High-Dimensional Knockoffs Inference for Time Series Data

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Abstract

The model-X knockoffs framework provides a flexible tool for achieving finite-sample false discovery rate (FDR) control in variable selection in arbitrary dimensions without assuming any dependence structure of the response on covariates. It also completely bypasses the use of conventional p-values, making it especially appealing in high-dimensional nonlinear models. Existing works have focused on the setting of independent and identically distributed observations. Yet time series data is prevalent in practical applications in various fields such as economics and social sciences. This motivates the study of model-X knockoffs inference for time series data. In this paper, we make some initial attempt to establish the theoretical and methodological foundation for the model-X knockoffs inference for time series data. We suggest the method of time series knockoffs inference (TSKI) by exploiting the ideas of subsampling and e-values to address the difficulty caused by the serial dependence. We also generalize the robust knockoffs inference in [5] to the time series setting and relax the assumption of known covariate distribution required by model-X knockoffs, because such an assumption is overly stringent for time series data. We establish sufficient conditions under which TSKI achieves the asymptotic FDR control. Our technical analysis reveals the effects of serial dependence and unknown covariate distribution on the FDR control. We conduct power analysis of TSKI using the Lasso coefficient difference knockoff statistic under linear time series models. The finite-sample performance of TSKI is illustrated with several simulation examples and an economic inflation study.

Running title: TSKI

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1 Introduction

Selecting important covariates contributing to a response variable from a set of candidate covariates is an important problem arising in various scientific fields including social and medical sciences. When the number of candidate variables is large, controlling the false discovery rate (FDR) of the variable selection procedure is an effective and popular way to control the error rate. Most existing works achieve this goal by building procedures based on the p-values constructed for assessing the importance of individual variables; see, e.g., the seminal works of [7, 8]. Yet, the high dimensionality in covariates and the possibly complicated nonlinear model structure that are frequently encountered in the big data era make many conventional ways of p-value calculations inapplicable or even completely fail [20]. To overcome such difficulties, the framework of knockoffs inference was proposed in [4, 11] to achieve the goal of exact FDR control in variable selection in finite samples completely bypassing the use of the conventional p-values in high-dimensional regression models. It allows arbitrary dependence structure of the response on covariates and arbitrary dimensionality of covariates at the cost of assuming the known joint covariate distribution. While various efforts have been made to ease the implementation and relax the technical assumptions on knockoffs inference [27, 19, 22, 3, 41], such endeavors are almost always in the setting of independent observations without serial dependence. As a result, it is unclear whether these existing works are applicable to the time series setting where serial dependence is present. Our work tries to fill the gap by developing a theoretical and methodological foundation of model-X knockoffs inference [11] in the time series setting.

We now briefly review the model-X knockoffs to better lay out the foundation. Let \( y \) be an \( n \)-dimensional response vector and \( X \) an \( n \times p \) matrix of covariates across \( n \) independent observations. The knockoffs inference aims at selecting relevant covariates according to Definition 2 (see Section 2.1) while keeping the FDR under control. To this end, the model-X knockoffs framework [11] constructs an \( n \times p \) matrix \( \tilde{X} = (\tilde{x}_1, \cdots, \tilde{x}_p) \) with \( \tilde{x}_j \in \mathbb{R}^n \), \( j = 1, \cdots, p \), using the joint distribution of \( X \) (assumed to be known) such that

\[
\tilde{X} \perp \perp y | X \quad \text{and} \quad (X, \tilde{X})_{\text{swap}(S)} \overset{d}{=} (X, \tilde{X})
\]

for each \( S \subset \{1, \cdots, p\} \), where \( \text{swap}(S) \) denotes the swapping operation meaning that for each \( j \in S \), columns \( j \) and \( j+p \) are swapped, and \( \overset{d}{=} \) stands for equal in distribution. Since \( \tilde{X} \) is constructed conditionally independent of \( y \), it holds that \( (X, \tilde{X}, y)_{\text{swap}(S)} \overset{d}{=} (X, \tilde{X}, y) \) for each \( S \) containing only irrelevant covariates. At a high level, the model-X knockoffs inference creates “fake” covariates \( \tilde{X} \) which perfectly mimic the “behavior” of the original covariates. By using these “fake” covariates as control, the importance of original covariates can be inferred. The fake covariates \( \tilde{x}_j \)'s are referred to as model-X knockoff variables (knockoffs for short) in [11].
Two important assumptions in [11] are that 1) the observations in \((X, y) \in \mathbb{R}^{n \times (p+1)}\) across the rows are independent and identically distributed (i.i.d.) and 2) the joint distribution of \(X\) is known for generating the knockoff matrix \(\tilde{X}\). The first assumption ensures that the knockoff variables can be constructed in a rowwise fashion independent of other rows. The second assumption makes it possible to construct ideal knockoffs satisfying the two critical conditions in (1). However, for time series data with serial dependence, it is unclear whether the rowwise knockoff variable construction still gives us nearly valid knockoffs inference and what the precise effect of serial dependence on FDR control is. Also, in time series applications when the covariates are lagged variables with stationarity assumption, assuming known covariate distribution directly gives us the set of important variables, invalidating the problem of variable selection. In this paper, we will address these challenges for time series applications by relaxing the two aforementioned assumptions.

Regarding the assumption of i.i.d. rows, we overcome the difficulties caused by serial dependence with the idea of subsampling. Meanwhile, to address the challenges related to known covariate distribution, we generalize the robust knockoffs inference in [5] to the time series setting, where the robust knockoffs inference [5] is a recent innovative work that allows for approximate covariate distribution, as opposed to known covariate distribution, in non-time series applications. We will name the knockoff variables generated using approximate covariate distribution as approximate knockoffs to ease the presentation. Specifically, our analyses reveal that with approximate knockoffs generated in a rowwise fashion ignoring the serial dependence, the FDR inflation has an upper bound depending on the Kullback–Leibler (KL) divergence between the distributions of data matrices corresponding to approximate and exact model-X knockoff variables (see Theorem 2). There is generally no guarantee that such KL divergence could asymptotically vanish in the existence of serial dependence, indicating that the corresponding FDR is generally uncontrolled. To address such difficulty, we apply the subsampling technique to obtain asymptotically independent rows [40] under the assumption that the time series are \(\beta\)-mixing. In contrast to most of the existing literature (e.g., [40]), our analysis of asymptotically independent rows takes into account the response variables and (approximate) knockoff covariates, creating additional technical challenges. We then apply the knockoffs inference method to the subsampled data. The asymptotically independent rows in the subsampled data make it possible for the KL divergence to asymptotically vanish. However, a major disadvantage of subsampling is the inefficient use of data. We propose to apply the knockoffs inference to each subsample of data, and then aggregate their results via the e-value method [37, 32]. The resulting knockoffs inference method with subsampling and e-value aggregation is presented in Section 2 and named as the time series knockoffs inference (TSKI). We provide an explicit characterization on how the serial dependence and the accuracy of the approximate knockoffs affect the FDR control. Particularly, the TSKI procedure can achieve asymptotic FDR control when the subsampling is done in an appropriate fashion.

It is well-known that the FDR and power are two sides of the same coin. We then turn to the power analysis of TSKI in Section 3. Assuming linear time series models and regularity conditions, we show that TSKI without subsampling, which is the e-value version
of the original knockoff plus inference [5, 4], enjoys the asymptotic sure screening property
[18] under a signal strength condition that is no stronger than the beta-min condition. For
TSKI with subsampling, our results reveal an interesting phenomenon that with asymptotic
probability one, the set of selected variables is either empty or enjoys the sure screening
property, when the tuning parameters are chosen appropriately. The event of no discovery
(i.e., the empty selected set) usually occurs when most individual knockoff filters for different
subsamples select an abundantly large number of false positives so that the resulting e-values
for all variables become too small to be selected. We further show that if the FDR for each
individual knockoff filter can be controlled, then an upper bound on the number of false
positives for each knockoff filter can be established. Consequently, the event of no discoveries
can be ruled out, and the set of selected variables by TSKI enjoys asymptotic power one.
These results are summarized formally in Theorem 3.

We test the empirical performance of TSKI on both simulated and real data. Our sim-
ulation results in Section 4 demonstrate that the TSKI with subsampling controls stably
the time series FDR for some popular $\beta$-mixing processes. The selection power is generally
satisfactory with sufficient sample size. Further, in Section 5 we apply the TSKI to study
the temporal relations between the inflation and other macroeconomic time series from the
U.S. economy during the recent ten years.

1.1 Notation

To facilitate the technical presentation, let us first introduce some necessary notation. Let
$(\Omega, \mathcal{F}, \mathbb{P})$ and $\mathcal{R}$ be the underlying probability space and the Borel $\sigma$-algebra
on the real line $\mathbb{R}$, respectively. We will use the boldface for random vectors and matrices, and
the tilde for the knockoff variables. The distribution of a random mapping $X$ is denoted as $\mu_X$.
For any vector $x$, define $x_{-j}$ as $x$ without the $j$th coordinate. We also use parentheses for
matrix concatenation. For a matrix $X$ and an index subset $S$, $X(S)$ represents a submatrix
of $X$ containing only columns with indices in $S$. For $\vec{x} := (x_1, \cdots, x_n)^T \in \mathbb{R}^n$, we define
$\|\vec{x}\|_k := (\sum_{i=1}^n |x_i|^k)^{1/k}$, $\|\vec{x}\|_\infty := \max_{1 \leq i \leq n} |x_i|$, and $\|\vec{x}\|_0 := \sum_{i=1}^n 1_{\{x_i \neq 0\}}$ with $1_{\{\cdot\}}$ being
the indicator function. Note that we use the vector notation $\vec{x}$ to denote vectors in the
Euclidean space. The total variation (TV) norm for any measures $\mu_1$ and $\mu_2$ on $(\Omega, \mathcal{F})$ is
defined as $\|\mu_1 - \mu_2\|_{TV} := 2 \sup_{D \in \mathcal{F}} |\mu_1(D) - \mu_2(D)|$. For any real sequences $\{a_n\}$ and $\{b_n\}$,
$a_n = O(b_n)$ means $\limsup_{n \to \infty} \frac{a_n}{b_n} < \infty$, and $a_n = o(b_n)$ means $\limsup_{n \to \infty} \frac{a_n}{b_n} = 0$. We
use $\#S$ to denote the cardinality of a given set $S$. Moreover, a transition kernel is defined as
a map $p : (\mathbb{R}^{k_1}, \mathcal{R}^{k_2}) \to [0, 1]$ for some positive integers $k_1$ and $k_2$ satisfying that (i) for each
$D \in \mathcal{R}^{k_2}$, $p(\cdot, D)$ is a measurable function and (ii) for each $x \in \mathbb{R}^{k_1}$, $p(x, \cdot)$ is a probability
measure.

2 Robust time series knockoffs inference with TSKI

Given an observed sample $\{Y, x_i\}_{i=1}^n$ that may involve stationary time series variables, we
are interested in selecting relevant features in the covariate vector $x_i$ with respect to response
Definition 2. A knockoff generator
Throughout this paper, we will consider the knockoff generator given in Definition 2 below.

2.1 Robust knockoffs inference framework

In this paper, we will develop an inference procedure for controlling the FDR for time series data with serial dependency. Our method builds on the recent work of robust knockoffs inference [5] proposed for the non-time series setting. We will introduce some key definitions motivated from [5] that will be used throughout the presentation next.

Definition 1. (Null covariate) Consider the response $Y$ and the covariate vector $x = (X_1, \cdots, X_p)^T$. Covariate $X_j$ with $j \in \{1, \cdots, p\}$ is said to be null if and only if $X_j$ is independent of response $Y$ conditional on $(X_1, \cdots, X_{j-1}, X_{j+1}, \cdots, X_p)^T$.

We denote the set of null features in $x_i$ with respect to response $Y_i$ as $\mathcal{H}_0 \subset \{1, \cdots, p\}$ for each $i$, where $\mathcal{H}_0$ is independent of $i$ because $(Y_i, x_i)$’s are assumed to have the same distribution. For a set of selected important features $\tilde{S} \subset \{1, \cdots, p\}$ returned by some algorithm, we are interested in controlling the false discovery rate (FDR) defined as

$$\text{FDR} := \mathbb{E} \left( \frac{\#(\tilde{S} \cap \mathcal{H}_0)}{\#\tilde{S} \lor 1} \right).$$

In this paper, we will develop an inference procedure for controlling the FDR for time series data with serial dependency. Our method builds on the recent work of robust knockoffs inference [5] proposed for the non-time series setting. We will introduce some key definitions motivated from [5] that will be used throughout the presentation next.

2.1 Robust knockoffs inference framework

Throughout this paper, we will consider the knockoff generator given in Definition 2 below.

Definition 2. A knockoff generator $\kappa : \mathbb{R}^p \times \mathbb{R}^p \mapsto \mathbb{R}^p$ is a transition kernel such that $\kappa(\tilde{z}, \cdot)$ is a probability measure for each $\tilde{z} \in \mathbb{R}^p$ and $\kappa(\cdot, A)$ is a measurable function for each $A \in \mathbb{R}^p$, where $\mathcal{R}$ is the smallest $\sigma$-algebra of $\mathbb{R}$.

Given a knockoff generator and a random vector $x$, we sample a knockoff random vector $\tilde{x}$ of $x$ from the distribution $\kappa(x, \cdot)$. From now on, we let $\tilde{x}_i$ be the knockoff vector of $x_i$ generated from the knockoff generator $\kappa$. Denote by $X = (x_1, \cdots, x_n)^T$, $\tilde{X} = (\tilde{x}_1, \cdots, \tilde{x}_n)^T$, and $Y = (Y_1, \cdots, Y_n)^T$. To facilitate our technical analysis, we will introduce some regularity conditions.

Condition 1. Assume that the density function of the distribution of $(X, \tilde{X}, Y)$ exists and $(Y_i, x_i)$’s are identically distributed. In addition, the supports of $(X, \tilde{X}, Y)$ and $[X, \tilde{X}, Y]_{\text{swap}(\{j\})}$ are the same for each $j \in \{1, \cdots, p\}$, where $[X, \tilde{X}, Y]_{\text{swap}(S)}$ is obtained by swapping the $j$th and $(j+p)$th columns of $(X, \tilde{X}, Y)$ for each $j \in S \subset \{1, \cdots, p\}$.

Condition 2. The knockoff generator $\kappa(\cdot, \cdot)$ is given before we observe $\{x_i, Y_i\}_{i=1}^n$.

Condition 1 is a basic regularity condition. Condition 2 may be relaxed if we apply the sample splitting to obtain an asymptotically independent training subsample for training the knockoff generator. With Condition 2, $Y_i$ is independent of $\tilde{x}_i$ conditional on $x_i$, and $(Y_i, x_i, \tilde{x}_i)$’s are identically distributed if $(Y_i, x_i)$’s are identically distributed. In addition, without Condition 2, $(x_i, \tilde{x}_i)$’s may not be i.i.d. even if $x_i$’s are i.i.d. themselves.
Let \((Y, \mathbf{x}, \tilde{\mathbf{x}})\) with \(\tilde{\mathbf{x}} = (\tilde{X}_1, \cdots, \tilde{X}_p)^T\) be an independent random vector identically distributed as \((Y_1, \mathbf{x}_1, \tilde{\mathbf{x}}_1)\). A good knockoff generator is expected to generate \(\tilde{\mathbf{x}}\) with distribution as close to the model-X knockoffs as possible, where the model-X knockoffs random vector \(\tilde{\mathbf{x}}^X \in \mathbb{R}^p\) of \(\mathbf{x}\) is such that 1) for each \(S \subset \{1, \cdots, p\}\), \([\mathbf{x}, \tilde{\mathbf{x}}^X]|_{\text{swap}(S)} \overset{d}{=} [\mathbf{x}, \tilde{\mathbf{x}}^X]\) with \(d\) standing for equal in distribution and 2) \(\tilde{\mathbf{x}}^X\) is independent of response \(Y\) conditional on \(\mathbf{x}\). However, generating the \textit{exact} model-X knockoffs requires the knowledge on the true underlying distribution of \(\mathbf{x}\), which is an impractical assumption for time series data. To understand this, note that for time series data, covariates \(\mathbf{x}\) may be lags of the response, and thus assuming a known distribution of \(\mathbf{x}\) gives us the serial distribution of the time series that leads directly to known variable importance in such a scenario.

To overcome such difficulty, we will allow certain deviation of the distribution of \(\tilde{\mathbf{x}}\) from that of the model-X knockoffs. In other words, \(\tilde{\mathbf{x}}\) generated from \(\kappa(\mathbf{x}, \cdot)\) is only a random vector of approximate knockoff variables. The use of approximate knockoffs instead of the exact model-X knockoffs may incur a potential FDR inflation. To control the FDR inflation, we require that our knockoff generator \(\kappa\) satisfies Condition 3 below, which is the pairwise exchangeability [5]. Specifically, in addition to the knockoff generator \(\kappa(\cdot, \cdot)\), let us assume that we have a coordinatewise knockoff generator \(\kappa_j : \mathbb{R}^{p-1} \times \mathbb{R}^{p-1} \mapsto \mathbb{R}\) for each \(j \in \{1, \cdots, p\}\) that generates \(\tilde{X}^\dagger_j\) given \(\mathbf{x}_{-j}\), where the distribution of \(\tilde{X}^\dagger_j\) conditional on \(\mathbf{x}_{-j}\) is an \textit{approximation} to the true underlying distribution of \(X_j\) conditional on \(\mathbf{x}_{-j}\). Condition 3 is an assumption on all \(p + 1\) knockoff generators \(\kappa(\cdot, \cdot), \kappa_1(\cdot, \cdot), \cdots, \kappa_p(\cdot, \cdot)\).

\textbf{Condition 3.} \textit{For each} \(1 \leq j \leq p, 1\) \textit{if} \(\tilde{\mathbf{z}} = (\tilde{Z}_1, \cdots, \tilde{Z}_p)^T\) \textit{is sampled from the conditional distribution} \(\kappa((X_1, \cdots, X_{j-1}, \tilde{X}_j, X_{j+1}, \cdots, X_p), \cdot)\), \textit{then} \((\tilde{X}^\dagger_j, \tilde{Z}_j, \mathbf{x}_{-j}, \tilde{\mathbf{x}}_{-j})\) \textit{and} \((\tilde{Z}_j, \tilde{X}^\dagger_j, \mathbf{x}_{-j}, \tilde{\mathbf{x}}_{-j})\) \textit{have the same distribution with} \(\tilde{X}^\dagger_j\) \textit{sampled from} \(\kappa_j(\mathbf{x}_{-j}, \cdot)\), \textit{and} \(2\) \textit{the density function of the distribution of} \((\tilde{X}^\dagger_j, \tilde{Z}_j, \mathbf{x}_{-j}, \tilde{\mathbf{x}}_{-j})\) \textit{exists.}

To avoid potential confusion, throughout the paper we distinguish the knockoff generator \(\kappa(\cdot, \cdot)\) from \(\kappa_j(\cdot, \cdot)\)'s by referring to the former as “the knockoff generator” and the latter as “the coordinatewise knockoff generators.” Also, the dagger tilde notation denotes a coordinatewise knockoff variable generated from \(\kappa_j(\cdot, \cdot)\)'s, while the tilde notation represents a knockoff variable produced by the knockoff generator \(\kappa(\cdot, \cdot)\).

We would like to point out that for practical implementation, only \(\kappa(\cdot, \cdot)\) is needed for generating the knockoff variables, and \(\kappa_j(\cdot, \cdot)\)'s are not needed. Nevertheless, from a theoretical viewpoint, the existence of some \(\kappa_j(\cdot, \cdot)\)’s such that our knockoff generator satisfies Condition 3 is crucial for controlling the FDR inflation. Some examples of the knockoff generator that satisfy Condition 3 with respect to some coordinatewise knockoff generators are given in [5]. When Condition 3 is satisfied, the FDR inflation can be measured by the Kullback–Leibler (KL) divergence between the distribution of \(\tilde{X}^\dagger_j\) conditional on \(\mathbf{x}_{-j}\) and that of \(X_j\) conditional on \(\mathbf{x}_{-j}\), which will be summarized formally in Theorems 1–2 to be presented in the later sections.
2.2 Robust TSKI

Our robust time series knockoffs inference (TSKI) procedure applies the robust knockoffs inference \cite{5} to multiple subsamples of the given time series observations and then establishes an ensemble inference using the e-values \cite{37}. Specifically, we consider \( q + 1 \) subsamples and their index sets \( H_k = \{ k + s(q + 1) : s = 0, 1, \cdots, \lfloor \frac{q}{q+1} \rfloor \} \) for each \( k \in \{ 1, \cdots, q + 1 \} \). To simplify the technical presentation, let \( \{ V_i, u_i, \tilde{u}_i \}_{i=1}^N \) be a generic subsample of \( \{ Y_i, x_i, \tilde{x}_i \}_{i=1}^n \). Denote by \( v := (V_1, \cdots, V_N)^T, U := (u_1, \cdots, u_N)^T, \) and \( \tilde{U} := (\tilde{u}_1, \cdots, \tilde{u}_N)^T \).

Now the knockoff statistics \( W_j \)'s based on \( v \) and the augmented design \((U, \tilde{U})\) are calculated such that \( W_j \) satisfies the sign-flip property \cite{4, 11}: for each \( S \subset \{ 1, \cdots, p \} \) and each \( 1 \leq j \leq p \),

\[
W_j(v, U, \tilde{U})_{\text{swap}(S)} = \begin{cases} -W_j(v, U, \tilde{U}) & \text{if } j \in S, \\ W_j(v, U, \tilde{U}) & \text{otherwise}. \end{cases}
\]  \hspace{1cm} (2)

In fact, the condition can be weakened from “for each \( S \subset \{ 1, \cdots, p \} \)” to “for each \( S \subset H_0 \) with \( \#S = 1 \)” but we choose not to pursue such a direction for technical simplicity.

