))(g(X_{j}) - \mathbb{E}g(X_{j})) \right)|\mathcal{X}_0, \\
\mu_2 = \mathbb{E}(\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j})), \\
Q_1 = \left| \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (A_{2i} + A_{3i} + A_{4i}) \right|, \\
Q_2 = \sqrt{n}|\mu_2|\left| \mathbb{E}g(X_{j}) - n^{-1}\sum_{i=1}^{n} g(X_{ij}) \right|.
\]

**Lemma 4.** Assume that all the conditions of Theorem 2 are satisfied. Then for some constant \( C > 0 \), all large \( n \), each \( 0 < B_1 < 1 \), and each \( t > 0 \), there exist some events \( \{E_{n,B_1}\} \) such that 1) \( \mathbb{P}(E_{n,B_1}^C) \leq (-\log B_1)^{-1} + C(B_1^{1/4} + n^{-1/4}) \) and 2) on event \( E_{n,B_1} \), it holds that \( c \geq |\hat{\sigma}_{jN/n} - \sigma_{jN/n}| t + Q_1 + Q_2 + \sqrt{n}|\mu_1| \). Particularly, constant \( C \) is independent of \( 1 \leq j \leq p \).
**Proof.** The main idea of the proof for Lemma 4 is similar to that of the proof for Lemma 1 in Section B.5. Since $\hat{\sigma}^2_{JN/n} = \hat{\sigma}^2_{J0}$, in view of the definition of $\hat{\sigma}^2_{J0}$ we can write

$$
\hat{\sigma}^2_{JN/n} = n^{-1} \sum_{i=1}^{n} \left( \sum_{k=1}^{4} A_{ki} - n^{-1} \sum_{l=1}^{n} \sum_{k=1}^{4} A_{kl} \right)^2.
$$

Note that the additional terms $\mu_1$ and $\mu_2$ do not appear in the above expression. Similarly as in (A.75), we can establish that if $\sigma^2_{JN/n} \geq \left| n^{-1} \sum_{i=1}^{n} (A^2_{1i} - \sigma^2_{JN/n}) \right|$, it holds that

$$
|\hat{\sigma}_{JN/n} - \sigma_{JN/n}| \leq \left| \frac{1}{n\sigma_{JN/n}} \sum_{i=1}^{n} (A^2_{1i} - \sigma^2_{JN/n}) \right| + \sum_{k=2}^{4} \sqrt{n^{-1} \sum_{i=1}^{n} A^2_{ki}}
$$

(A.88)

Following the arguments in the proof of Lemma 1 in Section B.5, we will introduce some key events below

$$
E_1^c := \{ |n^{-1/2} \sum_{i=1}^{n} A_{2i}| \geq B_1^{1/4} \},
$$

$$
E_2^c := \{ |n^{-1/2} \sum_{i=1}^{n} (Y_i - E(Y_i|X_{-ij}))| \geq n^{1/4} \},
$$

$$
E_3^c := \{ |\frac{1}{\sqrt{n}} \sum_{i=1}^{n} [E(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}) - \mu_2]| \geq 1 \},
$$

$$
E_4^c := \{ |\frac{1}{n} \sum_{i=1}^{n} g(X_{ij}) - E g(X_j)| \geq \frac{\log n}{\sqrt{n}} \},
$$

$$
E_5^c := \{ |n^{-1/2} \sum_{i=1}^{n} A_{1i}| \geq n^{1/4} \},
$$

$$
E_6^c := \{ \frac{1}{n} \sum_{i=1}^{n} (E(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}))^2 \geq B_1^{1/2} \},
$$

$$
E_7^c := \{ n^{-1} \sum_{i=1}^{n} (Y_i - E(Y_i|X_{-ij}))^2 \geq \sqrt{n} \},
$$

$$
E_8^c := \{ |n^{-1/2} \sum_{i=1}^{n} (A^2_{1i} - \sigma^2_{JN/n})| \geq n^{1/4} \},
$$

$$
W_1^c := \{ |\mu_1| \geq B_1^{1/2} (\log B_1) \},
$$

$$
W_2^c := \{ |\mu_2| \geq B_1^{1/4} \},
$$

where the dependence on $n$ and $B_1$ is suppressed here for notational simplicity. Note that $- \log B_1 > 0$ since $0 < B_1 < 1$.