Examples 1–2 below are two important examples of the knockoff statistics that satisfy the sign-flip property. The random forests model in Example 2 can be replaced with other learning models such as the deep learning model.

**Example 1** (Lasso coefficient difference (LCD)). For a given sample \((v, U, \tilde{U})\) and a tuning parameter \( \lambda \geq 0 \), we define

\[
W_j = W_j(v, U, \tilde{U}) = |\hat{\beta}_j| - |\hat{\beta}_{j+p}|,
\]

where \((\hat{\beta}_1, \cdots, \hat{\beta}_{2p})^T = \arg\min_{\beta \in \mathbb{R}^p} \left\{ n^{-1} \sum_{i=1}^n (V_i - (u_i^T \beta_i \tilde{u}_i^T \beta_i)^2 + \lambda \sum_{j=1}^{2p} |\beta_j|) \right\} \text{ with } \beta = (\beta_1, \cdots, \beta_{2p})^T.

**Example 2** (Random forests mean decrease accuracy (MDA)). For a given sample \((v, U, \tilde{U})\), we define

\[
W_j = W_j(v, U, \tilde{U}) = N^{-1} \sum_{i=1}^N \left\{ [V_i - \hat{m}(u_i^{(j)}, \tilde{u}_i)]^2 - [V_i - \hat{m}(u_i, \tilde{u}_i)]^2 \right\}
\]

for each \( j \in \{ 1, \cdots, p \} \), where \((u_i^{(j)}, \tilde{u}_i^{(j)}) = (u_i, \tilde{u}_i)_{\text{swap}(\{ j \})}\) and \( \hat{m} : \mathbb{R}^{2p} \to \mathbb{R} \) is the random forests regression function trained by regressing \( V_i \)'s on \((u_i, \tilde{u}_i)\)'s.
that is, and \( \hat{S} \) includes the intersection of variable sets selected by individual knockoff filters as a subset. 

1 can be viewed as a sophisticated majority voting procedure. In particular, if \( \hat{\{e_j\}} \) is the set of e-values obtained by applying individual knockoff filters via the e-value approach. The e-BH procedure is needed here since Condition 4 (the selection power loss compared to the underlying knockoffs procedure. See Theorem 3 in Meanwhile, the tuning parameter \( \tau \) is stationary distribution \( p \) is continuous with respect to the Lebesgue measure.\)

\[
\tilde{\kappa} = \max\{k : e_{(k)} \geq p(\tau^* \times k)^{-1}\},
\]

where \( e_{(j)} \)'s are the ordered statistics of \( e_j \)'s such that \( e_{(1)} \geq \cdots \geq e_{(p)} \).

Algorithm 1 above provides a way to combine the sets of variables selected by multiple individual knockoff filters via the e-value approach. The e-BH procedure is needed here since naively taking the intersection or union over multiple selected sets by the knockoff filters (i.e., \( \{j : W_j^k \geq T^k\} \) with \( k = 1, \cdots, q+1 \)) would not be guaranteed to control the FDR. Algorithm 1 can be viewed as a sophisticated majority voting procedure. In particular, if \( \hat{S} \neq \emptyset \), then \( \hat{S} \) includes the intersection of variable sets selected by individual knockoff filters as a subset and \( \hat{S} \) is also a subset of the union of all variable sets selected by individual knockoff filters; that is,

\[
\cap_{k=1}^{q+1}\{j : W_j^k \geq T^k\} \subset \hat{S} \subset \cup_{k=1}^{q+1}\{j : W_j^k \geq T^k\}.
\]

Meanwhile, the tuning parameter \( \tau_1 \) should be set to be smaller than \( \tau^* \) in order to reduce the selection power loss compared to the underlying knockoffs procedure. See Theorem 3 in Section 3 for details.

**Condition 4** (h-step \( \beta \)-mixing with exponential decay). Assume that the process \( \{x_t\} \) is a \( p \)-dimensional stationary Markov chain with a transition kernel \( p : \mathbb{R}^p \times \mathbb{R}^p \mapsto \mathbb{R} \) and a stationary distribution \( \pi \). There exist a positive integer \( h \), a measurable function \( V : \mathbb{R}^p \mapsto [0, \infty) \), and some constants \( 0 \leq \rho < 1 \) and \( 0 < C_0 < \infty \) such that for each \( \bar{x} \in \mathbb{R}^p \),

\[
\|p^h(\bar{x}, \cdot) - \pi(\cdot)\|_{TV} \leq C\rho^h V(\bar{x}),
\]

where \( C > 0 \) is some constant with \( C_0 \geq C \int_{\mathbb{R}^p} V(\bar{x})\,d\pi(\bar{x}) \) and \( \|\cdot\|_{TV} \) denotes the total variation (TV) norm associated with measures. Moreover, for each \( \bar{x} \in \mathbb{R}^p \), \( p(\bar{x}, \cdot) \) is absolutely continuous with respect to the Lebesgue measure.

Let \( \{x_i^\pi, \tilde{x}_i^\pi, Y_i^\pi\}_{i=1}^n \) be a sequence of i.i.d. random vectors such that \( \{x_1^\pi, \tilde{x}_1^\pi, Y_1^\pi\} \) and \( \{x_1, \tilde{x}_1, Y_1\} \) have the same distribution, \( X_k = \{x_i, \tilde{x}_i, Y_i\}_{i \in H_k} \), and \( X_k^\pi = \{x_i^\pi, \tilde{x}_i^\pi, Y_i^\pi\}_{i \in H_k} \)
for each \( k \in \{1, \ldots, q+1\} \). Let \( f_z(\cdot) \) be the density function of random vector \( z \). The FDR inflation due to the knockoff variable approximation can be measured and controlled by the KL divergence given in Theorem 1 below.

**Theorem 1.** Let \( \hat{S} \) be the set of selected variables by the TSKI with Algorithm 1. Then under Condition 1 and the assumption of positive \( T \) inflation due to the knockoff variable approximation can be measured and controlled by the conditional probability density function of (4)\[ \text{Assume that all the conditions of Theorem 1 hold. If further Condition 3 is satisfied,} \]

\[ \hat{S} = \{ i \in \mathcal{I} : \rho < 1 \} \]

where \( 0 < \tau^* < 1 \) is the target FDR level and for each \( 1 \leq k \leq q+1 \) and \( 1 \leq j \leq p \),

\[ \hat{S}^k_j = \sum_{i \in \mathcal{H}_k} \log \left( \frac{f_{X_{ij}}(X_{ij}^\pi, x_{ij}) f_{X_{ij}^\pi}^k(x_{ij}^\pi)}{f_{X_{ij}}(X_{ij}^\pi, x_{ij}) f_{X_{ij}^\pi}^k(x_{ij}^\pi)} \right). \]

The proof of Theorem 1 is provided in Section A.1 of the Supplementary Material. Recall that \((x, \bar{x}, y)\) and \((x_1, \bar{x}_1, y_1)\) have the same distribution. The KL divergence given in (5) that appears on the right-hand side of (4) can be simplified further below provided that some additional conditions are satisfied.

**Corollary 1.** Assume that all the conditions of Theorem 1 hold. If further Condition 3 is satisfied, then (4) holds with

\[ \hat{S}^k_j = \sum_{i \in \mathcal{H}_k} \log \left( \frac{f_{X_{ij}}(X_{ij}^\pi, x_{ij}) f_{X_{ij}^\pi}^k(x_{ij}^\pi)}{f_{X_{ij}}(X_{ij}^\pi, x_{ij}) f_{X_{ij}^\pi}^k(x_{ij}^\pi)} \right) \]

where \( \tilde{X}_{ij}^1 \)'s are given in Condition 3 and \( f_{z_1|z_2}(z_1 | z_2) = f_{z_1,z_2}(z_1, z_2)[f_{z_2}(z_2)]^{-1} \) which is the conditional probability density function of \( z_1 \) given \( z_2 \).

**Corollary 2.** Assume that all the conditions of Theorem 1 hold. If further Condition 2 is satisfied, \( \{x_i\}_{i \geq 1} \) satisfies Condition 4 with \( q \)-step and constants \( C_0 > 0 \) and \( 0 \leq \rho < 1 \), and \( Y_i \) is \( x_{i+1} \)-measurable, then (4) holds with

\[ \sum_{k=1}^{q+1} \sup_{D \in \mathcal{R} \#H_k \times (2p+1)} |\mathbb{P}(X_k \in D) - \mathbb{P}(X_k^\pi \in D)| \leq C_0 \times \rho^{q} \times n. \]

Moreover, when \((Y_i, x_i)\)'s are i.i.d., (6) holds with \( \rho = 0 \).

To make our results more concrete, let us consider an example with decreasing KL divergence. Assume that \( \{x_i\} \) follows a stationary linear Gaussian process as in Example 3 in Section 2.3.1 with zero mean and covariance matrix \( \Theta = \mathbb{E}(x_i x_i^\top) \), and the knockoff generator is such that \( \kappa(\bar{z}, \cdot) \) follows a Gaussian distribution with mean \((I_p - D\bar{\Theta})\bar{z}\) and variance...
\[ 2D - D\hat{\Theta}D \] for each \( \hat{z} \in \mathbb{R}^p \), where \( I_p \) is the \( p \)-dimensional identity matrix, \( \hat{\Theta} \) is the estimated covariance matrix, and \( D \) is a diagonal matrix with nonnegative entries such that \( 2D - D\hat{\Theta}D \) is positive semidefinite. Then it has been shown in Lemma 5 of [5] that when the data consists of i.i.d. observations without serial dependency, it holds that for each \( \varepsilon > 0 \),

\[
\lim_{n \to \infty} \sum_{k=1}^{q+1} \mathbb{P}( \max_{1 \leq j \leq p} KL_j > \varepsilon ) = 0
\]

(7)
as long as Condition 3 is satisfied, \( p \gg q \), and

\[
\lim_{n \to \infty} \left\{ \max_{1 \leq j \leq p} \left\| \Theta^{-\frac{1}{2}} (\hat{\Theta}_j - \Theta_j) \right\|_2 \times \sqrt{n \log p} \right\} = 0,
\]

where \( \Theta_{jj} \) denotes the \( j \)th diagonal entry of \( \Theta \) and \( \Theta_j \) represents the \( j \)th column of \( \Theta \). We omit the dependence of the parameters on sample size \( n \) here for simplicity. More examples on asymptotically vanishing KL divergence for non-time series data can be found in the same paper above. Similar results can be proved for our applications of time series data using the proof techniques in [5] by replacing the concentration inequalities for i.i.d. observations with those for \( \beta \)-mixing data; we omit the details here because the proof modification is straightforward.

### 2.3 Stationary processes satisfying Condition 4

#### 2.3.1 Linear ARX process

Example 3 below is a benchmark model for describing the behavior of macroeconomic variables.

**Example 3** (Autoregressive models with exogenous variables (ARX)). For each \( t \), we define

\[
Y_t = \sum_{j=1}^{k_1} \alpha_j Y_{t-j} + \sum_{l=1}^{k_2} \sum_{j=1}^{k_3} \beta_{jl}^{(l)} H_{t-j+l}^{(l)} + \varepsilon_{t}
\]

with \( H_{t}^{(l)} = \epsilon_{t}^{(l)} + \sum_{j=1}^{k_3} b_{j}^{(l)} H_{t-j}^{(l)} \), where for some positive constants \( L_0, L_1, \) and \( L_2 \), it satisfies that \( 1 - \sum_{j=1}^{k_3} b_{j}^{(l)} \neq 0 \) and \( 1 - \sum_{j=1}^{k_1} \alpha_j z^j \neq 0 \) for each \( |z| \leq 1 + L_0 \) and each \( l \in \{1, \cdots, k_2\} \);

\[
\sum_{l=1}^{k_2} \sum_{j=1}^{k_3} |\beta_{jl}^{(l)}| < L_1 \quad \text{and} \quad k_1, k_{31}, \cdots, k_{3k_2} < L_2.
\]

Here, \( k_1, k_2, \) and \( k_{31}, \cdots, k_{3k_2} \) are all positive integers. Moreover, \( \epsilon_{1}^{(1)}, \cdots, \epsilon_{k_2}^{(k_2)}, \epsilon_{l}^{(l)} \)'s are \( (k_2+1) \)-dimensional i.i.d. Gaussian random vectors with zero mean and positive definite covariance matrix \( \Sigma_0 \) that satisfy \( \mathbb{E}(\varepsilon_l \varepsilon_l^{(l)}) = 0 \) for each \( l \).

It is seen that the covariate vector with respect to response \( Y_t \) is \( x_t = (Y_{t-1}, \cdots, Y_{t-k_1}, h_t)^T \) with \( h_t = (H_{t}^{(1)}, \cdots, H_{t-k_{31}+1}^{(1)}, \cdots, H_{t}^{(k_2)}, \cdots, H_{t-k_{3k_2}+1}^{(k_2)})^T \). It has been shown (e.g., [2]) that the stationary process \{\( x_t \)\} in Example 3 with fixed dimensionality satisfies Condition 4 with \( h \)-step and some constants \( \rho, C_0 \) for each positive integer \( h \). When the dimensionality of \( x_t \) increases, certain growth conditions such as (8) below...
on the value of $h$ and the dimensionality of $\mathbf{x}_t$ are needed for Condition 4 to hold. Hence, we make the dependence of the stationary processes on $h$ explicit: hereafter $\{\mathbf{x}_t^{(h)}\}$ denotes a $p_h$-dimensional stationary process satisfying Condition 4 for $h = 1, 2, \cdots$. Proposition 1 below provides some sufficient conditions on the growth rate of $p_h$ as a function of $h$.

**Proposition 1.** Let $\{\mathbf{x}_t^{(h)}\}$ be a sequence of $p_h$-dimensional linear process in Example 3 with constant $L_i$'s and uniformly positive definite $\Sigma_0^{(h)}$'s. Assume that for some constant $C_2 > 0$ and sufficiently small $s_2 > 0$,

$$\sup_{h>0}\{p_h \exp (-s_2h)\} \leq C_2. \quad (8)$$

Then for some constants $0 \leq \rho < 1$ and $C_0 > 0$ and all large $h$, $\{\mathbf{x}_t^{(h)}\}$ satisfies Condition 4 with $h$-step.

Let arbitrary constants $K_0 > 0$ and $\delta > 0$ be given. In view of Theorem 1 and Proposition 1, if we perform subsampling such that $q = q_n = \lceil \log n \rceil^{1+\delta}$ in the TSKI algorithm (Algorithm 1) and assume Example 3 with $p = p_n = O(n^{K_0})$, then the $\beta$-mixing convergence rate required by Theorem 1 (Condition 4 with $q_n$-step and constants $C_0, \rho$) is satisfied by the subsampled data for all large $n$ according to Proposition 1.

### 2.3.2 Various nonlinear AR-type processes

Other than Example 3, many time-homogeneous Markov chains also satisfy Condition 4. To name a few, [35, 2] showed that with some additional mild regularity conditions, $\{(Y_{t-1}, \cdots, Y_{t-k_1})\}$ of Example 4 below satisfies Condition 4 for all $h > 0$ with some constants $C_0$ and $0 \leq \rho < 1$.

**Example 4 (Nonlinear AR [35, 2]).** Let a measurable function $G : \mathbb{R}^{k_1} \rightarrow \mathbb{R}$ be given such that $\sup_{\mathbf{z} \in \mathbb{R}^{k_1}} |G(\mathbf{z})| < \infty$, and $\{\epsilon_t\}$ a sequence of i.i.d. model errors. For each $t$, we define

$$Y_t = G(Y_{t-1}, \cdots, Y_{t-k_1}) + \epsilon_t.$$

The self-exciting threshold autoregressive models (SETAR) [36, 23] also satisfies Condition 4 for all $h > 0$ according to [2]. For more examples such as the exponential AR models, see [31, 2] and the references therein.

### 2.3.3 ARCH-type process

**Example 5 (AR($k_1$)-X-ARCH($k_3$) [14, 30]).** Let $\epsilon_t$'s be i.i.d. random variables with zero mean and $\mathbb{E} \epsilon_t^2 = 1$, and $\{h_t := (H_{t,1}, \cdots, H_{t,k_2})\}$ a sequence of $k_2$-dimensional time series covariates that is independent of $\epsilon_t$'s. Let measurable functions $G_1 : \mathbb{R}^{k_3} \rightarrow (0, \infty)$, $G_2 : \mathbb{R}^{k_2} \rightarrow \mathbb{R}$, and $\gamma_j : \mathbb{R}^{k_1} \rightarrow \mathbb{R}$ where $1 \leq j \leq k_1$ be given such that $\sum_{j=1}^{k_1} \sup_{\mathbf{z} \in \mathbb{R}^{k_1}} |\gamma_j(\mathbf{z})| < 1$. The functional-coefficient ARX-ARCH model [12] is given by

$$Y_t = \sum_{j=1}^{k_1} \gamma_j(Y_{t-1}, \cdots, Y_{t-k_1})Y_{t-j} + G_2(h_t) + \sigma_t \epsilon_t$$
with \( \sigma_t = G_1(\sigma_{t-1} \varepsilon_{t-1}, \cdots, \sigma_{t-k_3} \varepsilon_{t-k_3}) \).

Example 5 above is an ARCH model with the mean function consisting of an AR component and exogenous covariates. The covariate vector is \( x_t = (Y_{t-1}, \cdots, Y_{t-k_1-k_3}, h_t, \cdots, h_{t-k_3})^T \) for response \( Y_t \). In particular, Model 3 in Section 4 is an example of the ARX-ARCH model above when \( \gamma_j \)'s are constants and the model error follows a standard ARCH process [17].

The AR component in Example 5 above can be a general functional-coefficient autoregressive model [12], and the ARCH component can take the form of smooth transition ARCH model [26]. With \( G_2 = 0 \) and additional mild regularity conditions, the Markov chain \( \{Y_t, \cdots, Y_{t-k_1-k_3+1}\}_t \) satisfies Condition 4 for each \( h > 0 \) with constants \( C_0 > 0 \) and \( 0 \leq \rho < 1 \) according to [14, 30]. In the presence of exogenous covariates \( h_t \), additional regularity conditions on \( h_t \)'s are needed for Condition 4 to hold for the Markov chain; such study is beyond the scope of the current paper and is left for future investigation.

One challenge in variable selection problem with time series data is that there does not always exist an obvious definition of the covariate vector. Taking Example 5 for instance, the existence of the ARCH component requires us to take into account both the mean function and variance function when selecting the set of non-null variables in the broad sense according to Definition 1. To better understand this, let us consider an ARX-ARCH(1) model with a standard ARCH component such that \( \sigma_t = \sqrt{0.1 + 0.9(\sigma_{t-1} \varepsilon_{t-1})^2} \), and write

\[
\sigma_{t-1} \varepsilon_{t-1} = Y_{t-1} - \sum_{j=1}^{k_1} \gamma_j (Y_{t-2}, \cdots, Y_{t-1-k_1}) Y_{t-1-j} - G_2(h_{t-1}). \tag{9}
\]

In this example, in addition to variables \( (Y_{t-1}, \cdots, Y_{t-k_1}, h_t) \) which affect the mean regression function, we should also take into account the lagged covariates in the ARCH component \( (Y_{t-1}, \cdots, Y_{t-k_1-k_3}, h_{t-1}) \) when conducting variable selection in the broad sense according to Definition 1. That is, one sensible choice of the covariate vector is \( x_t = (Y_{t-1}, \cdots, Y_{t-k_1-k_3}, h_t, h_{t-1})^T \). Omitting variables in the variance function (i.e., the ARCH component) and defining the covariate vector as \( (Y_{t-1}, \cdots, Y_{t-k_1}, h_t) \) may give us a non-sparse set of non-null variables according to Definition 1. Nevertheless, the actual variable selection performance of the TSKI depends on the specific choice of the knockoff statistics, as will be shown in the later sections. If the knockoff statistics are constructed based on the mean regression function alone (e.g., the LCD and MDA discussed earlier), then the corresponding TSKI cannot be expected to have power in selecting variables that affect only the variance function. In this sense, our results in such scenario should be interpreted as for selecting the important variables contributing to the mean regression function alone.

Remark 1. We have left out the GARCH-type process [9] in our discussion because it can be challenging to formulate meaningful covariates for variable selection purpose in such a setting. Note that a GARCH-type process can be represented as an ARCH-type process with infinite order. Thus, if the covariates vector is not well-formulated such that some active covariates are not included, the resulting regression model may no longer be sparse, rendering
the FDR control problem invalid. We shall leave the variable selection problem for GARCH-type process in future work.

2.4 Robust TSKI without subsampling

In this section, we consider a special case of the TSKI with Algorithm 1 when we set \( q = 0 \), that is, no subsampling is used. We provide a full description of the corresponding algorithm in Algorithm 2 below since the related method and theory have standalone value to the time series literature. Two major contributions here are 1) extending the robust knockoffs inference [5] to the e-value setting and 2) further extending the results to time series applications. By similar analysis as in Theorem 2 below, we can show that the robust knockoffs inference [5] (without using the e-values) can also be extended to time series applications, but the details are omitted here for simplicity. We emphasize that our results (11)–(12) in Theorem 2 below assume neither i.i.d. observations nor the pairwise exchangibility Condition 3.

Algorithm 2: Robust time series knockoffs inference (TSKI) via e-values without subsampling

1. Let \( 0 < \tau_1 < 1 \) be a constant and \( 0 < \tau^* < 1 \) the target FDR level.
2. Calculate the knockoff statistics \( W_1, \ldots, W_p \) satisfying (2) with the full sample \( \{Y_i, x_i, \tilde{x}_i\}_{i=1}^n \).
3. Let \( W_+ = \{|W_s| : |W_s| > 0\} \). Calculate the e-value statistics \( e_j \)'s such that

\[
e_j = \frac{p \times 1_{\{W_j \geq T\}}}{1 + \sum_{s=1}^p 1_{\{W_s \leq -T\}}}, \quad T = \min \left\{ t \in W_+ : \frac{1 + \#\{j : W_j \leq -t\}}{\#\{j : W_j \geq t\} \vee 1} \leq \tau_1 \right\}. \quad (10)
\]

4. Let \( \hat{S} = \{j : e_j \geq p(\tau^* \times \hat{k})^{-1}\} \) with \( \hat{k} = \max\{k : e_{(k)} \geq p(\tau^* \times k)^{-1}\} \), where \( e_{(j)} \)'s are the ordered statistics of \( e_j \)'s such that \( e_{(1)} \geq \cdots \geq e_{(p)} \).

\[\text{min} \emptyset \text{ and } \max \emptyset \text{ are defined as } \infty \text{ and } 0, \text{ respectively.}\]

Let \( X_{-j} \) be the submatrix of \( X \) with the \( j \)th column removed, and \( X_j \) and \( \tilde{X}_j \) the \( j \)th columns of \( X \) and \( \tilde{X}, \) respectively. Recall that \((Y, x, \tilde{x})\) is an independent copy of \((Y_1, x_1, \tilde{x}_1)\) and \( \tilde{X}_j \) is given in Condition 3 by the \( j \)th coordinatewise knockoff generator.

Theorem 2. Let \( \hat{S} \) be the set of selected variables by the TSKI with Algorithm 2 and \( 0 < \tau^* < 1 \) the target FDR level. Assume that Condition 1 holds and \( T \) in (10) is positive. Then we have

\[
\text{FDR} \leq \inf_{\varepsilon > 0} \left[ \tau^* \times e^\varepsilon + \mathbb{P} (\max_{1 \leq j \leq p} \tilde{KL}_j > \varepsilon) \right], \quad (11)
\]

where for each \( 1 \leq j \leq p, \)

\[
\tilde{KL}_j = \log \left( \frac{\int_{X_j} \int_{\tilde{X}_j} \int_{X_{-j}} \int_{\tilde{X}_{-j}} \mathbb{P}(X_j, \tilde{X}_j, X_{-j}, \tilde{X}_{-j}, Y)}{\int_{X_j} \int_{\tilde{X}_j} \int_{X_{-j}} \int_{\tilde{X}_{-j}} \mathbb{P}(X_j, X_{-j}, \tilde{X}_j, \tilde{X}_{-j}, Y)} \right). \quad (12)
\]
If we further assume that Condition 2 is satisfied and $X_j$ is independent of $Y$ conditional on $X_{-j}$ for each $j \in \mathcal{H}_0$, then we have
\[
\tilde{K}_L_{ij} = \log \left( \frac{f_{X_{ij}x_{-j}x_{-j}}(X_{ij}x_{ij}, X_{-j}x_{-j})}{f_{X_{ij}x_{-j}x_{-j}}(X_{ij}x_{ij}, X_{-j}x_{-j})} \right). \tag{13}
\]
Moreover, if $(x, \tilde{x}), (x_1, \tilde{x}_1), \ldots, (x_n, \tilde{x}_n)$ are further assumed to be i.i.d., then we have
\[
\tilde{K}_L = \sum_{i=1}^{n} \log \left( \frac{f_{X_{ij}x_{-j}x_{-j}}(X_{ij}x_{ij}, X_{-j}x_{-j})}{f_{X_{ij}x_{-j}x_{-j}}(X_{ij}x_{ij}, X_{-j}x_{-j})} \right). \tag{14}
\]
If further Condition 3 is satisfied, then we have
\[
\tilde{K}_L = \sum_{i=1}^{n} \log \left( \frac{f_{X_{ij}x_{-j}x_{-j}}(X_{ij}x_{ij}, X_{-j}x_{-j})}{f_{X_{ij}x_{-j}x_{-j}}(X_{ij}x_{ij}, X_{-j}x_{-j})} \right) = \sum_{i=1}^{n} \log \left( \frac{f_{X_{ij}x_{-j}x_{-j}}(X_{ij}x_{ij}, X_{-j}x_{-j})}{f_{X_{ij}x_{-j}x_{-j}}(X_{ij}x_{ij}, X_{-j}x_{-j})} \right), \tag{15}
\]
where $f_{z_1|z_2}(z_1|z_2)$ denotes the conditional probability density function of $z_1$ given $z_2$.

The proof of Theorem 2 follows mainly those in [5, 32, 37] and is presented in Section A.2 of the Supplementary Material. Comparing (15) to (14), we see that the KL divergences become invariant to $\tilde{x}_{-j}$ thanks to the additional assumption Condition 3. The simplified form in (15) is important in proving the asymptotic FDR control as in (7). In addition, Condition 3 allows for deviation of the conditional distribution of $\tilde{X}_{ij}|x_{-j}$ from the true underlying conditional distribution of $X_{ij}|x_{-j}$, making the procedure more practically applicable, as verified in examples given in [5].

3 Selection power analysis of TSKI under linear models

In this section, we will analyze the selection power of TSKI with Algorithms 1–2 in time series data applications. Since the selection power of any procedure would depend on the signal strength in the data, we showcase the power analysis using linear time series models where the signal strength can be measured conveniently by regression coefficients. Correspondingly, we consider the LCD knockoff statistic which is used popularly in linear models for variable selection.

Given the augmented data $\{Y_i, x_i, \tilde{x}_i\}_{i=1}^{n}$ with both original covariate vectors $x_i$’s and their knockoff copies $\tilde{x}$’s, the Lasso estimate of the regression coefficient vector with tuning parameter $\lambda_n \geq 0$ is given by
\[
(\hat{\beta}_1, \cdots, \hat{\beta}_p)^T = \arg \min_{\beta \in \mathbb{R}^p} \left\{ n^{-1} \sum_{i=1}^{n} (Y_i - (x_i^T \beta) \beta)^2 + \lambda_n \sum_{j=1}^{2p} |\beta_j| \right\},
\]
where $\tilde{\beta} = (\beta_1, \cdots, \beta_{2p})^T$. We also denote by $\tilde{\beta}^* := (\beta_1^*, \cdots, \beta_{2p}^*)^T$ and $S^* = \{j : |\beta_j^*| > 0\}$ the true coefficient vector and the set of relevant features, respectively, in the linear regression model

$$Y_i = (x_i^T, \tilde{x}_i^T)\tilde{\beta} + \epsilon_i,$$

where $\epsilon_i$ is the model error. It is seen that $\beta_j^* = 0$ for all $j = p + 1, \cdots, 2p$ because they correspond to the knockoff variables.

For the time series setting when $(Y_i, x_i, \tilde{x}_i)$ exhibits serial dependency across $i$, the Lasso estimation error has been investigated thoroughly under various model settings and serial dependence structures; see, for example, [25, 39, 6, 29, 38, 1]. Specifically, the linear AR and ARCH model with sub-Weibull model errors has been considered in [38], the AR distributed lag models with GARCH errors are discussed in [1, 29], and the misspecified AR models and AR models with weak sparsity have been studied in [1]. Rather than reproducing these existing results, we summarize the generic condition needed for the TSKI power analysis in Condition 5 below. We remark that Condition 5 have been proved to hold in the aforementioned works with appropriately chosen $\lambda_n$ and their corresponding regularity conditions.

**Condition 5.** For some constant $c_0 > 0$ and sequence $k_{3n} > 0$ with $\lim_{n \to \infty} k_{3n} = 0$, it holds that \( P \left( \sum_{j=1}^{2p} |\tilde{\beta}_j - \beta_j^*| \leq c_0 (#S^*)\lambda_n \right) \geq 1 - k_{3n} \).

**Condition 6.** There exists some sequence $k_{1n} > 0$ with $k_{1n}q^{-1} \to \infty$ as $n \to \infty$ such that $\min_{j \in S^*} |\beta_j^*| > k_{1n}\lambda_n$.

**Condition 7.** For some constant $c_1 \in (0, 1)$ and sequence $\{k_{2n}\}$ with $\lim_{n \to \infty} k_{2n} = 0$, it holds that $2c_1(\#S^*)^{-1} < c_1, P(\# \{j : |W_j| \geq T\} \geq c_1(\#S^*)) \geq 1 - k_{2n}$ for Algorithm 2, and $P(\# \{j : W_j^k \geq T^k\} \geq c_1(\#S^*)) \geq 1 - k_{2n}$ with $k \in \{1, \cdots, q + 1\}$ for Algorithm 1.

Recall that $q + 1$ is the number of subsamples in Algorithm 1, $W_j^k$’s and $T^k$’s are given in Algorithm 1, and $W_j$’s and $T$’s are given in Algorithm 2. Also, we set $q = O((\log n)^{1+\delta})$ for some small $\delta > 0$ in our applications. Thus, when $\#S^* \gg (\log n)^{1+\delta}$, Condition 6 is weaker than the popularly imposed beta-min assumption which requires that $\min_{j \in S^*} |\beta_j^*| > (\#S^*) \times \lambda_n$ for ensuring the Lasso model selection consistency.

Condition 7 is a high-level assumption that can be shown to hold when the following Lasso estimation error under the $L_2$-norm is imposed additionally

$$P \left( \sum_{j=1}^{2p} (\tilde{\beta}_j - \beta_j^*)^2 \leq c_0 \sqrt{\#S^*\lambda_n} \right) \geq 1 - k_{2n}. \quad (16)$$

See [19] for details on deriving Condition 7 under Condition 5 and (16). Note that the error bounds in Condition 5 and (16) are the standard Lasso error bounds and have been derived in, for example, [25, 39, 6, 29, 38, 1], in time series settings, where $k_{1n}, k_{2n}, k_{3n}$ decrease generally with sample size $n$ at some polynomial rates. For technical simplicity in the power analysis, we assume that there are no ties in the magnitude of nonzero knockoff statistics and the Lasso solutions, and that $\max_{1 \leq k \leq q+1} \{T, T^k\} < \infty$ in (3) and (10) almost surely.
**Theorem 3.** Assume that \( S^* \subset \{1, \cdots, p\} \) with \( \#S^* > 0 \).

1) Let \( \hat{S} \) be returned by the TSKI with Algorithm 2 with constant tuning parameters \( 0 < \tau_1 \leq \tau_s < 1 \). Then under Conditions 5–7, it holds that for all large \( n \),

\[
P \left( \frac{\#(S^* \cap \hat{S})}{\#S^*} \geq 1 - 4c_0k_1^{-1} \right) \geq 1 - k_2n - k_3n. \tag{17}
\]

2) Let \( \hat{S} \) be returned by the TSKI with Algorithm 1 with \( \tau_1 \in (0, 1) \) and \( \tau_s \in (0, 1) \). Assume that Conditions 6–7 are satisfied and Condition 5 holds for the Lasso estimates applied to each subsample in \( H_k \) in Algorithm 1. Then it holds that for all large \( n \),

\[
P \left( \{\hat{S} = \emptyset\} \cup \left\{ \frac{\#(S^* \cap \hat{S})}{\#S^*} \geq 1 - 4c_0(1 + q)k_1^{-1} \right\} \right) \geq 1 - (q + 1) \times (k_2n + k_3n). \tag{18}
\]

If we further assume that \( \tau_1 = \tau^* \times K^{-1} \times (1 - 4(q + 1)c_0k_1^{-1}) \), then we have that for each \( K > 1 \) and all large \( n \),

\[
E \left( \frac{\#(S^* \cap \hat{S})}{\#S^*} \right) \geq \left( 1 - \frac{(q + 1)(\tau_1 + \theta_e)}{K - 1} - (q + 1) \times (k_2n + k_3n) \right) \times k_4n, \tag{19}
\]

where \( \{k_4n\} \) is some increasing sequence with \( \lim_{n \to \infty} k_4n = 1 \) and

\[
\theta_e = \inf \left\{ \theta \geq 0 : \max_{1 \leq k \leq q + 1} E \left( \frac{\#\{j : W_j^k \geq T_k \} \cap (S^*)^c}{\#\{j : W_j^k \geq T_k \} \vee 1} \right) \leq \tau_1 + \theta \right\}. \tag{20}
\]

The proof of Theorem 3 is provided in Section A.3 of the Supplementary Material. As discussed previously, \( k_{2n} \) and \( k_{3n} \) converge generally to zero at some polynomial rates of \( n \). If we set \( q = O((\log n)^{1+\delta}) \) for some \( \delta > 0 \) as discussed earlier, then the second term in the parentheses on the right-hand side of (18) is asymptotically negligible. In addition, we need \( (\tau_1 + \theta_e)q \) to be asymptotically negligible for making the probability of \( \{\hat{S} = \emptyset\} \) vanish asymptotically, which further ensures the high selection power, in view of (18)–(19).

The intuition is that when \( (\tau_1 + \theta_e)q \) is sufficiently small, the false discovery proportion for each knockoff filter is well controlled, yielding an upper bound on \( \sum_{s=1}^{p} 1_{\{W_s^k \leq -T_k\}} \) for each \( k = 1, \cdots, q + 1 \). This further entails that the \( j \)th e-value statistic given in Algorithm 1 is sufficiently large for each \( j \in S^* \) so that it can be selected by the e-value procedure and hence \( \hat{S} \neq \emptyset \). In implementation, in light of the definition of \( \tau_1 \), we can make \( \tau_1q \) asymptotically negligible by choosing \( K \gg q = O((\log n)^{1+\delta}) \).

### 4 Simulation studies

We now investigate the finite-sample performance of the TSKI procedure with Algorithm 1 and Algorithm 2. Two selection methods considered in this section are TSKI with LCD and TSKI with random forests mean decrease accuracy (MDA), which are abbreviated as
TSKI-LCD and TSKI-MDA, respectively. The theoretical foundation of the TSKI inference with \(q = 0\) and \(q > 0\) for time series application has been established in Theorem 2 and Theorem 1, respectively.

4.1 Simulation settings

We begin with introducing the data generating processes for three simulation examples. Specifically, we will consider below three popular time series models: the autoregressive model with exogenous variables (ARX), the self-exciting threshold autoregressive model with exogenous variables (SETARX) [36], and the autoregressive conditional heteroskedasticity model with exogenous variables (ARX-ARCH) [17]. In Models 1–3 below, \(\beta\) denotes the magnitude of the autoregressive coefficient, \(H_{t,j}\)'s represent the time series covariates, and \(\epsilon_t\)'s are model errors.

**Model 1** (AR model). For each integer \(t\), we define

\[
Y_t = \sum_{j=1}^{2} (-0.5)^{j-1} \beta Y_{t-j} + \sum_{j=1}^{15} 0.6 \times H_{t,j} + \epsilon_t.
\]

**Model 2** (SETAR model). For each integer \(t\), we define

\[
Y_t = \begin{cases} 
\sum_{j=1}^{2} (-0.5)^{j-1} \beta Y_{t-j} + \sum_{j=1}^{15} 0.6 \times H_{t,j} + \epsilon_t & \text{if } Y_{t-d} > r, \\
\sum_{j=1}^{2} -(-0.5)^{j-1} \beta Y_{t-j} + \sum_{j=1}^{15} 0.6 \times H_{t,j} + \epsilon_t & \text{otherwise,}
\end{cases}
\]

where we choose \(r = 0.5\) and \(d = 1\) as the threshold value and the threshold lag, respectively.

**Model 3** (AR-X-ARCH model). For each \(t\), we define

\[
Y_t = \sum_{j=1}^{2} (-0.5)^{j-1} \beta Y_{t-j} + \sum_{j=1}^{15} 0.6 \times H_{t,j} + \sigma_t \epsilon_t
\]

with \(\sigma_t^2 = 0.1 + 0.9(\sigma_{t-1} \epsilon_{t-1})^2\).

The set of model errors \(\{\epsilon_t\}\) is an independent sequence of i.i.d. zero-mean Gaussian random variables with \(\mathbb{E}\epsilon_t^2 = 1\), and the magnitude of the autoregressive coefficient is such that \(\beta \in \{0.3, 0.7\}\). The time series covariates are given by \(H_{t,j} = 0.2 \times H_{t-1,j} + \epsilon_{t,j}\) with \(j \in \{1, \cdots, 50\}\), where \((\epsilon_{t,1}, \cdots, \epsilon_{t,50})\)'s are i.i.d. Gaussian random vectors with zero mean and \(\mathbb{E}(\epsilon_{t,k} \epsilon_{t,l}) = 0.2^{k-l}\) for all \(k, l\). We formulate the covariate vector with respect to response \(Y_t\) as \(x_t = (Y_{t-1}, \cdots, Y_{t-20}, h_{t}, h_{t-1}, h_{t-2}, h_{t-3}, h_{t-4})\), where \(h_{t} = (H_{t,1}, \cdots, H_{t,50})\) and \(p = 270\).

In Models 1 and 3, the mean functions both depend linearly on the covariates, while in Model 2 the mean function is a piecewise linear function of the covariates. For Models 1–2, the relevant index set according to Definition 1 is \(S_0 = \{1, 2, 21, \cdots, 35\}\), giving rise to the set of null variables \(\mathcal{H}_0 = \{3, \cdots, 20, 36, \cdots, 270\}\). For Model 3, the relevant set is \(S_{arch} = \{1, 2, 3, 21, \cdots, 35, 71, \cdots, 85\}\) and the null set is \(\mathcal{H}_{arch} = \{4, \cdots, 20, 36, \cdots, 70, 86, \cdots, 270\}\),

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while \( S_0 \) and \( H_0 \) defined before are the sets of active and null covariates, respectively, in the mean regression function. Although \( S_0 \) and \( H_0 \) differ from \( S_{arch} \) and \( H_{arch} \), respectively, in Model 3, we examine the empirical power and FDR of the TSKI with respect to \( S_0 \) and \( H_0 \) for two reasons: 1) this is an interesting problem in time series inference and 2) random forests and Lasso are both algorithms designed for fitting the mean regression and thus are not expected to detect variables that affect only the variance function.

For implementation, the target FDR level is set as \( \tau^* = 0.2 \), and the R packages \texttt{glmnet} and \texttt{randomForest} are used for calculating the Lasso estimates and the random forests MDA, respectively. We generate the approximate knockoff variables using the idea of the second-order approximation where we pretend that \( x_t \) had a multivariate Gaussian distribution, and then use equation (3) of [19] to simulate the knockoff variables from a conditional Gaussian distribution with the precision matrix estimated using the method developed in [21]. Note that such knockoff variables have the first two moments approximately match the those of the original covariates and thus, this procedure is named as the second-order approximation. The TSKI Algorithm 1 with subsampling parameter \( q \in \{0, 1, 2\} \), \( \tau_1 \in \{0.066, 0.1, 0.2\} \), and \( \tau^* = 0.2 \) is considered in our simulation. The R code for the simulation experiments is available in the online Supplementary Material.

Let \( \hat{S} \) be the set of selected features returned by the TSKI-LCD or TSKI-MDA. Then the empirical versions of the FDR and power are given by

\[
\text{FDP} := \frac{\#(\hat{S} \cap H_0)}{\max\{\#\hat{S}, 1\}} \quad \text{and} \quad \text{Sample power} := \frac{\#(\hat{S} \cap S_0)}{\#S_0},
\]

respectively, where the FDP stands for the false discovery proportion. The values of \((\beta, q, n)\) are included in both Tables 1–2 and we choose \( \tau_1 = \tau^*/(q + 1) \).

| \( n/\beta \) | Method    | \( q \) | FDR    | Power |
|-------------|-----------|---------|--------|-------|
| 200/0.7     | TSKI-LCD 0 | 0.237   | 0.992  |
|             | TSKI-LCD 1 | 0.108   | 0.529  |
|             | TSKI-LCD 2 | 0.013   | 0.016  |
|             | TSKI-MDA 0 | 0.273   | 0.391  |
|             | TSKI-MDA 1 | 0.026   | 0.021  |
|             | TSKI-MDA 2 | 0       | 0      |
| 500/0.7     | TSKI-LCD 0 | 0.188   | 1      |
|             | TSKI-LCD 1 | 0.142   | 0.999  |
|             | TSKI-LCD 2 | 0.121   | 0.999  |
|             | TSKI-MDA 0 | 0.208   | 0.729  |
|             | TSKI-MDA 1 | 0.068   | 0.164  |
|             | TSKI-MDA 2 | 0.009   | 0.011  |

| \( n/\beta \) | Method    | \( q \) | FDR    | Power |
|-------------|-----------|---------|--------|-------|
| 200/0.7     | TSKI-LCD 0 | 0.203   | 0.985  |
|             | TSKI-LCD 1 | 0.122   | 0.755  |
|             | TSKI-LCD 2 | 0.027   | 0.057  |
|             | TSKI-MDA 0 | 0.220   | 0.292  |
|             | TSKI-MDA 1 | 0.044   | 0.021  |
|             | TSKI-MDA 2 | 0       | 0      |
| 500/0.7     | TSKI-LCD 0 | 0.181   | 0.999  |
|             | TSKI-LCD 1 | 0.166   | 0.996  |
|             | TSKI-LCD 2 | 0.141   | 0.996  |
|             | TSKI-MDA 0 | 0.142   | 0.476  |
|             | TSKI-MDA 1 | 0.037   | 0.076  |
|             | TSKI-MDA 2 | 0.006   | 0.005  |

Table 1: The simulation results on the empirical FDR and power for the TSKI with \( \tau_1 = \tau^*/(q + 1) \) and \( \tau^* = 0.2 \) under Model 1 (left panel) and Model 3 (right panel) in Section 4.1.
Table 2: The simulation results on the empirical FDR and power for the TSKI with $\tau_1 = \tau^*/(q + 1)$ and $\tau^* = 0.2$ under Model 2 in Section 4.1.