With the aid of the events introduced above, we will bound the RHS of (A.88) and terms
\[ Q_1, Q_2, \text{ and } \mu_1. \] On event \( E_8 \), it holds that
\[
\left| \frac{1}{n\sigma_{jN/n}^2} \sum_{i=1}^{n} (A_{1i}^2 - \sigma_{jN/n}^2) \right| \leq n^{-\frac{1}{2}} \sigma_{jN/n}^{-1}.
\]

From \( 0 \leq g(x) \leq 1 \) and \( 0 < B_1 < 1 \), on event \( E_6 \cap W_1 \cap E_1 \) we can deduce that
\[
n^{-1} \sum_{i=1}^{n} A_{2i}^2 = n^{-1} \sum_{i=1}^{n} (A_{2i} + \mu_1 - \mu_1)^2
\]
\[
\leq \mu_1^2 + n^{-1} \sum_{i=1}^{n} (A_{2i} + \mu_1)^2 + 2|\mu_1| \left| \sum_{i=1}^{n} (A_{2i} + \mu_1) \right| n^{-1}
\]
\[
\leq \mu_1^2 + n^{-1} \sum_{i=1}^{n} (A_{2i} + \mu_1)^2 + 2|\mu_1| \left( n^{-1} \sum_{i=1}^{n} A_{2i} + |\mu_1| \right)
\]
\[
\leq B_1 (-\log B_1)^2 + B_1^{1/2} + 2B_1^{3/4} (-\log B_1)^2 n^{-1/2} + 2B_1 (-\log B_1)^2
\]
\[
\leq 6B_1^{1/2} (-\log B_1)^2.
\]

Moreover, on event \( E_4 \cap E_6 \cap W_2 \), we have
\[
n^{-1} \sum_{i=1}^{n} A_{4i}^2 \leq \frac{(\log n)^2}{n} n^{-1} \sum_{i=1}^{n} \left( (E(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}))^2 + \mu_2^2
\right.
\]
\[
\left. + 2|\mu_2| \left| E(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}) \right| \right)
\]
\[
\leq \frac{(\log n)^2}{n} n^{-1} \sum_{i=1}^{n} \left( (E(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}))^2 + \mu_2^2
\right.
\]
\[
\left. + 2|\mu_2| \left| n^{-1} \sum_{i=1}^{n} (E(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}))^2 \right) \right)
\]
\[
\leq (\log n)^2 n^{-1} (B_1^{1/2} + B_1^{1/2} + 2B_1^{1/2})
\]
\[
= 4(\log n)^2 n^{-1} B_1^{1/2},
\]
where the second inequality is due to Jensen’s inequality. On event \( E_4 \cap E_7 \), we can show that
\[
\sqrt{n^{-1} \sum_{i=1}^{n} A_{3i}^2} \leq (\log n)n^{-1/4},
\]
and on event \( \cap_{k=1}^{5} E_k \), we can deduce that
\[
\left| n^{-1} \sum_{i=1}^{n} \sum_{k=1}^{4} A_{ki} \right| \leq n^{-1/4} + B_1^{1/4} n^{-1/2} + n^{-3/4} \log n + n^{-1} \log n.
\]

Hence, from these results, we can obtain that there exists some \( C > 0 \) such that for all large \( n \), each \( 0 < B_1 < 1 \), and each \( t > 0 \), it holds on event \( \cap_{k=1}^{8} E_k \) that
\[
\text{RHS of (A.88)} \leq C((\log n)n^{-1/4} + B_1^{1/4}).
\]
We next proceed with bounding terms $Q_1$, $Q_2$, and $\mu_1$. For all large $n$, each $B_1 > 0$, and each $t > 0$, it holds on event $\cap_{k=1}^4 E_k$ that

$$Q_1 \leq B_1^{1/4} + n^{-1/4} \log n + n^{-1/2} \log n.$$  

We can further establish that for all large $n$, each $0 < B_1 < 1$, and each $t > 0$, on event $E_4 \cap W_2$ we have

$$Q_2 \leq B_1^{1/4} \log n,$$

whereas for all large $n$, each $0 < B_1 < 1$, and each $t > 0$, on event $W_1$ we have

$$\sqrt{n}|\mu_1| \leq \sqrt{nB_1^{1/2}}(-\log B_1).$$

Let us define $E_{n,B_1} := (\cap_{k=1}^8 E_k) \cap W_2 \cap W_1$. Recall that

$$c = (\log n)(2B_1^{1/4} + n^{-1/4} \log n)(1 + t) + \sqrt{nB_1(-\log B_1)}.$$  

Thus, combining the above results yields that for all large $n$, each $0 < B_1 < 1$, and each $t > 0$, on event $E_{n,B_1}$ we have

$$c \geq |\hat{\sigma}_j N/n - \sigma_j N/n| t + Q_1 + Q_2 + \sqrt{n}|\mu_1|,$$

which gives the second assertion of Lemma 4.