### 4.2 Empirical performance of TSKI

For all simulation experiments reported in Tables 1–2, both TSKI-LCD and TSKI-MDA with $q > 0$ control the FDR in finite samples at the target value of $\tau^* = 0.2$, but at the cost of lower selection power compared to the case of $q = 0$. In contrast, TSKI with $q = 0$ (i.e., no subsampling) has FDR exceeding the target FDR level in Model 1 when the sample size is small (i.e., $n = 200$). When $q = 2$ and the sample size is small, TSKI becomes overly conservative with both low FDR and low power in most cases, with the MDA based method suffering more severely.

In all but one settings (Table 2, $(n, \beta) = (500, 0.3)$), the LCD based method outperforms the MDA based method in terms of power. Three plausible explanations for this are 1) the mean regression functions in all three models are not too far away from linear functions, 2) MDA is a nonparametric method which requires larger sample size to perform well compared to LCD, and 3) MDA suffers from the potential bias issue due to correlations between covariates [34, 13].

Overall, our simulation experiments show that the time series FDR is controlled stably by the TSKI procedure with subsampling parameter $q > 0$ in finite samples, whereas the selection power depends on the sample size, the subsampling parameter $q \geq 0$, the signal strength $\beta$, and the choice of the feature importance measure. Regarding the subsampling parameter $q$, we remark that by the construction of (3) in Algorithm 1, TSKI may have decent asymptotic power only when the number of relevant features is no less than $\tau^-_1 = (q + 1)/\tau^*$. To see the intuition, let us consider a case when the number of relevant features is less than $\tau^-_1$ and their knockoff statistics are the few largest (positive) statistics asymptotically. Then even if the other knockoff statistics are all zero, we have $T^k = \infty$ in (3), and hence the knockoff filter screens out all features. It is worth mentioning that a similar but more restrictive requirement is assumed in Condition 7 for the asymptotic power.
5 Real data application

Identifying important time series economic variables that can affect the inflation has been an active research problem with a long history [24, 15], due to the importance of inflation. In this section, we will analyze the temporal relations between the U.S. inflation and other major time series covariates of the U.S. economy from May 2013 \( (t = 1) \) to January 2023 \( (t = 117) \) using monthly data in this period. From Figure 1, we see that the inflation series consists of two nonstationary points at January 2015 and April 2020, corresponding to events A and B, respectively. Event A corresponds to a sharp gasoline index decline, whereas event B is due to the onset of the COVID-19 pandemic. These events cannot be predicted based on the available information before their occurrences. In addition, the U.S. economy has been experiencing economic recovery in the post-COVID-19 era, and there seem to be effects of Russia–Ukraine war, as revealed by the clear structural change during time period C indicated in Figure 1. In light of these versatile time varying patterns of the inflation series, we facilitate our analysis by considering five-year rolling windows, where the ends of the rolling windows start from April 2018 to January 2023 (a total of 58 rolling windows).

Specifically, we apply the TSKI-LCD with \( q \in \{0, 1\} \) to each five-year rolling window to investigate the temporal relations between the inflation and other time series lags. These monthly economic time series, including numerous types of consumer price indices, unemployment rates, and housing prices, can be obtained from the FRED-MD database [28] and the U.S. Bureau of Labor Statistics. These time series have been adjusted according to the instruction of the FRED-MD database, which can be found in the work of [28] or the codes provided in the paper. In particular, the inflation at time \( t \) is defined as the adjusted consumer price index for all goods

\[
\text{Inflation}_t := \left( \frac{\text{CPI}_t - \text{CPI}_{t-1}}{\text{CPI}_{t-1}} \times 100 \right) \%,
\]

\footnote{The website URL: \url{https://research.stlouisfed.org/econ/mccracken/fred-databases/}.}
Figure 2: The left panel displays the averages of “having any selections” indicators over 100 repetitions, where the indicator at each rolling window is one if and only if any covariates are selected, and the $x$-axis indicates the ending time of each rolling window. The right panel shows the analogous results, but with the indicator being one at each covariate index if that covariate is selected at any rolling windows. The first 127 covariates are current time covariates, and the 128th to 254th covariates are one month lag covariates in the AR(2) model. Covariates measuring similar economic values are clustered closer (see [28] for detailed definitions of these covariates). The selection method here is the TSKI-LCD without subsampling ($q = 0$).

Figure 3: These two figures are analogous to Figure 2 but with $q = 1$ for the TSKI-LCD procedure.
Figure 4: The black curves in the three panels are the inflation series at time $t + 1$. The red curve in panel (a) is the number of new orders for consumer goods at time $t$, the red curve in panel (b) indicates the U.S./Canada exchange rate at time $t$, and the red curve in panel (c) is the U.S. initial claims for unemployment benefits at time $t$. All curves here are standardized and adjusted for visual comparison, and hence the values of these time series are not reported on the $y$-axis.
where $CPI_t$ is the consumer price index for all goods at time (month) $t$. Each time series has a FRED-MD code. For example, CPIAUCSL is the FRED-MD code of the inflation series.

To reduce randomness resulting from the use of the knockoffs construction, we repeat the inference procedure 100 times, and report the average results in Figure 2 with $q = 0$, where the left panel displays whether any significant covaraites have been found at each rolling window period, and the right panel shows the selection frequency over 58 rolling window periods of the 127 time series covariates and their one month lags. That is, we model the one month ahead inflation series $\text{Inflation}_{t+1}$ (response) using an AR(2) model with 127 time series covariates at current time $t$ and 127 one month lags of these time series covariates. So the covariate dimensionality is $p = 254$.

As can be seen in Figure 2, the TSKI-LCD with $q = 0$ identifies some active windows around the B and C periods, and the selection frequency concentrates on a sparse set of covariates. The majority of the selected variables are covariates at current time $t$. The top 10 most frequently selected covariates by the TSKI-LCD with $q = 0$ are employment related series (HWI, CLAIMSx), consumption related indices (ACOGNO, CPIAUCSL), housing related series (PERMITS), U.S. bond yields (GS5, GS10), stock market indices (S.P.div.yield, S.P.500), and exchange rates (EXCAUSx) at their current time $t$, where their FRED-MD codes are given in the parentheses.

The simulation results in Section 4 suggest that the choice of $q = 1$ has better FDR control especially when the sample size is limited. Motivated by our simulation results, we next apply the TSKI-LCD with subsampling $q = 1$ in Figure 3 with the expectation of better FDR control. The results of Figure 3 are more conservative in comparison to those in Figure 2. Despite being conservative, these new results also suggest some active windows in the B and C periods, and the selected variables are also mostly covariates at current time $t$. In addition, most covariates selected by the TSKI-LCD with $q = 1$ belong to the set selected by the TSKI-LCD with $q = 0$. In particular, the top 10 selected covariates are CPIAUCSL, CLAIMSx, PERMITS, AMDMUOx, GS10, ACOGNO, EXCAUSx, EXUSUKx, INDPRO, IPFUELS, where only PERMITS is one month lag covariate at $t - 1$ in the AR(2) model. Among them, EXUSUKx, AMDMUOx, INDPRO, and IPFUELS are new in comparison to the list of selected set when $q = 0$, where the first two are the U.S./U.K. exchange rate and another type of consumption related index (the number of unfilled orders for durable goods), respectively, and the last two are industrial production indices that are related to consumption price indices. The difference in the selected sets of covariates are attributed to the fact that some economic covariates are designed to track similar economic factors and tend to be highly correlated.

The recent literature [33] suggests that the inflation foresting is a difficult task in the sense that AR models with additional time series covariates rarely outperform simple AR models with only inflation lags. In other words, conditional on the lagged inflation series, additional covariates do not carry strong signals in the inflation forecasting. The fact that the TSKI-LCD with $q = 1$ selects only a few time series covariates indeed supports such argument. It is also interesting to notice that the stock market indices are not considered as important covariates by the TSKI-LCD with subsampling (i.e., $q = 1$), but are selected as
important covariates when \( q = 0 \). In particular, the selection frequencies of S&P dividend yields and S&P 500 (both at lag \( t - 1 \)) are 100% and 79%, respectively, in Figure 2, while only 5% and 1%, respectively, in Figure 3, suggesting that stock market indices could be spurious findings.

The selection results by the TSKI-LCD motivate us to further investigate the dependency of inflation on a few time series covariates. In Figure 4, we further plot three selected series, namely ACOGNO, EXCAUSx, and CLAIMSx, that are among the top 10 lists both when \( q = 0 \) and \( q = 1 \). These three selected covariates are all at their current time \( t \) in the AR(2) model. ACOGNO is the number of new orders for consumer goods which is an important consumption index, EXCAUSx is the exchange rate from U.S. dollar to Canadian dollar, and CLAIMSx is the initial claim for unemployment benefits. We also include the inflation series at time \( t + 1 \) in the same period (the black curve in each panel). For better visual comparison, all curves in Figure 4 have been standardized and adjusted.

A visual inspection of Figure 4 shows that the impacts of the COVID-19 pandemic in April 2020 on the U.S. economy are stronger than those of gasoline price shock in January 2015. This potentially explains why our empirical findings of significant covariates concentrate mostly around periods B and C. From Figure 4, we see that the gasoline price shock in January 2015 affects the consumption index series ACOGNO more mildly compared to the impact of COVID-19 in April 2020. Also, although there is some variation in the exchange rate EXCAUSx after January 2015, it is unclear whether such variation was caused by the gasoline price shock. In contrast, most time series of the U.S. economy responded clearly to the pandemic to an unignorable degree. Particularly, the exchange rate and the number of initial claims dropped in March 2020, suggesting that these covariates are one-month ahead indicators for the inflation drop in April 2020. In summary, we have applied the newly suggested tool of TSKI to study the U.S. economy. Our empirical results illustrate the potential of the TSKI on obtaining more instructive findings in real data applications.

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Supplementary Material to “High-Dimensional Knockoffs Inference for Time Series Data”

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This Supplementary Material contains the proofs of all main results and technical lemmas, and some additional technical details. All the notation is the same as defined in the main body of the paper.

A Proofs of Theorems 1–3, Corollaries 1–2, and Proposition 1

A.1 Proof of Theorem 1

For simplicity, in this proof we use the notation $U, \tilde{U}, V$ to denote a generic subsample of $\{x_i, \tilde{x}_i, Y_i\}_{i=1}^n$ or their independent and identically distributed (i.i.d.) counterparts $\{x_i^\pi, \tilde{x}_i^\pi, Y_i^\pi\}_{i=1}^n$, where their exact meaning will be made explicit whenever confusion is possible. Let us define

$$\hat{KL}_j^k \equiv \log \left( \frac{f(U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j}, V(U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j}, V))}{f(U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j}, V(\tilde{U}_j, U_j, U_{-j}, \tilde{U}_{-j}, V))} \right), \quad (A.1)$$

where $U = (x_i, i \in H_k)^T$, $\tilde{U} = (\tilde{x}_i, i \in H_k)^T$, and $V = (Y_i, i \in H_k)^T$. We can use (A.7) in the proof of Theorem 2 in Section A.2 to conclude that for each $k \in \{1, \ldots, q+1\}$,

$$\mathbb{E}(\sum_{j \in H_0} e_j^k \times 1_{\{\hat{KL}_j^k \leq \varepsilon\}}) \leq p \times e^\varepsilon.$$

Then it holds that

$$\mathbb{E}(\sum_{j \in H_0} e_j^{(e)}) \leq p \times e^\varepsilon,$$

where

$$e_j^{(e)} = (q + 1)^{-1} \sum_{k=1}^{q+1} e_j^k \times 1_{\{\hat{KL}_j^k \leq \varepsilon\}}.$$

Denote by $\hat{S}_\varepsilon$ be the set of selected features when applying the e-BH method to $e_j^{(e)}$’s at the target FDR level $\tau^*$. Then using similar arguments to those for (A.8) in Section A.2, we can show that

$$\mathbb{E} \left( \frac{\#(\hat{S}_\varepsilon \cap H_0)}{(\#\hat{S}_\varepsilon) \vee 1} \right) \leq \tau^* \times e^\varepsilon.$$

Thus, it follows that

$$\mathbb{E} \left( \frac{\#(\hat{S} \cap H_0)}{(\#\hat{S}) \vee 1} \right) \leq \mathbb{E} \left( \frac{\#(\hat{S}_\varepsilon \cap H_0)}{(\#\hat{S}_\varepsilon) \vee 1} \times 1_{\{\hat{S}=\hat{S}_\varepsilon\}} + 1_{\{\hat{S} \neq \hat{S}_\varepsilon\}} \right) \leq \tau^* \times e^\varepsilon + \sum_{k=1}^{q+1} \mathbb{P}(\max_{1 \leq j \leq p} \hat{KL}_j^k > \varepsilon) \quad (A.2)$$
in view of \( \{ \tilde{S} \neq \tilde{S}_i \} \subset \{ \max_{1 \leq k \leq q+1} \max_{1 \leq j \leq k} \tilde{KL}_j^k > \varepsilon \} \). Since (A.2) holds for each \( \varepsilon > 0 \), we can further obtain that

\[
\mathbb{E}\left( \frac{|\tilde{S} \cap \mathcal{H}_0|}{|\tilde{S}|} \right) \leq \inf_{\varepsilon > 0} \left\{ \tau^* \varepsilon + \sum_{k=1}^{q+1} \mathbb{P}\left( \max_{1 \leq j \leq p} \tilde{KL}_j^k > \varepsilon \right) \right\}
\]

\[
+ \sum_{k=1}^{q+1} \left( \mathbb{P}\left( \max_{1 \leq j \leq p} \tilde{KL}_j^k > \varepsilon \right) - \mathbb{P}\left( \max_{1 \leq j \leq p} \tilde{KL}_j^k > \varepsilon \right) \right).
\]

(A.3)

It remains to bound the second term on the right-hand side of (A.3) above. Recall that \( \tilde{KL}_j^k \) is defined analogously to (A.1) but based on i.i.d. sample \( \{x_i^\pi, \tilde{x}_i^\pi, Y_i^\pi\}_{i=1}^n \). With \( U = (x_i^\pi, i \in H_k)^T, \tilde{U} = (\tilde{x}_i^\pi, i \in H_k)^T \), and \( V = (Y_i^\pi, i \in H_k)^T \), we can deduce that

\[
\tilde{KL}_j^k = \sum_{i \in H_k} \log \left( \frac{f_{x_j, \tilde{x}_j, x_{-j}, \tilde{x}_{-j}}(X_j^\pi, \tilde{X}_j^\pi, x_{-j}^\pi, \tilde{x}_{-j}^\pi)}{f_{X_j, \tilde{X}_j, x_{-j}, \tilde{x}_{-j}}(X_j^\pi, \tilde{X}_j^\pi, x_{-j}^\pi, \tilde{x}_{-j}^\pi)} \right)
\]

\[
= \log \left( \frac{f_{U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j}}(U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j})}{f_{U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j}}(U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j})} \right)
\]

\[
= \log \left( \frac{f_{U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j}}(U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j})}{f_{U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j}}(U_j, \tilde{U}_j, U_{-j}, \tilde{U}_{-j})} \right).
\]

(A.4)

where the third equality above follows from similar analysis to that of (13) in Theorem 1. The conditional column independence required by (13) holds for each \( j \in \mathcal{H}_0 \) because (A.4) involves i.i.d. samples.

We can now see that \( \tilde{KL}_j^k \) is well-defined thanks to Condition 1. Moreover, by the fact that the supports of \( (x, \tilde{x}) \) and \( (x, \tilde{x})_{\text{swap}(j)} \) are the same (as guaranteed by Condition 1) and the definition of \( (x_i^\pi, \tilde{x}_i^\pi)'s \), \( \tilde{KL}_j^k \) is well-defined. Hence, in light of (A.1) and (A.4), there exists some measurable function \( g : \mathbb{R}^{#H_k \times (2p+1)} \rightarrow \mathbb{R} \) such that \( \tilde{KL}_j^k = g(X_j^k) \) and \( \tilde{KL}_j^k = g(X_j^k) \) for each \( \varepsilon \geq 0 \), which entails that there exists some \( D \in \mathcal{R}^{#H_k \times (2p+1)} \) such that

\[
\{ X_k \in D \} = \{ \max_{1 \leq j \leq p} \tilde{KL}_j^k > \varepsilon \},
\]

\[
\{ X_k^\pi \in D \} = \{ \max_{1 \leq j \leq p} \tilde{KL}_j^k > \varepsilon \}.
\]

(A.5)

With the aid of (A.5), it holds that

\[
|\mathbb{P}(\max_{1 \leq j \leq p} \tilde{KL}_j^k > \varepsilon) - \mathbb{P}(\max_{1 \leq j \leq p} \tilde{KL}_j^k > \varepsilon)| \leq \sup_{D \in \mathcal{R}^{#H_k \times (2p+1)}} |\mathbb{P}(X_k \in D) - \mathbb{P}(X_k^\pi \in D)|.
\]

(A.6)

Therefore, from (A.3)–(A.4) and (A.6) we can obtain the desired conclusion, which completes the proof of Theorem 1.
A.2 Proof of Theorem 2

Let us first make a useful claim that with $\hat{KL}_j$’s given in (12), it holds that for each $\varepsilon > 0$,

$$\sum_{j \in H_0} \mathbb{E}(e_j \times 1_{\{\hat{KL}_j \leq \varepsilon\}}) \leq p \times e^\varepsilon. \quad (A.7)$$

Then we consider an application of the e-BH method [37] to $e_j^{(e)} := e_j \times 1_{\{\hat{KL}_j \leq \varepsilon\}}$ with the target FDR level $\tau^*$, yielding a set of selected features $\hat{S}_\varepsilon \subset \{1, \cdots, p\}$ defined as

$$\hat{S}_\varepsilon = \{j : e_j^{(e)} \geq p(\tau^* \times \hat{k}_\varepsilon)^{-1}\}$$

with $\hat{k}_\varepsilon \equiv \max\{k : e_j^{(e)}(k) \geq p(\tau^* \times k)^{-1}\}$. Here, $e_j^{(e)}$’s are the ordered statistics of $e_j^{(e)}$’s such that $e_j^{(e)}(1) \geq \cdots \geq e_j^{(e)}(p)$. It is easy to see that $\#\hat{S}_\varepsilon = \hat{k}_\varepsilon$.

In view of the definition of $\hat{k}_\varepsilon$, we can deduce that

$$\mathbb{E}\left(\frac{\#(\hat{S}_\varepsilon \cap H_0)}{(#\hat{S}_\varepsilon) \vee 1}\right) \leq \mathbb{E}\left(\frac{\sum_{j \in H_0} 1_{\{j \in \hat{S}_\varepsilon\}}}{\hat{k}_\varepsilon \vee 1}\right) \leq \mathbb{E}\left(\frac{\sum_{j \in H_0} 1_{\{j \in \hat{S}_\varepsilon\}} \times \tau^* \times e_j^{(e)}}{p}\right) \leq \tau^* p^{-1} \times \mathbb{E}\left(\sum_{j \in H_0} e_j^{(e)}\right) \leq \tau^* e^\varepsilon, \quad (A.8)$$

where the last inequality above is from (A.7). Then combining (A.8) and $\{\hat{S} \neq \hat{S}_\varepsilon\} \subset \cup_{j=1}^p \{\hat{KL}_j > \varepsilon\}$ leads to

$$\mathbb{E}\left(\frac{\#(\hat{S}_\varepsilon \cap H_0)}{(#\hat{S}_\varepsilon) \vee 1}\right) \leq \mathbb{E}\left(1_{\{\hat{S} = \hat{S}_\varepsilon\}} \times \frac{\#(\hat{S}_\varepsilon \cap H_0)}{(\#\hat{S}_\varepsilon) \vee 1} + 1_{\{\hat{S} \neq \hat{S}_\varepsilon\}}\right) \leq \tau^* e^\varepsilon + P(\max_{1 \leq j \leq p} \hat{KL}_j > \varepsilon)$$

for each $\varepsilon \geq 0$. This concludes the proof for the desired result (11). We will provide the proofs of (A.7) and (13)–(15), separately.

Proof of (A.7). Let us define

$$T_j \equiv \min \left\{t \in \mathbb{W}_+^j : \frac{1 + \#(s : W_s^j \leq -t)}{\#(s : W_s^j \geq t) \vee 1} \leq \tau_1\right\},$$

where $W_k^j = W_k$ if $k \neq j$ and $W_j^j = |W_j|$, $\mathbb{W}_+^j = \{|W_s^j| : |W_s^j| > 0\}$, and $\min \emptyset$ is defined as infinity. We further define $X_j^{(0)}$ and $X_j^{(1)}$ such that $X_j^{(0)} = X_j$ and $X_j^{(1)} = \tilde{X}_j$ if $W_j \geq 0$, and $X_j^{(1)} = X_j$ and $X_j^{(0)} = \tilde{X}_j$ if $W_j < 0$. 

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Furthermore, we will show that it holds almost surely that

\[
\sum_{j \in H_0} \mathbb{E} \left( \frac{1_{\{W_j \geq T\}} \times 1_{\{\tilde{KL}_j \leq \epsilon\}}}{1 + \sum_{s=1}^P 1_{\{W_s \leq -T\}}} \right) = \sum_{j \in H_0} \mathbb{E} \left( \frac{1_{\{W_j \geq T\}} \times 1_{\{\tilde{KL}_j \leq \epsilon\}}}{1 + \sum_{s=1}^P 1_{\{W_s \leq -T\}}} \right)
\]

where the first three equalities above hold because when \(1_{\{W_j \geq T\}} = 1\), we have \(W_j > 0\), \(T = T_j\), and \(1_{\{W_s \leq -T\}} = 0\), and the last equality above holds since \(|W_j|, T_j, W_1, \cdots, W_{j-1}, W_{j+1}, \cdots, W_P\) are functions of \((X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)\) due to the sign-flip property (2).

From the definitions of \(X_j^{(0)}, X_j^{(1)}, \text{and } \tilde{KL}_j\), we can obtain that

\[
\mathbb{P}(W_j > 0, \tilde{KL}_j \leq \epsilon \mid X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y) = \mathbb{P}(W_j > 0, \tilde{KL}_j^{(01)} \leq \epsilon \mid X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)
\]

where

\[
\tilde{KL}_j^{(01)} = \log \left( \frac{f_{X_j, X_{-j}, \bar{X}_{-j}, Y}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)}{f_{X_j, X_{-j}, \bar{X}_{-j}, Y}(X_j^{(1)}, X_j^{(0)}, X_{-j}, \bar{X}_{-j}, Y)} \right).
\]

Furthermore, we will show that it holds almost surely that

\[
\mathbb{P}(W_j > 0 \mid X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y) \leq \mathbb{P}(W_j < 0 \mid X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)
\]

where Condition 1 is assumed to avoid division by zero on the right-hand side (RHS) of the second inequality above. The proof of (A.11) is deferred to right after the proof of (A.7).
Lemma 6 in [5]. Hence, by resorting to (A.9), (A.12), and the fact that

where RHS is short for the right-hand side and the third inequality above follows from Lemma 6 in [5]. Hence, by resorting to (A.9), (A.12), and the fact that

we can establish (A.7).

Proof of (A.11). Denote by $F_{>0}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)$ and $F_{<0}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)$ the versions of $\mathbb{P}(W_j > 0| X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)$ and $\mathbb{P}(W_j < 0| X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)$, respectively. We will show that functions $F_{>0}: \mathbb{R}^{n(2p+1)} \mapsto \mathbb{R}$ and $F_{<0}: \mathbb{R}^{n(2p+1)} \mapsto \mathbb{R}$ satisfy that

$$
F_{>0}(\bar{z}) = \frac{1_{\{w_j(\bar{z}) > 0\}} \times f_{X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y}(\bar{z})}{f_{X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y}(\bar{z})},
$$

$$
F_{<0}(\bar{z}) = \frac{1_{\{w_j(\bar{z}_{swap}) < 0\}} \times f_{X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y}(\bar{z}_{swap})}{f_{X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y}(\bar{z})},
$$

(A.13)

respectively, where $\bar{z} = (\bar{z}_1, \bar{z}_2, \bar{z}_3, \bar{z}_4, \bar{z}_5)$, $\bar{z}_{swap} = (\bar{z}_2, \bar{z}_1, \bar{z}_3, \bar{z}_4, \bar{z}_5)$ with $\bar{z}_1 \in \mathbb{R}^n$, $\bar{z}_2 \in \mathbb{R}^n$, $\bar{z}_3 \in \mathbb{R}^{n(p-1)}$, $\bar{z}_4 \in \mathbb{R}^{n(p-1)}$, $\bar{z}_5 \in \mathbb{R}^{n}$, and $w_j: \mathbb{R}^{n(2p+1)} \mapsto \mathbb{R}$ denotes the knockoff statistic function of $W_j$. From the definitions of $X_j^{(0)}$, $X_j^{(1)}$, and $w_j(\cdot)$ along with the sign-flip property (2), we have that almost surely,

$$
w_j(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y) \geq 0,
$$

$$
w_j(X_j^{(1)}, X_j^{(0)}, X_{-j}, \bar{X}_{-j}, Y) < 0.
$$

(A.14)

Then an application of (A.13)–(A.14) and the fact that the probability density function
is nonnegative yields that

\[
F_{>0}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y) \leq \frac{f_{X_j, \bar{X}_j, X_{-j}, \bar{X}_{-j}, Y}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)}{f_{X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)}
\]

\[
F_{<0}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y) = \frac{f_{X_j, \bar{X}_j, X_{-j}, \bar{X}_{-j}, Y}(X_j^{(1)}, X_j^{(0)}, X_{-j}, \bar{X}_{-j}, Y)}{f_{X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)}
\]

which entail that

\[
\mathbb{P}(W_j > 0 | X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)
= \frac{f_{X_j, \bar{X}_j, X_{-j}, \bar{X}_{-j}, Y}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)}{f_{X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)},
\]

\[
\mathbb{P}(W_j < 0 | X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)
= \frac{f_{X_j, \bar{X}_j, X_{-j}, \bar{X}_{-j}, Y}(X_j^{(1)}, X_j^{(0)}, X_{-j}, \bar{X}_{-j}, Y)}{f_{X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y}(X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y)}.
\]

Hence, a combination of (A.15) and Condition 1 (which ensures that the denominator is nonzero) establishes the result in (A.11).

It remains to prove (A.13). To this end, observe that for any Borel sets \(A_1 \in \mathcal{R}^n\), \(A_2 \in \mathcal{R}^n\), \(A_3 \in \mathcal{R}^{n(p-1)}\), \(A_4 \in \mathcal{R}^{n(p-1)}\), and \(A_5 \in \mathcal{R}^n\), it holds that

\[
\int_{\mathcal{X} \in A_1 \times \cdots \times A_5} F_{>0}(\vec{z}) f_{X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y}(\vec{z}) d\mathbb{P}\]

\[
= \mathbb{P}(W_j > 0, X_j \in A_1, \bar{X}_j \in A_2, X_{-j} \in A_3, \bar{X}_{-j} \in A_4, Y \in A_5)
= \mathbb{P}(W_j > 0, X_j^{(0)} \in A_1, X_j^{(1)} \in A_2, X_{-j} \in A_3, \bar{X}_{-j} \in A_4, Y \in A_5)
= \int_{\{X_j^{(0)} \in A_1, X_j^{(1)} \in A_2, X_{-j} \in A_3, \bar{X}_{-j} \in A_4, Y \in A_5\}} \mathbb{P}(W_j > 0 | X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y) d\mathbb{P},
\]

where the second equality above holds by the definitions of \(X_j^{(0)}\) and \(X_j^{(1)}\). Similarly, for any Borel sets \(A_1 \in \mathcal{R}^n\), \(A_2 \in \mathcal{R}^n\), \(A_3 \in \mathcal{R}^{n(p-1)}\), \(A_4 \in \mathcal{R}^{n(p-1)}\), and \(A_5 \in \mathcal{R}^n\), we have

\[
\int_{\mathcal{X} \in A_1 \times \cdots \times A_5} F_{<0}(\vec{z}) f_{X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y}(\vec{z}) d\mathbb{P}\]

\[
= \mathbb{P}(W_j < 0, \bar{X}_j \in A_1, X_j \in A_2, X_{-j} \in A_3, \bar{X}_{-j} \in A_4, Y \in A_5)
= \mathbb{P}(W_j < 0, X_j^{(0)} \in A_1, X_j^{(1)} \in A_2, X_{-j} \in A_3, \bar{X}_{-j} \in A_4, Y \in A_5)
= \int_{\{X_j^{(0)} \in A_1, X_j^{(1)} \in A_2, X_{-j} \in A_3, \bar{X}_{-j} \in A_4, Y \in A_5\}} \mathbb{P}(W_j < 0 | X_j^{(0)}, X_j^{(1)}, X_{-j}, \bar{X}_{-j}, Y) d\mathbb{P},
\]

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where the second equality above holds by the definitions of \(X_j^{(0)}\) and \(X_j^{(1)}\). With the aid of (A.16)–(A.17), we can resort to the \(\pi - \lambda\) Theorem [16] and the definition of the conditional expectation to obtain (A.13). Thus, we have established (A.11).

**Proof of (13).** We now aim to show (13) under Condition 2 and the assumption that \(X_j\) is independent of \(Y\) conditional on \(X_{-j}\) for each \(j \in \mathcal{H}_0\). First, in light of Condition 2 and Definition 2 of the knockoff generator, we see that \(Y\) is independent of \(\tilde{X}\) conditional on \(X\). Next, we can deduce that

\[
\begin{align*}
 f_{X_j, \tilde{X}_j, x_{-j}, \tilde{x}_{-j}, Y}(\tilde{z}_1, \tilde{z}_2, \tilde{z}_3, \tilde{z}_4, \tilde{z}_5) \\
 = f_X(\tilde{z}_1, \tilde{z}_3) \times f_{\tilde{X}_j, \tilde{x}_{-j}, Y|X}(\tilde{z}_2, \tilde{z}_4, \tilde{z}_5 | \tilde{z}_1, \tilde{z}_3) \\
 = f_X(\tilde{z}_1, \tilde{z}_3) \times f_{Y|X}(\tilde{z}_5 | \tilde{z}_1, \tilde{z}_3) \times f_{\tilde{X}_j}(\tilde{z}_2, \tilde{z}_4 | \tilde{z}_3) \\
 = f_{X, \tilde{X}}(\tilde{z}_1, \tilde{z}_3, \tilde{z}_2, \tilde{z}_4) \times f_{Y|X}(\tilde{z}_5 | \tilde{z}_1, \tilde{z}_3),
\end{align*}
\]

(A.18)

where the second equality above follows from the conditional independence property of the knockoffs and the last equality above holds because of the columnwise conditional independence assumption on the null features.

From (A.18), it holds that

\[
\begin{align*}
 f_{X_j, \tilde{X}_j, x_{-j}, \tilde{x}_{-j}, Y}(X_j, \tilde{X}_j, X_{-j}, \tilde{x}_{-j}, Y) \\
 = f_{X_j, \tilde{X}_j, x_{-j}, \tilde{x}_{-j} | X_j, \tilde{X}_j, X_{-j}}(X_j, \tilde{X}_j, X_{-j}, \tilde{x}_{-j}) \times f_{Y|X_{-j}}(Y | X_{-j})
\end{align*}
\]

and

\[
\begin{align*}
 f_{X_j, \tilde{X}_j, x_{-j}, \tilde{x}_{-j}, Y}(\tilde{X}_j, X_j, X_{-j}, \tilde{x}_{-j}, Y) \\
 = f_{X_j, \tilde{X}_j, x_{-j}, \tilde{x}_{-j} | X_j, \tilde{X}_j, X_{-j}}(\tilde{X}_j, X_j, X_{-j}, \tilde{x}_{-j}) \times f_{Y|X_{-j}}(Y | X_{-j}),
\end{align*}
\]

which establish (13).

**Proofs of (14) and (15).** The proof of (14) is straightforward using the additional assumption of i.i.d. observations and hence, is omitted here for simplicity. We now focus on proving (15). Fixing a feature index \(j\), let us consider a random vector \((\tilde{X}_j^1, x_{-j}, \tilde{z})\) such that \(\tilde{X}_j^1\) is generated by the \(j\)th coordinatewise knockoff generator \(\kappa_j(x_{-j})\), given \(x_{-j}\) and that \(\tilde{z} = (\tilde{Z}_j, \tilde{z}_{-j})\) is a knockoff vector of \((\tilde{X}_j, x_{-j})\) generated from the knockoff filter \(\kappa((\tilde{X}_j^1, x_{-j}), )\), where \(\kappa_j\) and \(\kappa\) are as given in Condition 3. In view of Condition 3, we see that \((\tilde{X}_j^1, \tilde{Z}_j, x_{-j}, \tilde{z}_{-j})\) and \((\tilde{Z}_j, \tilde{X}_j^1, x_{-j}, \tilde{z}_{-j})\) have the same distribution and the corresponding density functions exist, which entail that for each \((z_1, z_2, z_3, z_4) \in \mathbb{R}^{2p}\),

\[
f_{\tilde{X}_j^1, \tilde{Z}_j, x_{-j}, \tilde{z}_{-j}}(z_1, z_2, z_3, z_4) = f_{\tilde{X}_j^1, \tilde{Z}_j, x_{-j}, \tilde{z}_{-j}}(z_2, z_1, z_3, z_4).
\]

(A.19)
Moreover, we have that \( T < \infty \). We begin with proving the first assertion (17) in Theorem 3. The notation

\[
A.3 \text{ Proof of Theorem 3}
\]

Next, it follows from the definition of \((\tilde{X}_j, \tilde{Z}_j, \tilde{x}_{-j}, \tilde{z}_{-j})\) that

\[
f_{\tilde{X}_j, \tilde{Z}_j, \tilde{x}_{-j}, \tilde{z}_{-j}}(z_1, z_2, z_3, z_4) = f_{x_{-j}}(z_3)f_{\tilde{X}_j, \tilde{x}_{-j}}(z_1 | z_3)f_{\tilde{Z}_j, \tilde{z}_{-j}}(\tilde{z}_2 | z_1, z_3) = f_{x_{-j}}(z_3)f_{\tilde{X}_j, \tilde{x}_{-j}}(z_1 | z_3)f_{\tilde{X}_j, \tilde{x}_{-j} | X_j, x_{-j}}(z_2, z_4 | z_1, z_3),
\]

(A.20)

where \( f_{\tilde{Z}_j, \tilde{z}_{-j}}(\tilde{z}_2, \tilde{z}_4 | z_1, z_3) = f_{\tilde{X}_j, \tilde{x}_{-j} | X_j, x_{-j}}(\tilde{z}_2, \tilde{z}_4 | z_1, z_3) \) because a knockoff generator outputs random vectors with the same distribution if the input values are the same due to Definition 2. Similarly, it holds that

\[
f_{\tilde{X}_j, \tilde{Z}_j, \tilde{x}_{-j}, \tilde{z}_{-j}}(z_2, z_1, z_3, z_4) = f_{x_{-j}}(z_3)f_{\tilde{X}_j, \tilde{x}_{-j}}(z_2 | z_3)f_{\tilde{Z}_j, \tilde{z}_{-j}}(\tilde{z}_1 | z_2, z_3) = f_{x_{-j}}(z_3)f_{\tilde{X}_j, \tilde{x}_{-j}}(z_2 | z_3)f_{\tilde{X}_j, \tilde{x}_{-j} | X_j, x_{-j}}(z_1, z_4 | z_2, z_3).
\]

(A.21)

From (A.19)–(A.21), we can deduce that

\[
f_{\tilde{X}_j, \tilde{x}_{-j}}(z_1 | \tilde{z}_3)f_{\tilde{X}_j, \tilde{x}_{-j} | X_j, x_{-j}}(\tilde{z}_2, z_4 | z_1, z_3) = f_{\tilde{X}_j, \tilde{x}_{-j}}(z_2 | \tilde{z}_3)f_{\tilde{X}_j, \tilde{x}_{-j} | X_j, x_{-j}}(z_1, z_4 | z_2, z_3),
\]

which results in

\[
\frac{f_{X_j, \tilde{X}_j, x_{-j}, \tilde{x}_{-j}}(z_1, z_2, z_3, z_4)}{f_{X_j, \tilde{X}_j, x_{-j}, \tilde{x}_{-j}}(z_2, z_1, z_3, z_4)} = \frac{f_{X_j, \tilde{X}_j, x_{-j}}(z_2, \tilde{z}_3) \times f_{X_j, x_{-j}}(z_1, \tilde{z}_3)}{f_{X_j, \tilde{X}_j, x_{-j}}(z_1, \tilde{z}_3) \times f_{X_j, x_{-j}}(z_2, \tilde{z}_3)}.
\]

(A.22)

Setting \((z_1, z_2, z_3, z_4) = (X_{ij}, \tilde{X}_{ij}, x_{-ij}, \tilde{x}_{-ij})\) in (A.22) above, we can obtain that

\[
\sum_{i=1}^{n} \log \left( \frac{f_{X_j, \tilde{X}_j, x_{-j}, \tilde{x}_{-j}}(X_{ij}, \tilde{X}_{ij}, x_{-ij}, \tilde{x}_{-ij})}{f_{X_j, \tilde{X}_j, x_{-j}, \tilde{x}_{-j}}(X_{ij}, \tilde{X}_{ij}, x_{-ij}, \tilde{x}_{-ij})} \right)
= \sum_{i=1}^{n} \log \left( \frac{f_{X_j, x_{-j}}(X_{ij}, x_{-ij})f_{\tilde{X}_j, x_{-j}}(\tilde{X}_{ij}, x_{-ij})}{f_{X_j, x_{-j}}(X_{ij}, x_{-ij})f_{\tilde{X}_j, x_{-j}}(\tilde{X}_{ij}, x_{-ij})} \right),
\]

which establishes (15). This concludes the proof of Theorem 2.

A.3 Proof of Theorem 3

Proof of (17). We begin with proving the first assertion (17) in Theorem 3. The notation of \( W_j \) and \( T \) is the same as in Algorithm 2. By the definition of \( T \) and the assumption that \( T < \infty \), we can show that

\[
1 + \# \{ j : W_j \leq -T \} \leq \tau_1 \times \# \{ j : W_j \geq T \}.
\]

Moreover, we have that

\[
e_j = \frac{p}{\# \{ s : W_s \leq -T \} + 1} > 0.
\]
if and only if $j \in \{s : W_s \geq T\}$. Thus, for nonzero $c_j$’s or equivalently any $j \in \{s : W_s \geq T\}$, it holds that

$$e_j \geq p \times (\tau_1 \times \{j : W_j \geq T\})^{-1}$$

$$\geq p \times (\tau^* \times \{j : W_j \geq T\})^{-1},$$

where the second inequality above is from the assumption that $\tau_1 \leq \tau^*$. Using the above result and the construction of the e-BH procedure, we can show that

$$\{j : W_j \geq T\} \subset \tilde{S}. \quad (A.23)$$

In light of (A.23), we need only to prove that conditional on event $\{\sum_{j=1}^{2p} |\hat{\beta}_j - \beta^*_j| \leq c_0(#S^*) \lambda_n\} \cap \{\{j : W_j \geq T\} \geq c_1(#S^*)\}$, it holds that

$$\frac{{#(S^* \cap \{j : W_j \geq T\})}}{{#S^*}} \geq 1 - (1 + \phi)c_0k_{1n}^{-1}. \quad (A.24)$$

Then the first assertion of Theorem 3 follows from Conditions 5–6.

We now proceed with establishing (A.24). Assume without loss of generality that

$$|W_1| \geq \cdots \geq |W_p|.$$

Let $j^* \in \{1, \cdots, p\}$ be given such that $j^* \in \{s : |W_s| = T\}$. Such $j^*$ always exists because of the assumption that $T < \infty$. Then it follows that

$$-T < W_{j^*+1} \leq 0$$

by the definition of $T$ (because otherwise $T$ would take a smaller value than $|W_{j^*}|$) and the assumption that there are no ties in $\{|W_j| : W_j > 0\}$. We will analyze two cases separately, where the first case considers $W_{j^*+1} = 0$ and the second case considers $-T < W_{j^*+1} < 0$.

Let us consider the first case of $W_{j^*+1} = 0$. Denote by $\tilde{q} = \phi c_0 k_{1n}^{-1}$ with $\phi > 0$ and $\phi^2 - \phi - 1 = 0$. We will discuss the scenarios of $\#\{j : W_j < 0\} \leq \tilde{q}(#S^*)$ and $\#\{j : W_j < 0\} > \tilde{q}(#S^*)$ separately, where the former case will be examined here and the latter one will be left to a later part. For the scenario of $\#\{j : W_j < 0\} \leq \tilde{q}(#S^*)$, some simple calculations together with $W_{j^*+1} = 0$ give that

$$\#(\{j : W_j \geq T\} \cap S^*) = \#(\{j : |W_j| > 0\} \cap S^*) - \#(\{j : W_j < 0\} \cap S^*)$$

$$\geq \#(\{j : |W_j| > 0\} \cap S^*) - \tilde{q}(#S^*). \quad (A.25)$$

We will deal with the term $\#(\{j : |W_j| > 0\} \cap S^*)$ on the RHS of (A.25) below. On the event $\{\sum_{j=1}^{2p} |\hat{\beta}_j - \beta^*_j| \leq c_0(#S^*) \lambda_n\}$, we can deduce that

$$c_0 \lambda_n (#S^*) \geq \sum_{j \in \tilde{S}_1 \cap S^*} |\beta^*_j|$$

$$\geq #(\tilde{S}_1 \cap S^*) \times (\min_{j \in S^*} |\beta^*_j|).$$
where \( \hat{S}_1 = \{ j : |\hat{\beta}_j| = 0 \} \). Such result and Condition 6 entail that

\[
c_0(\#S^*)k_n^{-1} \geq \#(\hat{S}_1 \cap S^*).
\]

Hence, it follows from the assumption that there are no ties in \( \{|\hat{\beta}_j| : |\hat{\beta}_j| > 0 \} \) that

\[
\#(\{ j : |W_j| > 0 \} \cap S^*) = \#((\hat{S}_1)^c \cap S^*) \\
\geq (1 - c_0k_n^{-1}) \times (\#S^*).
\]

(A.26)

Then combining (A.25)–(A.26), we can obtain that conditional on event \( \{ \sum_{j=1}^{2p} |\hat{\beta}_j - \beta_j^*| \leq c_0(\#S^*)\lambda_n \} \),

\[
\frac{\#(\{ j : W_j \geq T \} \cap S^*)}{\#S^*} \geq 1 - c_0k_n^{-1} - \tilde{q} \\
= 1 - (1 + \phi)c_0k_n^{-1},
\]

which establishes (A.24). Moreover, observe that the second scenario of \( \#\{ j : W_j < 0 \} > \tilde{q}(\#S^*) \) when \( W_{j+1} = 0 \) implies that

\[
\#\{ j : W_j \leq -T \} = \#\{ j : W_j < 0 \} > \tilde{q}(\#S^*) > \tilde{q}(\#S^*),
\]

which reduces to the same form as in (A.28) below. Thus, the proof provided below can be applied here to conclude the proof for the first case \( W_{j+1} = 0 \).