It remains to bound the probabilities of all these events. We start with bounding $\mathbb{P}(E_1^c)$. To this end, let us observe that

$$\mathbb{E}A_{i}^2 \leq \left(\sqrt{\mathbb{V}ar\left((\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}))g(X_{ij}) - \mathbb{E}g(X_j)\right)} + \sqrt{\mathbb{E}\mu_1^2}\right)^2$$

$$\leq \left(2\sqrt{\mathbb{V}ar\left((\mathbb{E}(Y_i|X_{-ij}) - \hat{Y}(X_{-ij}))g(X_{ij}) - \mathbb{E}g(X_j)\right)}\right)^2$$

$$\leq 4\mathbb{E}\left(\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j})\right)^2,$$

where the first and second inequalities are due to Minkowski’s and Jensen’s inequalities, respectively, and the last one is because of the facts that $0 \leq g(x) \leq 1$ and that $(X_i, Y_i)$ and $(X_i, Y_i)$ have the same distribution for each $i$. Further, as in the application of the Burkholder–Davis–Gundy inequality for (A.77) in Section B.5, we see that $\{\sum_{t=1}^k \frac{A_{i,t}}{\sqrt{n}}\}_{k \geq 1}$ is a martingale sequence with respect to $\{\mathcal{F}_k\}$, where $\mathcal{F}_k := \sigma(X_0, A_{21}, \cdots, A_{2k})$ and $\mathcal{F}_0 := \sigma(X_0)$.

We are now ready to establish the upper bound of $\mathbb{P}(E_1^c)$. There exists some $K_1 > 0$ such
that for each \( n, B_1, t > 0 \),

\[
\Pr(E_1^c) \leq B_1^{-1/4} \mathbb{E}[n^{-1/2} \sum_{i=1}^n A_{2i}] \\
\leq B_1^{-1/4} K_1 \mathbb{E}(n^{-1} \sum_{i=1}^n A_{2i}^2)^{1/2} \\
\leq B_1^{-1/4} K_1 (n^{-1} \sum_{i=1}^n \mathbb{E}A_{2i}^2)^{1/2} \\
\leq B_1^{-1/4} K_1 (4 \mathbb{E}(\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j}))^2)^{1/2} \\
\leq 2K_1 B_1^{1/4},
\]

(A.90)

where the second inequality is due to the Burkholder–Davis–Gundy inequality, the third one is an application of Jensen’s inequality, the fourth one follows from (A.89), and the last one is by Condition 1. Note that in these arguments, the specific value of \( t \) is irrelevant in analyzing the probability upper bounds.

We next deal with term \( \Pr(E_2^c) \). It follows that there exists some \( K_2 > 0 \) such that for each \( n, B_1, t > 0 \),

\[
\Pr(E_2^c) \leq n^{-1/4} \mathbb{E}\left|\sum_{i=1}^n (Y_i - \mathbb{E}(Y_i|X_{-ij}))\right| \\
\leq n^{-1/4} K_2 \mathbb{E}\left(n^{-1} \sum_{i=1}^n (Y_i - \mathbb{E}(Y_i|X_{-ij}))^2\right)^{1/2} \\
\leq n^{-1/4} K_2 \left( n^{-1} \sum_{i=1}^n \mathbb{E}(Y_i - \mathbb{E}(Y_i|X_{-ij}))^2\right)^{1/2} \\
= n^{-1/4} K_2 \left( \mathbb{E}(Y - \mathbb{E}(Y|X_{-j}))^2\right)^{1/2} \\
\leq n^{-1/4} K_2 \{\text{Var}(Y)\}^{1/2},
\]

(A.91)

where the first to third inequalities are entailed by Markov’s inequality, the Burkholder–Davis–Gundy inequality (since \( X_j \) is assumed to be a null feature), and Jensen’s inequality, respectively, the equality above is because \((X, Y)\) and \((X_i, Y_i)\) have the same distribution for each \( i \), and the last inequality is due to the fact that \( \mathbb{E}(Y - \mathbb{E}(Y|X_{-j}))^2 \leq \text{Var}(Y) \).