We now consider the case of \(-T < W_{j+1} < 0\). From the definition of \( T \) and the assumption that there are no ties in \( \{|W_j| : |W_j| > 0\} \), it holds on event \( \{ \#\{ j : W_j \geq T \} \geq c_1(\#S^*) \} \) that

\[
\#\{ j : W_j \leq -T \} + 2 \geq \tau_1 \times \#\{ j : W_j \geq T \} \\
\geq \tau_1 c_1(\#S^*).
\]

(A.28)

Meanwhile, on the event \( \{ \sum_{j=1}^{2p} |\hat{\beta}_j - \beta_j^*| \leq c_0(\#S^*)\lambda_n \} \), since \( \beta_{j+p}^* = 0 \) for all \( j > 0 \) and \( |\hat{\beta}_{j+p}| \geq T + |\hat{\beta}_j| \) for all \( j \in \{ s : W_s \leq -T \} \), we have that

\[
c_0\lambda_n(\#S^*) \geq \sum_{j : W_j \leq -T} |\hat{\beta}_{j+p} - \beta_{j+p}^*| \\
= \sum_{j : W_j \leq -T} |\hat{\beta}_{j+p}| \\
\geq \#\{ j : W_j \leq -T \} \times T.
\]

(A.29)

Then from (A.28)–(A.29) and Conditions 6–7, we can obtain that conditional on event \( \{ \#\{ j : W_j \geq T \} \geq c_1(\#S^*) \} \cap \{ \#\{ j : W_j \geq T \} \geq c_1(\#S^*) \} \),

\[
T \leq \frac{c_0\lambda_n(\#S^*)}{c_1\tau_1(\#S^*)} - 2 \leq k_n\lambda_n\phi^{-1}
\]

(A.30)
for all large $n$.

Further, conditional on event $\{\sum_{j=1}^{2p} |\hat{\beta}_j - \beta_j^*| \leq c_0(\#S^*)\lambda_n\} \cap \{\#(j : W_j \geq T) \geq c_1(\#S^*)\}$, we can deduce that for all large $n$,

$$c_0\lambda_n(\#S^*) \geq \sum_{j \in S^* \cap \{j : W_j \geq T\}^c} (|\hat{\beta}_j - \beta_j^*| + |\hat{\beta}_{j+p}|) \geq \sum_{j \in S^* \cap \{j : W_j \geq T\}^c} (|\hat{\beta}_j - \beta_j^*| + |\hat{\beta}_j - T|) \geq \sum_{j \in S^* \cap \{j : W_j \geq T\}^c} (|\beta_j^*| - T) \geq \#(S^* \cap \{j : W_j \geq T\}) \times k_1 n (1 - \phi^{-1}) \lambda_n,$$

where the second inequality above is from the fact that $|\hat{\beta}_{j+p}| > |\hat{\beta}_j| - T$ for $j$ in $\{j : W_j \geq T\}^c$, the third inequality above is due to the triangle inequality, and the last inequality above results from Condition 6 and (A.30).

In light of (A.31), it holds on event $\{\sum_{j=1}^{2p} |\hat{\beta}_j - \beta_j^*| \leq c_0(\#S^*)\lambda_n\} \cap \{\#(j : W_j \geq T) \geq c_1(\#S^*)\}$ that for all large $n$,

$$\frac{\#(S^* \cap \{j : W_j \geq T\})}{\#S^*} = 1 - \frac{\#(S^* \cap \{j : W_j \geq T\}) \cap \{\#(j : W_j \geq T) < c_1(\#S^*)\}}{\#S^*} \geq 1 - \frac{c_0}{k_1 n (1 - \phi^{-1})} \geq 1 - (1 + \phi) c_0 k_1^{-1},$$

where the second equality above follows from the definition of $\phi$. This establishes (A.24). Thus, combining the above results concludes the proof for the first assertion of Theorem 3.

**Proof of (19).** We now aim to prove the third assertion (19) of Theorem 3, and will defer the proof of (18) to the end. Let the knockoff thresholds $T^k$’s, knockoff statistics $W_j^k$’s, statistics $e_j^k$’s, and e-values $e_j$’s be given as in Algorithm 1. Let us first outline the proof idea for (19) and we will build our proof on the first assertion of Theorem 3. Using the inclusion-exclusion principle, we will show that $\cap_{k=1}^{q+1} \{j : e_j^k > 0\}$ includes most features in $S^*$ with high probability. We then prove that each $e_j$ with $j$ in $\cap_{k=1}^{q+1} \{j : e_j^k > 0\}$ is sufficiently large to be selected by the e-BH procedure, that is, $\cap_{k=1}^{q+1} \{j : e_j^k > 0\} \subset \hat{S}$. Combining all these results will complete the proof of (19). We will provide the full details of the proof next.

First, recall that $\hat{S} = \{j : e_j \geq p(\tau^* \times \hat{k})^{-1}\}$ with $\hat{k} = \max\{k : e_{(k)} \geq p(\tau^* \times k)^{-1}\}$, where $e_{(j)}$’s are the ordered statistics of $e_j$’s such that $e_{(1)} \geq \cdots \geq e_{(p)}$. Let $K > 1$ be the constant specified in Theorem 3. Let us consider two events given by

$$\cap_{k=1}^{q+1} \{\#(j : W_j^k \geq T^k) \leq K(\#S^*)\} \quad \text{(A.33)}$$

and

$$\cap_{k=1}^{q+1} \left\{ \frac{\#(S^* \cap \{j : W_j^k \geq T^k\})}{\#S^*} \geq 1 - (1 + \phi) c_0 k_1^{-1} \right\}. \quad \text{(A.34)}$$
We will show that conditional on the two events in (A.33) and (A.34) above, it holds that

$$e(\#S) = \min_{j \in S} e_j \geq p(\tau^*(\#S))^{-1}, \quad (\text{A.35})$$

where

$$S := \bigcap_{k=1}^{q+1} \{ j : W_j^k \geq T^k \}. \quad (\text{A.36})$$

Then it follows from (A.35) and the definition of \( \hat{k} \) that \( \hat{k} \geq \#S \) and \( S \subset \hat{S} \). Such results along with an application of the inclusion–exclusion principle entail that conditional on the intersection of events (A.33) and (A.34), we have

$$\frac{\#(S^* \cap \hat{S})}{\#S^*} \geq \frac{\#(S^* \cap S)}{\#S^*} \geq 1 - (q + 1)(1 + \phi)c_0k_1^{-1}, \quad (\text{A.37})$$

Since it holds that

$$\mathbb{E} \left[ \frac{\#(S^* \cap \hat{S})}{\#S^*} \right] \geq \left( 1 - (q + 1)(1 + \phi)c_0k_1^{-1} \right) \times \mathbb{P} \left( \frac{\#(S^* \cap \hat{S})}{\#S^*} \geq 1 - (q + 1)(1 + \phi)c_0k_1^{-1} \right) \geq \left( 1 - (q + 1)(1 + \phi)c_0k_1^{-1} \right) \mathbb{P} \left( \text{event in (A.33) \cap event in (A.34)} \right), \quad (\text{A.38})$$

to establish (19) we need only to prove (A.35) and construct the probability lower bounds for events in (A.33) and (A.34).

To show (A.35), note that by the definition of \( T^k \)'s and the assumption that \( T^k < \infty \), we have that conditional on event given in (A.33),

$$1 + \# \{ j : W_j^k \leq -T^k \} \leq \tau_1(\# \{ j : W_j^k \geq T^k \}) \leq \tau_1K(\#S^*) \quad (\text{A.39})$$

for each \( k \in \{ 1, \cdots, q+1 \} \). In view of (A.39), it holds that for each nonzero \( e_j^k \),

$$e_j^k = \frac{p}{\# \{ s : W_s^k \leq -T^k \}} + 1 \geq \frac{p}{\tau_1K(\#S^*)} \geq \frac{p}{\tau^* \times (1 - (1 + q)(1 + \phi)c_0k_1^{-1}) \times (\#S^*)}, \quad (\text{A.40})$$

where we have used the definitions of \( e_j^k \)'s, \( \phi \), and \( \tau_1 \). Then from (A.40) and the definition \( e_j = (q + 1)^{-1} \sum_{k=1}^{q+1} e_j^k \), we can deduce that conditional on event (A.33),

$$\min_{j \in S} e_j \geq \frac{p}{\tau^* \times (1 - (1 + q)(1 + \phi)c_0k_1^{-1}) \times (\#S^*)},$$

which establishes (A.35).

It remains to provide the probability upper bounds for the complementary events of
(A.33) and (A.34), which are given in (A.43) and (A.41), respectively, below. By the result of the first assertion of Theorem 3 and the assumptions (Conditions 6–7 and that Condition 5 is satisfied for the Lasso estimates applied to each subsample in $H_k$ in Algorithm 1), it holds that

$$P(\text{complementary event of (A.34)}) \leq (q + 1) \times (k_2 n + k_3 n) \quad (A.41)$$

for all large $n$.

On the other hand, it follows from the assumption of $\#S^* > 0$ that conditional on event \{\#\{j : W_j^k \geq T^k\} \geq K(\#S^*)\},

$$\frac{\#(\{j : W_j^k \geq T^k\} \cap (S^*)^c)}{\#\{j : W_j^k \geq T^k\} \lor 1} \geq \frac{\#(\{j : W_j^k \geq T^k\} - \#S^*)}{\#\{j : W_j^k \geq T^k\} \lor 1} > \frac{\#(\{j : W_j^k \geq T^k\} - \#(\{j : W_j^k \geq T^k\} \times K^{-1})}{\#\{j : W_j^k \geq T^k\} \lor 1} \geq \frac{K - 1}{K}. \quad (A.42)$$

Therefore, from (20) and (A.42) some simple calculations give that

$$P(\#\{j : W_j^k \geq T^k\} > K(\#S^*)) \times \frac{K - 1}{K} + P(\#\{j : W_j^k \geq T^k\} \leq K(\#S^*)) \times 0 \leq E\left(\frac{\#(\{j : W_j^k \geq T^k\} \cap (S^*)^c)}{\#\{j : W_j^k \geq T^k\} \lor 1}\right) \leq \tau_1 + \theta_\epsilon,$$

which yields that

$$P(\text{complementary event of (A.33)}) \leq (q + 1) \times \frac{(\tau_1 + \theta_\epsilon)K}{K - 1}. \quad (A.43)$$

This establishes the desired conclusion in (19) of Theorem 3.

Proof of (18). Finally, we show the second assertion (18) of Theorem 3. Let us observe that by the construction of Algorithm 1 and the definition of $S$ in (A.36), it holds that

$$P(\{\hat{S} = \emptyset\} \cup \{S \subset \hat{S}\}) = 1.$$

Then by (A.34)–(A.37), (A.41), and the fact that $\phi \leq 3$ (recall that $\phi$ is defined at the beginning of this proof), we can obtain the desired result in (18). It is worth mentioning that we do not require $\tau_1 \leq \tau^*$ here. This completes the proof of Theorem 3.

A.4 Proof of Corollary 1

The conclusion of Corollary 1 follows from the proof of (15) in Theorem 2 given in Section A.2.
where we recall that $X_k = \{x_i, \tilde{x}_i, Y_i\}_{i \in H_k}$ and $X^\pi_k = \{x^\pi_i, \tilde{x}^\pi_i, Y^\pi_i\}_{i \in H_k}$ for each $k \in \{1, \cdots, q+1\}$. Combining (A.44) and $\sum_{k=1}^{q+1} \#H_k \leq n$ leads to the desired result in (6).

Next, we deal with the second assertion of Corollary 2. When Condition 2 holds and $\{Y_i, x_i\}_{i=1}^n$ is also an i.i.d. sample, $\{Y_i, x_i, \tilde{x}_i\}_{i=1}^n$ is an i.i.d. sample. Therefore, it follows from the fact that $(Y^\pi_i, x^\pi_i, \tilde{x}^\pi_i)$’s are i.i.d. with $(Y^\pi_i, x^\pi_i, \tilde{x}^\pi_i)$ having the same distribution as $(Y_1, x_1, \tilde{x}_1)$ that (A.44) holds with $\rho = 0$, which concludes the proof of Corollary 2.

A.6 Proof of Proposition 1

For the reader’s convenience, we provide some basic knowledge about time-homogeneous Markov chains here. Two sufficient conditions for a process $\{Q_t\}$ to admit a transition kernel are 1) for each Borel set $A$ and each $t$,

$$\mathbb{P}(Q_t \in A | Q_{t-1}) = \mathbb{P}(Q_t \in A | Q_{t-j}, j < 1),$$

the so-called the “Markov property,” and 2) the conditional distribution of $Q_t$ given $Q_{t-1}$ are the same for each $t$. Processes satisfying these two conditions are known as time-homogeneous Markov chains. A useful sufficient condition for verifying that a process is a time-homogeneous Markov chain is to check whether the process can be written as $Q_t = F(Q_{t-1}, \varepsilon_t)$ for some measurable $F(\cdot, \cdot)$ and identically distributed innovative random vectors $\{\varepsilon_t\}$ such that $\varepsilon_t$ is independent of $Q_{t-j}$ with $j \geq 1$. It can be shown that $\{x_t\}$ in Example 3 is a time-homogeneous Markov chain, and we omit the details on proving such claim for simplicity.

Next, let us consider Example 6 below, which is more general than Example 3. In particular, $\{x_t\}$ in Example 3 is a special case of $\{z_t\}$ in Example 6.

Example 6 (Gaussian linear processes). Let $\{z_t := (Y_{t1}, \cdots, Y_{tp})^T\}$ be such that for $l = 1, \cdots, p$, $Y_t = \sum_{i=0}^{\infty} (\tilde{w}_i(l))^T \delta_{t-i}$, where $\tilde{w}_i(l)$ is an $l$-dimensional coefficient vector such that for each $h \geq 0$,

$$\max_{1 \leq l \leq h} \sum_{i \geq h} \|\tilde{w}_i(l)\|_1 \leq C_1 e^{-s_1 h} \tag{A.45}$$

with some positive $C_1$ and $s_1$, and $\delta_t$’s are i.i.d. $l$-dimensional Gaussian random vectors with zero mean and covariance matrix $\Sigma$. In addition, assume that $\lambda_{\text{max}}(\Sigma) < L_3$ and $\lambda_{\text{min}}(\mathbb{E}(z_1 z_1^T)) > l_1$ for some positive $L_3$ and $l_1$, where $\lambda_{\text{max}}(\cdot)$ and $\lambda_{\text{min}}(\cdot)$ denote the largest and smallest eigenvalues of a given matrix, respectively.
We use Propositions 3.1.1–3.1.2 of Brockwell and Davis [10] to obtain the stationarity of Example 6; the details on this are omitted. Thus, \( \{x_t\} \) in Example 3 is a stationary time-homogeneous Markov chain; equivalently, the stationary distribution and transition kernel of \( \{x_t\} \) exist.

**Remark 2.** Notice that time-homogeneous Markov chains are not always stationary; particularly, a random walk process can be a time-homogeneous Markov chain. Also, note that Example 6 may not be a time-homogeneous Markov chain. With regularity conditions particularly, a random walk process can be a time-homogeneous Markov chain. Also, note that time-homogeneous Markov chains are not always stationary; par-

Let \( \{z_t^{(h)}\} \) in Example 6 with dimensionality \( p_h \) and stationary distribution \( \pi_h(\cdot) \) be given. Note that we do not assume a transition kernel for Example 6 and that all parameters (except for constant \( C_1, s_1, t_1, \) and \( L_3 \)) in Example 6 may change for each \( h \), but we drop the superscript or subscript \( h \) for simplicity of presentation whenever there is no confusion. Since Example 3 admits a transition kernel and it is a special case of Example 6, to prove Proposition 1 it suffices to show that for all large \( h \), there exist some constants \( 0 \leq \rho < 1, 0 < C_0 < \infty \), and measurable functions \( V_h : \mathbb{R}^{p_h} \rightarrow [0, \infty) \) such that for each integer \( t \),

\[
\sup_{D \in \mathbb{R}^{p_h}} \left| \mathbb{P}(z_{t+h} \in D) - \mathbb{P}(z_t^{(h)} \in D \mid z_t^{(h)}) \right| \leq V_h(z_t^{(h)}) \rho^h C_3 \quad (A.46)
\]

almost surely for some constant \( C_3 > 0 \), and

\[
C_0 \geq \sup_{h > 0} \int_{\mathbb{R}^{p_h}} V_h(x) \pi_h(dx).
\]

To ease the technical presentation, we first introduce some necessary notation. For each \( h \), denote by

\[
U_{1t}^{(h)} := \left( \sum_{i=h}^{\infty} (\bar{w}_i(1))^T \delta_{t-i}, \cdots, \sum_{i=h}^{\infty} (\bar{w}_i(p_h))^T \delta_{t-i} \right)^T,
\]

\[
U_{2t}^{(h)} := \left( \sum_{i=0}^{h-1} (\bar{w}_i(1))^T \delta_{t-i}, \cdots, \sum_{i=0}^{h-1} (\bar{w}_i(p_h))^T \delta_{t-i} \right)^T, \quad (A.47)
\]

and let \( V_{1t}^{(h)} \) and \( V_{2t}^{(h)} \) be independent copies of \( U_{1t}^{(h)} \) and \( U_{2t}^{(h)} \), respectively, where the superscript or subscript \( h \) represents the truncation length. Observe that \( U_{1t}^{(h)} + U_{2t}^{(h)} \) is an instance of \( z_t \) in Example 6. Due to the Gaussian innovations, the stationary distribution \( \pi_h \) is the distribution of \( V_{11}^{(0)} \), which is the same as that of \( V_{1t}^{(h)} + V_{2t}^{(h)} \) for each \( t \) and \( h \).

Let us repeat the needed statement (A.46) with the newly defined notation. For all large \( h \), there exist some constants \( 0 \leq \rho < 1, 0 < C_0 < \infty \), and measurable functions
\[ V_h : \mathbb{R}^{p_h} \rightarrow [0, \infty) \text{ such that for each integer } t, \]
\[
\sup_{D \in \mathbb{R}^{p_h}} \left| P(V_{1t}^{(h)} + V_{2t}^{(h)} \in D) - P(U_{1(t+h)}^{(h)} + U_{2(t+h)}^{(h)} \in D \mid U_{1t}^{(h)} + U_{2t}^{(h)}) \right| \leq V_h(U_{1t}^{(h)} + U_{2t}^{(h)}) \rho^h C_3 \tag{A.48}
\]

almost surely for some constant \( C_3 > 0 \), and
\[
C_0 \geq \sup_{h > 0} \int_{\mathbb{R}^{p_h}} V_h(x) \pi_h(dx). \tag{A.49}
\]

If (A.48) holds for some \( t \), it holds for each integer \( t \) because the process is stationary. Notice that the technical analysis here does not depend on the Markov property. For the remaining proof of Proposition 1, we tend to omit the term almost surely when the equality or inequality holds clearly almost surely.

Let us begin with establishing (A.48). In view of assumption (8), let \( s_3 > 0 \) and \( 0 < \delta_0 < 1 \) be given such that \( 0 < s_3 < s_1 \) and \( s_2 < \delta_0 s_3 \). For each positive integer \( h \), we have
\[
\rho^h \exp (-\delta_0 s_3 h) \leq C_2 \exp ((s_2 - \delta_0 s_3) h). \tag{A.50}
\]

We claim that for all large \( h \) and each \( t \), it holds that for each \( D \in \mathbb{R}^{p_h}, \)
\[
\left| P \left( V_{1t}^{(h)} + V_{2t}^{(h)} \in D \right) - P \left( U_{1(t+h)}^{(h)} + U_{2(t+h)}^{(h)} \in D \mid U_{1t}^{(h)} + U_{2t}^{(h)} \right) \right| \leq P \left( \left\| V_{11}^{(h)} \right\|_\infty \geq e^{-s_3 h} \right) + P \left( \left\| U_{1(t+h)}^{(h)} \right\|_\infty \geq e^{(-s_3 h)} \mid U_{1t}^{(h)} + U_{2t}^{(h)} \right) + 2 \rho^h \exp (-\delta_0 s_3 h), \tag{A.51}
\]

where \( c > 0 \) is some constant and \( \left\| z \right\|_\infty := \max_{1 \leq i \leq k} |z_i| \) for \( z = (z_1, \cdots, z_k)^T \in \mathbb{R}^k \). The proof of claim (A.51) above is presented in Section B.2.

We next construct some upper bounds for the first and third terms on the RHS of (A.51). It follows from \( \|v\|_1^2 \geq \|v\|_2^2 \) and (A.45) that for each \( q \) and \( t \),
\[
\text{Var} \left( \sum_{i \geq h} \bar{w}_i^T(q) \delta_{t-i} \right) \leq \sum_{i \geq h} \left\| \bar{w}_i(q) \right\|_2^4 \lambda_{\max}(\Sigma_h)
\leq \left( \sum_{i \geq h} \left\| \bar{w}_i(q) \right\|_1 \right)^2 \lambda_{\max}(\Sigma_h)
\leq (C_1 \exp (-s_1 h))^2 \lambda_{\max}(\Sigma_h),
\]

where \( \Sigma_h \) denotes the covariance matrix of the underlying Gaussian random vectors \( \delta_t \)'s (the superscript \( h \) is dropped) associated with \( \{z_t^{(h)}\} \) in Example 6. Combining this, the fact that
\(\delta_i\)'s are Gaussian random vectors, and Markov’s inequality, it holds that for each \(h \geq 0\),

\[
\Pr \left( \left\| V_{11}^{(h)} \right\|_\infty \geq \exp (-s_3 h) \right) \\
\leq \rho h \Pr \left( C_1 \exp (-s_1 h) \sqrt{\lambda_{\max}(\Sigma_h)} |Z| \geq \exp (-s_3 h) \right) \\
\leq \rho h \mathbb{E}(e^{\|Z\|}) \exp \left[ - \left( C_1 \sqrt{\lambda_{\max}(\Sigma_h)} \right)^{-1} \exp ((s_1 - s_3) h) \right],
\]

where \(Z\) denotes a Gaussian random variable with zero mean and unit variance. Similarly, we can show that for all large \(h\), it holds that

\[
\Pr \left( \left\| V_{21}^{(h)} \right\|_\infty \geq \exp ((1 - \delta_0) s_3 h) - 2 \exp (-s_3 h) \right) \\
\leq \rho h \Pr \left( C_1 \sqrt{\lambda_{\max}(\Sigma_h)} |Z| \geq \exp ((1 - \delta_0) s_3 h) - 1 \right) \\
\leq \rho h \mathbb{E}(e^{\|Z\|}) \exp \left[ - \left( C_1 \sqrt{\lambda_{\max}(\Sigma_h)} \right)^{-1} \exp ((1 - \delta_0) s_3 h) - 1 \right].
\]

We are now ready to construct the \(V_h\) function. Let \(g\) be a measurable function such that \(g(U_{1t}^{(h)} + U_{2t}^{(h)})\) is a version of \(\Pr \left( \left\| U_{1t}^{(h)} + U_{2t}^{(h)} \right\|_\infty \geq \exp (-s_3 h) \mid U_{1t}^{(h)} + U_{2t}^{(h)} \right)\). It follows from the assumption that \(\lambda_{\max}(\Sigma_h)\) is bounded by a constant, \(\mathbb{E}(e^{\|Z\|}) < \infty\), (A.50), (A.52), and (A.53) that there exist some constants \(C_3 > 0\) and \(0 \leq \rho < 1\) such that for each positive \(h\), \(C_3 \rho^h\) is larger than the summation of the first, third, and fourth terms on the RHS of (A.51). For each \(h\), let us define function \(V_h\) as

\[
V_h(x) := \begin{cases} 
2 & \text{if } g(x) \leq C_3 \rho^h, \\
2 \rho^{-h} C_3^{-1} & \text{otherwise}.
\end{cases}
\]

Then combining (A.51) and the definitions of \(\rho\), \(C_3\), and \(V_h\) leads to (A.48).

Finally, we deal with (A.49). By Markov’s inequality, the definition of \(g\), and \(\Pr \left( \left\| V_{11}^{(h)} \right\|_\infty \geq \exp (-s_3 h) \right) = \Pr \left( \left\| U_{11}^{(h)} \right\|_\infty \geq \exp (-s_3 h) \right)\), we can deduce that

\[
\int V_h(x)d\pi_h(x) = \mathbb{E}(V_h(U_{1t}^{(h)} + U_{2t}^{(h)})) \\
\leq 2 + 2(C_3 \rho^h)^{-1} \Pr(g(U_{1t}^{(h)} + U_{2t}^{(h)}) > C_3 \rho^h) \\
\leq 2 + 2(C_3 \rho^h)^{-2} \mathbb{E}(g(U_{1t}^{(h)} + U_{2t}^{(h)})) \\
= 2 + 2(C_3 \rho^h)^{-2} \mathbb{P} \left( \left\| V_{11}^{(h)} \right\|_\infty \geq \exp (-s_3 h) \right).
\]

For the first equality, recall that \(U_{1t}^{(h)} + U_{2t}^{(h)}\) has the stationary distribution. Therefore, by (A.54), (A.52), and (A.50), for all large \(h\), it holds that \(\int V_h(x)d\pi_h(x)\) is bounded by a constant, which leads to (A.49). This completes the proof of Proposition 1.
B Some key lemmas and additional technical details

We will provide in this section the additional technical details and some key lemmas. In particular, we rely on measure theory for valid arguments for the manipulation of integration when the conditional distributions are involved.

B.1 Proof of Claim (A.44)

Let us first make a simple observation. For any $q_1$-dimensional random vectors $X_1, Y_1$ and $q_2$-dimensional random vectors $X_2, Y_2$ such that $X_2 = F(X_1)$ and $Y_2 = F(Y_1)$ for some measurable $F : \mathbb{R}^{q_1} \mapsto \mathbb{R}^{q_2}$, it holds that

$$
\sup_{D \in \mathbb{R}^{q_2}} |\mu_{X_2}(D) - \mu_{Y_2}(D)| = \sup_{D \in \mathbb{R}^{q_2}} |\mu_{X_1}(F^{-1}(D)) - \mu_{Y_1}(F^{-1}(D))| \\
\leq \sup_{A \in \mathbb{R}^{q_1}} |\mu_{X_1}(A) - \mu_{Y_1}(A)|,
$$

where $F^{-1}(\cdot)$ denotes the inverse mapping of $F(\cdot)$. With the aid of (A.55), we now deal with the case of $k = 1$ below. Let $M$ be given as in (A.77) with $l = 2$, $h = q - 1$, and $z_i = x_i$. Similarly, let $M^\pi$ be given as in (A.77) with $l = 2$, $h = q - 1$, and i.i.d. random vectors $(z_i^{\pi_1}, z_i^{\pi_2})$'s such that $(z_i^{\pi_1}, z_i^{\pi_2})$ and $(x_1, x_2)$ have the same distribution. Then it follows from Lemma 1 in Section B.3 that

$$
\sup_{D \in \mathbb{R}^{#H_1 \times (2p)}} |\mathbb{P}((x_{i+1}, x_i, i \in H_1) \in D) - \mathbb{P}((z_2^{\pi_1}, z_1^{\pi_1}, i \in H_1) \in D)| \\
\leq \#H_1 \times \rho^q \times C_0.
$$

By the assumption that $Y_i$ is $x_{i+1}$-measurable, we have that $Y_i, x_i = F(x_{i+1}, x_i)$ for some measurable $F : \mathbb{R}^{2p} \mapsto \mathbb{R}^{1+p}$. Then it follows from the assumption that each $(Y_i, x_i)$ and $(Y_1, x_1)$ have the same distribution and the assumption that each $(z_i^{\pi_1}, z_i^{\pi_2})$ and $(x_1, x_2)$ have the same distribution that

$$
\{F(z_2^{\pi_1}, z_1^{\pi_1})\}_{i=1}^n \text{ and } \{(Y_i, x_i)\}_{i=1}^n
$$

have the same distribution. Hence, from (A.55)–(A.57), we can deduce that

$$
\sup_{D \in \mathbb{R}^{#H_1 \times (1+p)}} |\mathbb{P}((Y_i, x_i, i \in H_1) \in D) - \mathbb{P}((Y_i, x_i, i \in H_1) \in D)| \\
= \sup_{D \in \mathbb{R}^{#H_1 \times (1+p)}} |\mathbb{P}((x_{i+1}, x_i, i \in H_1) \in F^{-1}(D)) - \mathbb{P}((z_2^{\pi_1}, z_1^{\pi_1}, i \in H_1) \in F^{-1}(D))| \\
\leq \#H_1 \times \rho^q \times C_0.
$$

Finally, we can apply Lemma 7 in Section B.9 to control the distributional variation results from the inclusion of knockoffs. Using Definition 2 and Conditions 1–2, we can show that 1) $(Y_i, x_i, \tilde{x}_i)$'s are identically distributed; 2) $(\tilde{x}_i, i \in H_1)$ are independent conditional on $(x_i, i \in H_1)$, and that $\tilde{x}_i$ is independent of $(x_q, q \in H_1 \setminus \{i\})$ conditional on $x_i$ for each $i \in H_1$; 3) $(Y_i, i \in H_1)$ is independent of $(\tilde{x}_i, i \in H_1)$ conditional on $(x_i, i \in H_1)$; and 4)
the above results also hold for \((Y_{i}^{x}, x_{i}^{x}, \bar{x}_{i}^{x})'s\). By these results, an application of the first assertion of Lemma 7 concludes the proof of (A.44) for the case with \(k = 1\). The other cases with \(2 \leq k \leq q + 1\) can be dealt with similarly. This concludes the proof of Claim (A.44).

### B.2 Proof of Claim (A.51)

We denote by \(f_{h}(x)\) the density function of \(V_{21}^{(h)}\), that is,

\[
f_{h}(x) := \frac{1}{\sqrt{(2\pi)^{p_{h}}|\Sigma_{h}^{V}|}} \exp \left(-\frac{1}{2} x^{\top} (\Sigma_{h}^{V})^{-1} x\right),
\]

where \(\Sigma_{h}^{V}\) is the corresponding covariance matrix and \(|A|\) stands for the determinant of a given matrix \(A\). By the assumptions of Gaussian linear processes (this is where we need \(\lambda_{\min}(\mathbb{E}(z_{1}^{(h)}(z_{1}^{(h)})^{\top})) > l_{1}\)), there exist some constant \(c > 0\) and positive integer \(\bar{h}\) such that

\[
\min_{k \geq \bar{h}} \lambda_{\min}(\mathbb{E}(V_{21}^{(h)}V_{21}^{(h)\top})) > c > 0. \tag{A.59}
\]

In view of (A.59), for all \(h \geq \bar{h}\) we have \(\lambda_{\min}(\Sigma_{h}^{V}) > c\).

To facilitate the technical analysis, we will make use of the following facts.

1) For all \(x < 1.79\), it holds that

\[
\exp(x) \leq 1 + x + x^{2}. \tag{A.60}
\]

To get the specific value of 1.79, we use the first and second order derivatives of \(\exp(x)\) and \(1 + x + x^{2}\) to conclude that there exists some positive number \(x_{0}\) such that when \(x \leq x_{0}\), (A.60) holds, and when \(x > x_{0}\), it holds that \(\exp(x) > 1 + x + x^{2}\). Then a direct calculation shows that \(\exp(1.79) < 5.994 < 1 + 1.79 + 1.79^{2}\), which gives \(x_{0} \geq 1.79\).

2) By (A.59), for all large \(h\), we have that for each \(\Delta, x \in \mathbb{R}^{p_{h}}\) with \(\|\Delta\|_{2} \leq \|x\|_{2}\),

\[
|x^{\top} (\Sigma_{h}^{V})^{-1} \Delta + \frac{1}{2} \Delta^{\top} (\Sigma_{h}^{V})^{-1} \Delta| \leq 2 \|x\|_{2} \|\Delta\|_{2}\ c^{-1}. \tag{A.61}
\]

If furthermore \(2 \|x\|_{2} \|\Delta\|_{2}\ c^{-1} < 1.79\), then it follows from (A.60)–(A.61) that

\[
|f_{h}(x + \Delta) - f_{h}(x)| \leq f_{h}(x) \left|\exp \left(-x^{\top} (\Sigma_{h}^{V})^{-1} \Delta - \frac{1}{2} \Delta^{\top} (\Sigma_{h}^{V})^{-1} \Delta\right) - 1\right|
\leq f_{h}(x) \left(2 \|x\|_{2} \|\Delta\|_{2}\ c^{-1} + (2 \|x\|_{2} \|\Delta\|_{2}\ c^{-1})^{2}\right). \tag{A.62}
\]

3) We show that for each \(\mathcal{D} \in \mathcal{R}^{p_{h}}\), \(\mu_{V_{21}}(\mathcal{D} - V_{1t}^{(h)})\) is a version of \(\mathbb{P}(V_{1t}^{(h)} + V_{2t}^{(h)} \in \mathcal{D} \mid V_{1t}^{(h)})\) and in particular, for each \(t, h > 0\), and \(\mathcal{D} \in \mathcal{R}^{p_{h}}\),

\[
\mathbb{P}(V_{1t}^{(h)} + V_{2t}^{(h)} \in \mathcal{D} \mid V_{1t}^{(h)}) = \mu_{V_{21}}(\mathcal{D} - V_{1t}^{(h)}). \tag{A.63}
\]

To this end, let us define a measurable function \(g(x) := \int_{\mathbb{R}^{p_{h}}} \mu_{V_{21}}(dx_{2}) \mathbf{1}_{x_{2} \in \mathcal{D} - x}\) with
$D - x := \{ z - x : z \in D \}$ and write $\mu_{V_1^{(h)}}(D - V_{1t}^{(h)}) = g(V_{1t}^{(h)})$ to see that $\mu_{V_1^{(h)}}(D - V_{1t}^{(h)})$ is $\sigma(V_{1t}^{(h)})$-measurable. Observe that if we can show that for each $A \in \mathcal{R}^p$, we have that

$$\int_A \mu_{V_1^{(h)}}(dx_1) \mu_{V_2^{(h)}}(D - x_1) = \int_{\{V_1^{(h)} \in A\}} \mathbb{P}(V_{1t}^{(h)} + V_{2t}^{(h)} \in D | V_{1t}^{(h)}) d\mathbb{P}, \quad (A.63)$$

then we can apply the change of variables formula to the left-hand side of (A.63) and use the definition of conditional expectation to obtain the desired result. It remains to prove (A.63).

Since $V_{1t}^{(h)}$ and $V_{2t}^{(h)}$ are independent for each $t$ and $h > 0$, it holds that for each $D, A \in \mathcal{R}^p$,

$$\mathbb{P}(\{V_{1t}^{(h)} + V_{2t}^{(h)} \in D\} \cap \{V_{1t}^{(h)} \in A\})$$

$$= \int_{\mathbb{R}^p} \mu_{V_1^{(h)}}(dx_1) \mu_{V_2^{(h)}}(dx_2) 1_{x_1 + x_2 \in D} 1_{x_1 \in A}$$

$$= \int_{\mathbb{R}^p} \mu_{V_1^{(h)}}(dx_1) \mu_{V_2^{(h)}}(dx_2) 1_{x_1 + x_2 \in D} 1_{x_1 \in A}$$

$$= \int_{\mathbb{R}^p} 1_{(x_1 \in A)} \mu_{V_1^{(h)}}(dx_1) \int_{\mathbb{R}^p} \mu_{V_2^{(h)}}(dx_2) 1_{x_2 \in D - x_1} \quad (A.64)$$

$$= \int_{\mathbb{R}^p} 1_{(x_1 \in A)} \mu_{V_1^{(h)}}(dx_1) \mu_{V_2^{(h)}}(D - x_1)$$

$$= \int_{\mathbb{R}^p} 1_{(x_1 \in A)} \mu_{V_1^{(h)}}(dx_1) \mu_{V_2^{(h)}}(D - x_1)$$

$$= \int_A \mu_{V_1^{(h)}}(dx_1) \mu_{V_2^{(h)}}(D - x_1),$$

where the second equality above is due to the independence. Moreover, since $\mathbb{P}(\{V_{1t}^{(h)} + V_{2t}^{(h)} \in D\} \cap \{V_{1t}^{(h)} \in A\} | V_{1t}^{(h)}) = 1_{V_1^{(h)} \in A} \mathbb{P}(V_{1t}^{(h)} + V_{2t}^{(h)} \in D | V_{1t}^{(h)})$, by the law of total expectation we have that

$$\mathbb{P}(\{V_{1t}^{(h)} + V_{2t}^{(h)} \in D\} \cap \{V_{1t}^{(h)} \in A\})$$

$$= \mathbb{E}[\mathbb{P}(\{V_{1t}^{(h)} + V_{2t}^{(h)} \in D\} \cap \{V_{1t}^{(h)} \in A\} | V_{1t}^{(h)})]$$

$$= \int_{\{V_{1t}^{(h)} \in A\}} \mathbb{P}(V_{1t}^{(h)} + V_{2t}^{(h)} \in D | V_{1t}^{(h)}) d\mathbb{P}. \quad (A.65)$$

Hence, combining (A.64)–(A.65) leads to (A.63).

4) Observe that $U_{2(t+h)}^{(h)}$ is independent of $U_{1t}^{(h)} + U_{2t}^{(h)}$ and $U_{1(t+h)}^{(h)}$. Thus, for each $D \in \mathcal{R}^p$, we have that

$$\mathbb{P}(U_{1t}^{(h)} + U_{2t}^{(h)} \in D \mid U_{1t}^{(h)} + U_{2t}^{(h)}, U_{1(t+h)}^{(h)})$$

$$= \mathbb{P}(U_{1(t+h)}^{(h)} + U_{2(t+h)}^{(h)} \in D \mid U_{1(t+h)}^{(h)}).$$

Using such representation, similar arguments as in 3) above, and the fact that $\mu_{U_2^{(h)}}$
is identical to $\mu_{V_2^{(h)}}$, we can show that

$$
\mathbb{P}(U_{1(t+h)}^{(h)} + U_{2(t+h)}^{(h)} \in D \mid U_{1t}^{(h)} + U_{2t}^{(h)} = \mu_{V_2^{(h)}}(D - U_{1(t+h)}^{(h)}))
$$

5) Denote by $Q := \left\{ \left\| V_{1t}^{(h)} \right\|_{\infty} \geq e^{-s_3 h} \right\}$ and $G := \left\{ \left\| U_{1(t+h)}^{(h)} \right\|_{\infty} \geq e^{-s_3 h} \right\}$. Then it follows from the definition of $\mu_{V_2^{(h)}}$ that for each $D \in \mathcal{R}^{PH}$,

$$
1_{Q \cap G} \left( \mu_{V_2^{(h)}}(D - V_{1t}^{(h)}) \biggclip \mu_{V_2^{(h)}}(D - U_{1(t+h)}^{(h)}) \right)
\leq \sup_{\left\| \Delta \right\|_{\infty} \leq e^{-s_3 h}} \left\| \int_{D - \Delta_2} (f_h(x + \Delta_2 - \Delta_1) - f_h(x)) \, dx \right\|.
$$

We are now ready to establish the desired upper bound. For each integer $h > 0$, $t$, and $D \in \mathcal{R}^{PH}$, it holds that

$$
\left\| \mathbb{P}(V_{1t}^{(h)} + V_{2t}^{(h)} \in D) - \mathbb{P}(U_{1(t+h)}^{(h)} + U_{2(t+h)}^{(h)} \in D \mid U_{1t}^{(h)} + U_{2t}^{(h)}) \right\|
= \left\| \mathbb{E} \left[ \mathbb{P}(V_{1t}^{(h)} + V_{2t}^{(h)} \in D \mid V_{1t}^{(h)}) \right) - \mathbb{E} \left[ \mathbb{P}(U_{1(t+h)}^{(h)} + U_{2(t+h)}^{(h)} \in D \mid U_{1t}^{(h)} + U_{2t}^{(h)}) \right) \right]\right\|.
$$

By 3) and 4) above, for each $D \in \mathcal{R}^{PH}$, we have

$$
\text{RHS of (A.67)} = \mathbb{E} \left[ \mu_{V_2^{(h)}}(D - V_{1t}^{(h)}) \right] - \mathbb{E} \left[ \mu_{V_2^{(h)}}(D - U_{1(t+h)}^{(h)}) \mid U_{1t}^{(h)} + U_{2t}^{(h)} \right].
$$

Since $V_{1t}^{(h)}$ is an independent copy, it follows that

$$
\text{RHS of (A.68)} = \mathbb{E} \left[ \mu_{V_2^{(h)}}(D - V_{1t}^{(h)}) \biggclip \mu_{V_2^{(h)}}(D - U_{1(t+h)}^{(h)}) \right] U_{1t}^{(h)} + U_{2t}^{(h)} \right].
$$

Next, we separate the expectation according to events $Q$ and $G$ as

$$
\text{RHS of (A.69)}
= \mathbb{E} \left[ (1_{Q \cup G} + 1_{Q \cap G}) \mu_{V_2^{(h)}}(D - V_{1t}^{(h)}) - \mu_{V_2^{(h)}}(D - U_{1(t+h)}^{(h)}) \right] U_{1t}^{(h)} + U_{2t}^{(h)} \right].
$$

Then by (A.66) and some simple calculations, we can show that

$$
\text{RHS of (A.70)}
\leq \mathbb{P}(G \cup Q \mid U_{1t}^{(h)} + U_{2t}^{(h)}) + \sup_{\left\| \Delta \right\|_{\infty} \leq e^{-s_3 h}} \left\| \int_{D - \Delta_2} (f_h(x + \Delta_2 - \Delta_1) - f_h(x)) \, dx \right\|.
$$

For the first term on the RHS of (A.71), it follows from the definitions of $Q$ and $G$ and the
For the second term on the RHS of (A.71), it holds that
\[ R(A.62), (A.74), \text{and the fact that} \]
The theoretical foundation of our subsampling method is provided by Lemma 1, which concerns the asymptotical independence of the β-mixing random vectors in each subsample.

For the second term on the RHS of (A.71), it holds that
\[
\sup_{\|\Delta\|_\infty < e^{-3h}} \left| \int_{D-\Delta_2} (f_h(x + \Delta_2 - \Delta_1) - f_h(x)) \, dx \right|
\leq 2\mathbb{P}\left( \left\| V_{21}^{(h)} \right\|_\infty \geq \exp((1 - \delta_0) s_3 h) - 2 \exp(-s_3 h) \right)
+ \sup_{\|\Delta\|_\infty < e^{-3h}} \int_{x \in D-\Delta_2, \|x\|_\infty < e^{(1-\delta_0)s_3 h}} (f_h(x + \Delta_2 - \Delta_1) - f_h(x)) \, dx.
\] (A.73)

Let us define \( \Delta := \Delta_2 - \Delta_1 \). In light of the fact that \( \|z\|_2 \leq \sqrt{\mathbb{P}} \|z\|_\infty \) for all \( z \in \mathbb{R}^p \), (A.62), (A.74), and the fact that \( \int_{x \in \mathbb{R}^p} f_h(x) \, dx = 1 \), it holds that for all large \( h \),
\[
\sup_{\|\Delta\|_\infty < e^{-3h}} \left| \int_{x \in D-\Delta_2, \|x\|_\infty < e^{(1-\delta_0)s_3 h}} (f_h(x + \Delta_2 - \Delta_1) - f_h(x)) \, dx \right|
\leq \sup_{\|\Delta\|_\infty < e^{-3h}, \|\Delta_1\|_\infty < e^{-3h}} \left| \int_{x \in D-\Delta_2, \|x\|_\infty < e^{(1-\delta_0)s_3 h}} (f_h(x + \Delta) - f_h(x)) \, dx \right|
\leq \sup_{\|\Delta\|_\infty < e^{-3h}, \|\Delta_1\|_\infty < e^{-3h}} (2 \|x\|_2 \|\Delta\|_2 \mathcal{L}^{-1} + (2 \|x\|_2 \|\Delta\|_2 \mathcal{L}^{-1})^2)\] (A.75)

Therefore, combining (A.67)–(A.73), (A.75), and the stationarity of the process yields the desired conclusion. This completes the proof of Claim (A.51).