The rest of the upper bounds can be established using similar arguments as in (A.90)–(A.91), and hence we will omit the full technical details here for simplicity. Similar to (A.90), we can show that there exists some \( K_3 > 0 \) such that for each \( n, B_1, t > 0 \),

\[
\Pr(E_3^c) \leq K_3 B_1^{1/2}.
\]

(A.92)

An application of Hoeffding’s inequality yields that for each \( n, B_1, t > 0 \), we have

\[
\Pr(E_4^c) \leq 2 \exp\left(-2(\log n)^2\right).
\]

(A.93)
Similar to (A.91), we can also obtain that there exists some $K_4 > 0$ such that for each $n, B_1, t > 0$,
\[
\mathbb{P}(E_n^c) \leq n^{-1/4}K_4\{\text{Var}(Y)\}^{1/2}.
\] (A.94)

Moreover, it follows from the Markov inequality, the construction of $\hat{Y}$, and Condition 1 that for each $n, B_1, t > 0$,
\[
\mathbb{P}(E_n^c) \leq \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}(\mathbb{E}(Y_i | X_{-ij}) - \hat{Y}(X_{-ij}))^2 \\
\leq B_1^{1/2}.
\] (A.95)

Similar to (A.91), we can show that for each $n, B_1, t > 0$,
\[
\mathbb{P}(E_n^c) \leq n^{-1/2}\text{Var}(Y).
\] (A.96)

As in (A.84), we can establish that there exists some $K_5 > 0$ such that for each $n, B_1, t > 0$,
\[
\mathbb{P}(E_n^c) \leq n^{-1/4}4K_5\sqrt{\mathbb{E}Y^4}.
\] (A.97)

Finally, from Condition 1 and $0 \leq g(x) \leq 1$, an application of the Markov inequality and Jensen’s inequality yields that for each $n, t > 0$ and $0 < B_1 < 1$,
\[
\mathbb{P}(W_1^c) \leq B_1^{-1/2}(-\log B_1)^{-1}\mathbb{E}|\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j})| \leq (-\log B_1)^{-1},
\]
\[
\mathbb{P}(W_2^c) \leq B_1^{-1/4}\mathbb{E}|\mathbb{E}(Y|X_{-j}) - \hat{Y}(X_{-j})| \leq B_1^{1/4}.
\] (A.98)

Therefore, by (A.90)–(A.98) and the assumption of $\mathbb{E}Y^4 < D_2$ (Condition 3), we can obtain that there exists some $C > 0$ such that for all large $n$, each $0 < B_1 < 1$ ($B_1^{1/2} \leq B_1^{1/4}$ if $0 < B_1 < 1$), and each $t > 0$,
\[
\mathbb{P}(E_n^{c, B_1}) \leq C(B_1^{1/4} + n^{-1/4}) + (-\log B_1)^{-1}.
\]

This concludes Lemma 4.

### B.9 Lemma 5 and its proof

**Lemma 5.** Given (A.70), it holds that $\mathbb{E}(Y|X_{-j}) = \mathbb{E}(Y|X).

**Proof.** The proof of this lemma involves an application of the $\pi - \lambda$ theorem [22]; see, e.g., the textbook [22] for the definitions of the $\pi$ and $\lambda$ systems. Let $\mathcal{G}$ be the collection of sets in $\sigma(X)$ such that if $A \in \mathcal{G}$, then it holds that

\[
\mathbb{E}(1_A \mathbb{E}(Y|X_{-j})) = \mathbb{E}(1_A Y).
\]

Then we can resort to the result in (A.70) to show that $\mathcal{G}$ contains a $\pi$-system. Provided that $\mathcal{G}$ is a $\lambda$-system, with the $\pi - \lambda$ theorem we can establish that $\mathcal{G}$ contains the smallest
σ-algebra generated by this π-system, which is \( \sigma(X) \). Such a result will lead to the desired conclusion of the lemma.

It remains to show that \( \mathcal{G} \) is a \( \lambda \)-system. To this end, we will make a few claims. First, event \( \Omega \) of the probability space \((\Omega, \mathcal{F}, \mathbb{P})\) is an event in \( \mathcal{G} \) by the law of the total expectation. Second, for any two events \( D_1, D_2 \in \mathcal{G} \) with \( D_1 \subset D_2 \), we can deduce that

\[
\mathbb{E}(1_{D_2 \setminus D_1} \mathbb{E}(Y|X_{-j})) = \mathbb{E}(1_{D_2} - 1_{D_1}) \mathbb{E}(Y|X_{-j}) \\
= \mathbb{E}(1_{D_2} \mathbb{E}(Y|X_{-j})) - \mathbb{E}(1_{D_1} \mathbb{E}(Y|X_{-j})) \\
= \mathbb{E}(1_{D_2} Y) - \mathbb{E}(1_{D_1} Y) \\
= \mathbb{E}(1_{D_2 \setminus D_1} Y),
\]

where the third equality is due to the definition of events \( D_i \)'s. We see from (A.99) that \( D_2 \setminus D_1 \in \mathcal{G} \). Third, for a sequence of \( D_i \in \mathcal{G} \) with \( D_i \subset D_{i+1} \), it holds that

\[
\mathbb{E}(1_{\cup_{i=1}^{\infty} D_i} \mathbb{E}(Y|X_{-j})) = \lim_{k \to \infty} \mathbb{E}(1_{\cup_{i=1}^{k} D_i} \mathbb{E}(Y|X_{-j})) \\
= \lim_{k \to \infty} \mathbb{E}(1_{\cup_{i=1}^{k} D_i} Y) \\
= \mathbb{E}(1_{\cup_{i=1}^{\infty} D_i} Y),
\]

where the first and third equalities follow from the definitions of \( D_i \)'s and \( Y \) and an application of the dominated convergence theorem, and the second one is due to the definition of \( D_i \)'s and the arguments as in (A.99). In particular, (A.100) shows that \( \cup_{i=1}^{\infty} D_i \in \mathcal{G} \). Therefore, combining these results yields that \( \mathcal{G} \) is a \( \lambda \)-system, which establishes the desired result. This completes the proof of Lemma 5.

C Some additional numerical results

C.1 Additional simulation results

In this section, we provide a summary of some basic statistics for the data generating model (28). In particular, Table 4 reports the out-of-sample root mean-squared errors (RMSEs) for these two models. The theoretical RMSE is given by

\[
\sqrt{\mathbb{E}(m(X) - \hat{Y}(X))^2},
\]

where \( \hat{Y} \) is the predicted response by random forests trained on a simulated data set from model (28) with \( n \in \{500, 1000\} \), \( \sigma = 5 \), \( p = 50 \), and \( \lambda = 0 \). The sample RMSE is calculated as

\[
\sqrt{\frac{1}{10000} \sum_{i=1}^{10000} (m(X_i) - \hat{Y}(X_i))^2}
\]

based on an independent data set of 10,000 test points \( X_1, \ldots, X_{10000} \). The reported RMSE is the average of these sample RMSEs over 50 simulation repetitions.
Table 4: The root mean-squared errors (RMSEs) are computed using 10,000 independent test points and averaged over 50 repetitions. The signal-to-noise ratios (SNRs) are calculated based on Monte Carlo simulations. For all reported statistics, we set $\lambda = 0$.

In addition, we report in Table 4 the signal-to-noise ratios (SNRs) for each additive component $\frac{\text{Var}(Z)}{\sigma^2}$, where $Z$ denotes a generic additive component in model (28). The reported ratios are calculated through Monte Carlo simulations. From these basic statistics, we can see that the random forests model fitting in this simulation is only moderately accurate, and the SNRs are generally weak with high noise level $\sigma = 5$. The candidate model (28) indeed challenges the capability of random forests in learning interactive and additive components in rather noisy environments.

C.2 Additional real data results

C.2.1 Features for forecasting

Let us present some details for the 12 selected features in Table 3. First, the IP Index stands for the Industrial Production Index which measures the levels of production and capacity in the manufacturing, mining, electric, and gas industries. Second, the housing variable HOUST is the number of new starting construction projects. Third, the FEDFUNDS is the interest rate that banks charge each other for overnight loans to meet their reserve requirements. It is set by the central bank of the U.S. (the Fed) and is the most influential interest rate in the U.S. economy. Fourth, the 3-month treasury bill rate is the yield received for investing in a government issued treasury security that has a maturity of three months. Fifth, the PPI stands for the Producer Price Index. The PPI of the finished goods measures the average change in the sale prices for the finished goods, which are commodities that will not undergo further processing and are ready for sale to the end users. Sixth, the FRED code for the overall Consumer Price Index is “CPIAUCSL.” The Consumer Price Index measures the average change in prices over time that consumers pay for a basket of goods and services. The kinds of goods and services included by the PPI and Consumer Price Index are different, but these indices are both natural measures of the inflation. In particular, all time series have been transformed following [39] except for CPIAUCSL, which has been transformed by $\log(\text{CPIAUCSL}_t) - \log(\text{CPIAUCSL}_{t-1})$ at time $t$ to measure the inflation.

The 81 features are categorized into 12 groups. Three of them contain only a single feature, which are RPI, S&P 500, and FEDFUNDS, respectively, while the other 9 groups of the remaining 78 features are listed in Table 5. Our groups of features are similar to the categories in [39], but are smaller than theirs. For example, the new starting constructions and new housing permits are in the same group called “Housing” in [39]. All the groups in Table 5 contain features that measure the same aspect of economy; these aspects are displayed at the top of each column in the table. The boldface features in the table are the selected...
| Industrial production | Unemployment | Employment | New starting constructions |
|-----------------------|-------------|------------|---------------------------|
| INDPRO                | HWI         | PAYEMS     | HOUST                     |
| IPFPNSS               | HWIURATIO   | USGOOD     | HOUSTNE                   |
| IPFINAL               | CLF16OV     | CES1021000001 | HOUSTMW                  |
| IPCONGD               | CE16OV      | USCONS     | HOUSTS                    |
| IPDCONGD              | UNRATE      | MANEMP     | HOUSTW                    |
| IPNCONGD              | UEMPMEAN    | DMANEMP     |                           |
| IPBUSEQ               | UEMPLT5     | NDMANEMP    |                           |
| IPMAT                 | UEMP5TO14   | SRVPRD     |                           |
| IPDMAT                | UEMP15OV    | USTPU      |                           |
| IPNMAT                | UEMP15T26   | USWTRADE   |                           |
| IPMANSICS             | UEMP27OV    | USTRADE    |                           |
| IPB51222S             |             | USFIRE     |                           |
| IPFUELS               |             | USGOVT     |                           |

| New housing permits | Money supply | Interest rates | PPI | CPI |
|---------------------|--------------|----------------|-----|-----|
| PERMIT              | M1SL         | TB3MS          | WPSFD49207 | CPIAUUCSL |
| PERMITNE            | M2SL         | TB6MS          | WPSFD49502 | CPIAPPSL  |
| PERMITMWM           | M2REAL       | GS1            | WPSID61    | CPITRNSL  |
| PERMITS             | GS5          | GS10           | WPSID62    | CPIMEDSL  |
| PERMITW             | AAA          | AAA            |             | CUSR0000SAC |
|                     | BAA          | T1YFFM         |             | CUSR0000SAD |
|                     |              | T5YFFM         |             | CUSR0000SAS |
|                     |              | T10YFFM        |             | CPIULFSL  |
|                     |              | ABAFFM         |             | CUSR6000S2A0L2 |
|                     |              | BAAFFM         |             | CUSR6000S2A0L5 |

Table 5: The 9 groups of the remaining 78 features and their FRED codes.
ones and each group has only one selected feature. For more details of these features, see [39] and the FRED website https://fred.stlouisfed.org/.

C.2.2 Grouping features for enhanced power

In this section, we provide details on how we process the time series in each group listed in Table 5. We also illustrate the effects of grouping features on improving the selection power through additional numerical analysis. For each feature in a group listed in Table 5 that is not a selected one (i.e., non-boldface), we replace it with the residual obtained by regressing it on the selected one (i.e., the boldface one in this group) with random forests. This way, we can remove the effects of selected features on the other features in their respective groups.

To investigate the effects of grouping features, we conduct a numerical study in the identical way as that for FEDFUNDS in the left panel of Figure 3 expect for no feature grouping. The results are reported in the right panel of Figure 5. To ease the reading, we reproduce the left panel of Figure 3 here in the left panel of Figure 5, with two additional vertical dashed lines indicating the indices of features in the group “Interest rates” in Table 5. The x-axis of Figure 5 displays the feature indices, which are the same as those in Figure 3.

We can observe from the right panel of Figure 5 that for the FACT statistics, more features take larger values compared to the results from the left panel, but none of the features are significant when adjusted for multiplicity in testing with the false discovery rate (FDR) controlled at the 0.2 level, where the p-values are calculated using (17). In addition, the grouping technique makes the relative importance of some features more stand out under the MDI measure. Particularly, with the grouping technique, the MDI measure of feature TB3MS is clearly more distinguished from other features in the same group of “Interest rates” (i.e., between the two vertical dashed lines).

From Figure 5, we see that without grouping features, it is less clear which features are relatively more active than others, illustrating the effects of grouping features for the FRED-
MD data set. Grouping features here relies only on the basic economic knowledge given in [39]. It is possible that more advanced economic knowledge can be exploited to further improve the selection power.