### B.3 Lemma 1 and its proof

The theoretical foundation of our subsampling method is provided by Lemma 1, which concerns the asymptotical independence of the β-mixing random vectors in each subsample. Since (A.77) below for Lemma 1 involves stacking up stationary elements columnwise (there are \( l \) elements in a row of matrices in (A.77) below), it is unclear whether we can directly apply Lemma 4.1 of [40] to our setting. Thus, we provide our self-contained proof for
Lemma 1. Our technical analysis of Lemma 1 seems to be the first formal proof for results on the asymptotically independent blocks due to the $\beta$-mixing and subsampling.

Consider a $p$-dimensional vector-valued stationary process $\{z_t\}$. Let $n, \bar{n}, h, \text{ and } l$ be positive integers such that

$$\bar{n} = \sup\{s \in \mathbb{N} : s(l + h) - h \leq n\} > 0. \tag{A.76}$$

We construct two $\bar{n} \times (lp)$ design matrices as

$$M := \begin{pmatrix} z_{(1-1)\times(l+h)+1}^T, \cdots, z_{(2-1)\times(l+h)-h}^T \\ \vdots \\ z_{(\bar{n}-1)\times(l+h)+1}^T, \cdots, z_{\bar{n}\times(l+h)-h}^T \end{pmatrix}$$

and

$$M^\pi := \begin{pmatrix} (z_1^\pi)^T, \cdots, (z_l^\pi)^T \\ \vdots \\ (z_{\bar{n}}^\pi)^T, \cdots, (z_{\bar{n}}^\pi)^T \end{pmatrix}, \tag{A.77}$$

where $\{(z_1^\pi, \cdots, z_l^\pi)\}_t$ is an i.i.d. sequence such that $(z_1^\pi, \cdots, z_l^\pi)$ has the same distribution as $(z_1, \cdots, z_l)$. Here, matrix $M$ is obtained by removing $h$ random vectors in the process after each consecutive $l$ random vectors, and then stacking up the remaining random vectors. Lemma 1 below characterizes the distributional distance between $M$ with dependent rows and $M^\pi$ with i.i.d. rows.

**Lemma 1.** Assume that the $p$-dimensional process $\{z_t\}$ satisfies Condition 4 with $(h+1)$-step and constants $0 \leq \rho < 1$ and $C_0 > 0$. Then it holds that

$$\sup_{D \in \mathbb{R}^{lp\bar{n}}} \left| \mathbb{P}(M \in D) - \mathbb{P}(M^\pi \in D) \right| \leq n\rho^{h+1}C_0, \tag{A.78}$$

where random matrices $M$ and $M^\pi$ are defined in (A.77).

**Proof.** If we view the rows of $M$ as random mappings, a simple version of this problem is to establish an upper bound of the total variation distance between the distributions of $U_1, \cdots, U_\bar{n}$ and their i.i.d. counterparts denoted as $U_1^\pi, \cdots, U_\bar{n}^\pi$. The main technique used here is to separate the total variation distance into $TV_1, \cdots, TV_\bar{n}$ introduced below and control them separately as

$$U_1, U_2, U_3, \cdots, U_\bar{n} \leftrightarrow_{TV_1} U_1^\pi, U_2, U_3, \cdots, U_\bar{n} \leftrightarrow_{TV_2} U_1^\pi, U_2^\pi, U_3, \cdots, U_\bar{n}^\pi \leftrightarrow_{TV_3} \cdots \leftrightarrow_{TV_\bar{n}} U_1^\pi, U_2^\pi, \cdots, U_\bar{n}^\pi. \tag{A.79}$$

By the technique in (A.79) above, for each step we can focus on the total variation distance between two processes with only one distinct part. For example, for the $j$th and $(j + 1)$th processes, the distinct part is $U_j$ and $U_j^\pi$. We will present the formal proof next.

To ease the technical presentation, let us first introduce some notation. Denote the
and $D \in \mathbb{R}$ is a well-defined integral. 3) For each measurable function $f \in \mathcal{D}$, $\mu_j$ admits the following representation follow from the first two properties, and the details on deriving it can be found in Section 5.2 of [16]. For each distribution of $\mu_j$ and $\mathcal{R}^n$, we state some important properties of the transition kernel $p : \mathbb{R}^p \times \mathcal{R}^p \rightarrow [0, 1]$ of a stationary Markov chain with stationary distribution $\pi$. 1) For each integer $t$ and $\mathcal{D} \in \mathcal{R}^p$, $p(z_t, \mathcal{D})$ is a version of $\mathbb{P}(z_{t+1} \in \mathcal{D}|z_t)$. 2) For each measurable function $f$ and $\mathcal{D} \in \mathcal{R}^p$, $\int_\mathcal{D} p(\vec{x}, d\vec{y}) f(\vec{y})$ is a measurable function of $\vec{x}$, and hence for each $\mathcal{D}_k \in \mathcal{R}^p$,

$$\int_{\mathcal{D}_1} \pi(d\vec{x}_1) \int_{\mathcal{D}_2} p(\vec{x}_1, d\vec{x}_2) \cdots \int_{\mathcal{D}_k} p(\vec{x}_{k-1}, d\vec{x}_k) f(\vec{x}_k)$$

is a well-defined integral. 3) For each measurable function $f$ and $\mathcal{D} \in \mathcal{R}^p$,

$$\int_{\mathbb{R}^p} \pi(d\vec{x}) \int_{\mathcal{D}} p(d\vec{x}, d\vec{y}) f(\vec{y}) = \int_{\mathcal{D}} \pi(d\vec{x}) f(\vec{x}).$$

4) We have an expression of $\mu_j$ as given in (A.82) below, where we indicate each part of the distribution of $\mu_j$ according to

$$\mathcal{Z}_1^{\pi_1}, \cdots, \mathcal{Z}_{(j-1)(l+h)+1}^{(j-1)(l+h)+1} : j(l+h) - h, \cdots, \mathcal{Z}_{(n-1)(l+h)+1}^{(n-1)(l+h)+1} : n(l+h) - h.$$ 

Such representation follows from the first two properties, and the details on deriving it can be found in Section 5.2 of [16]. For each $\mathcal{D} \in \mathcal{R}^{lp^\mathcal{D}}$, $\mu_j(\mathcal{D})$ admits the following representation

$$\mu_j(\mathcal{D}) = \int_{\mathcal{D}} \pi(d\vec{x}_1) \times \cdots \times p(\vec{x}_{l-1}, d\vec{x}_j) \times \cdots \times \pi(d\vec{x}_{(j-1)(l+h)+1}) \times \cdots \times p(\vec{x}_{j(l+h)-h-1}, d\vec{x}_j) \times \cdots \times p^{h+1}(\vec{x}_j(l+h) - h, d\vec{x}_j(l+h) - h) \times \cdots \times \pi^{(j+1)th part}(d\vec{x}_{(n-1)(l+h)-h}, d\vec{x}_{(n-1)(l+h)+1}) \times \cdots \times p^{(j+1)th part}(\vec{x}_{n(l+h)-h-1}, d\vec{x}_{n(l+h)-h}) \times \cdots \times \pi^{(n)th part}(d\vec{x}_{n(l+h) - h}),$$

where $\vec{x}_1, \cdots, \vec{x}_{l-1}, \vec{x}_{(j-1)(l+h)+1}, \cdots, \vec{x}_{(n-1)(l+h)-h}$ stand for the corresponding running variables with $\vec{x}_k \in \mathbb{R}^p$ for each $k$. 24
Let us make use of a critical observation that
\[
\frac{1}{2}\|\mu_1 - \mu_{n+1}\|_{TV} \leq \sum_{j=1}^{n} \sup_{D \in \mathbb{R}^p} |\mu_j(D) - \mu_{j+1}(D)|. \tag{A.83}
\]
We will bound each term in the above summation separately. Let us fix $1 \leq j \leq n$. We notice that $\mu_j$ and $\mu_{j+1}$ are almost identical except for the $(j + 1)$th part in (A.82). By a careful comparison, we see that for $\mu_j$, the $(j + 1)$th part starts with $p^{h+1}(\vec{x}_{j(l+h)-h}, d\vec{x}_{j(l+h)+1})$, whereas the $(j + 1)$th part of $\mu_{j+1}$ starts with $\pi(d\vec{x}_{j(l+h)+1})$. To see the difficulty for bounding each term on the right-hand side (RHS) of (A.83) using such observation, note that $\int_D |\mu_1(dx) - \mu_2(dx)|$ is not a well-defined integral for a Borel set $D$ and two measures $\mu_1$ and $\mu_2$ since there are two $dx$’s inside the integration. To have a valid argument for this bound, we use the Radon–Nikodym theorem \cite{16} to replace the underlying measures with measurable functions (the Radon–Nikodym derivatives). The arguments follow mainly those for the proof of Lemma 5 in Section B.7.

By Condition 4, for each $\vec{x} \in \mathbb{R}^p$ it holds that $p(\vec{x}, \cdot)$ is dominated by the Lebesgue measure. Since $p$ is the transition kernel of the stationary Markov chain, this entails that 1) $p^{h+1}(\vec{x}, \cdot)$ is dominated by the Lebesgue measure for each $\vec{x} \in \mathbb{R}^p$ and 2) $\pi(\cdot)$ is also dominated by the Lebesgue measure. By 1) and the Radon–Nikodym Theorem, there exists a nonnegative measurable function on $\mathbb{R}^{2p}$, which is denoted as $r$, such that for each $\vec{x} \in \mathbb{R}^p$ and $D \in \mathbb{R}^p$,
\[
p^{h+1}(\vec{x}, D) = \int_D r(\vec{x}, \vec{y}) \, d\vec{y}.
\]
This measurable function is simply the Radon–Nikodym derivative \cite{16}, and $r(\vec{x}, \vec{y})$ is also called the probability density functions of $z_{t+h+1}$ conditional on $z_t$. In particular, for each $D_1, D_2 \in \mathbb{R}^p$, we have that
\[
\mathbb{P}((z_t, z_{t+h+1}) \in D_1 \times D_2) = \int_{\vec{x} \in D_1} \pi(d\vec{x}) \int_{\vec{y} \in D_2} r(\vec{x}, \vec{y}) d\vec{y}.
\]

For more details on the conditional probability density functions, see Example 4.1.6 of \cite{16}. Furthermore, by 2) we denote by $r_\pi(\vec{x})$ the Radon–Nikodym derivative such that for each $D \in \mathbb{R}^p$,
\[
\pi(D) = \int_D r_\pi(\vec{x}) d\vec{x}.
\]
Thus, we can obtain that
\[
\mu_j(D) = \int_D \cdots \times r(\vec{x}_{j(l+h)-h}, \vec{x}_{j(l+h)+1}) d\vec{x}_{j(l+h)+1} \times \cdots \times p(\vec{x}_{(j+1)(l+h)-h-1}, d\vec{x}_{(j+1)(l+h)-h}) \times \cdots \times p^{h+1}(\vec{x}_{(n-1)(l+h)-h}, d\vec{x}_{(n-1)(l+h)+1}) \times \cdots \times p(\vec{x}_{n(l+h)-h-1}, d\vec{x}_{n(l+h)-h}) \tag{A.84}
\]

\[
\text{\textsuperscript{(j+1)th part}} \quad \text{\textsuperscript{n\textsuperscript{th} part}}
\]
A similar expression also holds for \( \mu_{j+1} \) with \( r_\pi \). We will bound \( |\mu_j(D) - \mu_{j+1}(D)| \) next.

It follows from (A.84) and the fact of \( p \leq 1 \) that for each \( D \in \mathbb{R}^{lpn} \),

\[
|\mu_j(D) - \mu_{j+1}(D)| = \left| \int_{D} \cdots \times (r(\tilde{x}_{j(l+h)} - h, \tilde{x}_{j(l+h)+1}) - r_\pi(\tilde{x}_{j(l+h)+1})) \, d\tilde{x}_{j(l+h)+1} \times \cdots \right |
\]

\[
\leq \int_{D} \cdots \times |r(\tilde{x}_{j(l+h)} - h, \tilde{x}_{j(l+h)+1}) - r_\pi(\tilde{x}_{j(l+h)+1})| \, d\tilde{x}_{j(l+h)+1} \times \cdots
\]

\[
\leq \int_{\mathbb{R}^{lpn}} \cdots \times |r(\tilde{x}_{j(l+h)} - h, \tilde{x}_{j(l+h)+1}) - r_\pi(\tilde{x}_{j(l+h)+1})| \, d\tilde{x}_{j(l+h)+1}.
\]

To bound the RHS of (A.85), we separate the modulus into positive and negative parts and get rid of the modulus operation. Let \( D_+ \) and \( D_- \) be two disjoint Borel sets such that

\[
\int_{\mathbb{R}^{lpn}} \cdots \times |r(\tilde{x}_{j(l+h)} - h, \tilde{x}_{j(l+h)+1}) - r_\pi(\tilde{x}_{j(l+h)+1})| \, d\tilde{x}_{j(l+h)+1} = \int_{D_+} \cdots \times (r(\tilde{x}_{j(l+h)} - h, \tilde{x}_{j(l+h)+1}) - r_\pi(\tilde{x}_{j(l+h)+1})) \, d\tilde{x}_{j(l+h)+1} + \int_{D_-} \cdots \times (r_\pi(\tilde{x}_{j(l+h)+1}) - r(\tilde{x}_{j(l+h)} - h, \tilde{x}_{j(l+h)+1})) \, d\tilde{x}_{j(l+h)+1}.
\]

To proceed, we exploit arguments involving “cross-sections.” For any \( D \in \mathbb{R}^{k_1+k_2} \) and \( \tilde{x} \in \mathbb{R}^{k_1} \) with \( k_1 \) and \( k_2 \) some positive integers, let us define the cross-section at \( \tilde{x} \) as \( D_{\tilde{x}} := \{ \tilde{y} : (\tilde{x}, \tilde{y}) \in D \} \). See Section B.4 for more detail on cross-sections. The it holds that

\[
\int_{D_+} \cdots \times (r(\tilde{x}_{j(l+h)} - h, \tilde{x}_{j(l+h)+1}) - r_\pi(\tilde{x}_{j(l+h)+1})) \, d\tilde{x}_{j(l+h)+1} = \int_{D_+} \cdots \times p_{h+1}(\tilde{x}_{j(l+h)} - h, d\tilde{x}_{j(l+h)+1}) - \int_{D_-} \cdots \times \pi(d\tilde{x}_{j(l+h)+1})
\]

\[
= \int_{\mathbb{R}^{lpj}} \cdots \times p_{h+1}(\tilde{x}_{j(l+h)} - h, (D_+)_z) - \int_{\mathbb{R}^{lpj}} \cdots \times \pi((D_+)_z)
\]

\[
= \int_{\mathbb{R}^{lpj}} \cdots \times \pi((D_+)_z),
\]

where \( z \) represents \((\tilde{x}_{j+1}, \cdots, \tilde{x}_{j(l+h)+1})^{T} \) in the integration. Here, we have used the definition of the Radon–Nikodym derivative to get the first equality in (A.87). The second equality in (A.87) is justified by the fact that \( \pi \) is a distribution and hence a transition kernel, and an application of Lemma 3 in Section B.5. To apply Lemma 3 in (A.87), we can regard \( z_{j(l+h)+1} \) as \( X_3 \), \( z_{j(l+h)} \) as \( X_2 \), and the remaining variables as \( X_1 \) in Lemma 3, and notice that (A.90) is satisfied due to the Markov property. Similar arguments can be applied to \( D_- \) too.

In view of (A.86) and (A.87), it follows from the fact of \( D_+ \cap D_- = \emptyset \), (A.81), and
Condition 4 that

\[
\begin{align*}
\text{RHS of (A.85)} &= \int_{\mathbb{R}^{p_j}} \cdots \times \left[ \left( p^{h+1}(\bar{x}_{j(l+h)}^{(l+h)}, (D_+)_x) - \pi((D_+)_x) \right) \\
&\quad - \left( p^{h+1}(\bar{x}_{j(l+h)}^{(l+h)}, (D_-)_x) - \pi((D_-)_x) \right) \right] \\
&\leq \int_{\mathbb{R}^{p_j}} \cdots \times \left\| p^{h+1}(\bar{x}_{j(l+h)}^{(l+h)}, \cdot) - \pi(\cdot) \right\|_{TV} \\
&= \int_{\mathbb{R}^p} \pi(d\bar{x}_{j(l+h)}) \left\| p^{h+1}(\bar{x}_{j(l+h)}^{(l+h)}, \cdot) - \pi(\cdot) \right\|_{TV} \\
&\leq \int_{\mathbb{R}^p} V(\bar{x})\pi(d\bar{x})p^{h+1}C,
\end{align*}
\]

where \( C > 0 \) is given in Condition 4. By Condition 4, we can further show that

\[
\text{RHS of (A.88)} \leq C_0\rho^{h+1},
\]

where \( C_0 > 0 \) is a constant such that \( \int_{\mathbb{R}^p} V(\bar{x})\pi(d\bar{x})C \leq C_0 \). Therefore, combining (A.83), (A.88), and the fact of \( \bar{n} \leq n \), we can see that the upper bound is given by \( n\rho^{h+1}C_0 \), which concludes the proof of Lemma 1.

### B.4 Lemma 2 and its proof

To ease the technical presentation, let us first introduce some notation. For any \( \mathcal{D} \subset \mathbb{R}^{k_1+k_2} \) and \( x \in \mathbb{R}^{k_1} \) with \( k_1 \) and \( k_2 \) some positive integers, we define the cross-section at \( x \) as \( \mathcal{D}_x := \{ y : (x, y) \in \mathcal{D} \} \). A standard operation on \( \mathcal{D}_x \) is as follows. If \( \mathcal{D}_1 \subset \mathcal{D}_2 \), then we have that for each \( x \), \( (\mathcal{D}_1)_x \subset (\mathcal{D}_2)_x \) and \( (\mathcal{D}_2 \setminus \mathcal{D}_1)_x = (\mathcal{D}_2)_x \setminus (\mathcal{D}_1)_x \). In addition, for any set \( \mathcal{D} \subset \mathbb{R}^k \) and \( x \in \mathbb{R}^k \), we denote by \( \mathcal{D} - x \) the set \( \{ y-x : y \in \mathcal{D} \} \). The expectation \( \int f(x)\mu(dx) \) for a measurable function \( f \) with respect to some random vector \( \mathbf{X} \) with distribution \( \mu \) is written as \( \int_{\mathbb{R}^k} f d\mu \) whenever the running variables are obvious. We also use the product notation in the integration to specify the running variables such as \( \int f(x_2)\mu(dx_1 \times dx_2) \).

**Lemma 2.** Let \( \mathbf{X} \) and \( \mathbf{Y} \) be \( k_1 \)-dimensional and \( k_2 \)-dimensional random vectors, respectively. Assume that \( h : \mathbb{R}^{k_1} \times \mathbb{R}^{k_2} \rightarrow [0, 1] \) is a transition kernel such that for each \( \mathcal{D} \in \mathbb{R}^{k_2} \), \( h(\mathbf{X}, \mathcal{D}) \) is a version of \( \mathbb{P}(\mathbf{Y} \in \mathcal{D} \mid \mathbf{X}) \). Then it holds that

1) For each \( \mathcal{D} \in \mathbb{R}^{k_1+k_2} \) and \( x \in \mathbb{R}^{k_1} \), \( \mathcal{D}_x \in \mathbb{R}^{k_2} \).

2) For each \( \mathcal{D} \in \mathbb{R}^{k_1+k_2} \), \( h(\cdot, \mathcal{D}) \) is \( \mathbb{R}^{k_1} \)-measurable.

3) For each \( \mathcal{D} \in \mathbb{R}^{k_1+k_2} \), \( \mathbb{P}( (\mathbf{X}^T, \mathbf{Y}^T) \in \mathcal{D} ) = \int_{\mathbb{R}^{k_1}} \mu_X(dx)h(x, \mathcal{D}_x) \).

**Proof.** We begin with showing part 1). Let \( L \) be the collection of sets in \( \mathbb{R}^{k_1+k_2} \) satisfying the required conditions; that is, for each \( \mathcal{D} \in L \), it holds that for each \( x \in \mathbb{R}^{k_1} \), \( \mathcal{D}_x \in \mathbb{R}^{k_2} \). Then it is easy to verify that \( L \) contains all the rectangles of form \( A \times B \), where \( A \in \mathbb{R}^{k_1} \) and \( B \in \mathbb{R}^{k_2} \). By the basic set operations, it holds that for each \( x \in \mathbb{R}^{k_1} \) and \( E, E_i \in \mathbb{R}^{k_1+k_2} \),

- a) \( (E_x)^c = (\{ y : (x, y) \in E \})^c = \{ y : (x, y) \in E^c \} = (E^c)_x \);
b) $\cup_i(E_i)_x = \cap_i((E_i)_x)^c = \cap_i(E_i^c)_x = (\cap_i E_i^c)_x = (\cup_i E_i)_x$.

Thus, for $E, E_1 \in L$, we have that $E^c, \cup_i E_i \in L$. This shows that $L$ is a $\sigma$-algebra. Since $L$ contains all the rectangles, we obtain the conclusion in part 1) of Lemma 2.

We next proceed to establish part 2). Since $D_x$ is a measurable set, $h(x, D_x)$ is a well-defined function of $x$. Let $L$ be the collection of sets such that for each $D \in L$, $h(\cdot, D)$ is $\mathcal{R}^{k_1}$-measurable. Since for each $A \in \mathcal{R}^{k_1}$ and $B \in \mathcal{R}^{k_2}$, it holds that

$$h(x, (A \times B)_x) = h(x, B) 1_{\{x \in A\}},$$

which is a measurable function of $x$, we can see that $L$ contains all such rectangles. Moreover, if $D_1, D_2 \in L$ with $D_1 \subset D_2$, then it follows that for each $x$, $(D_1)_x \subset (D_2)_x$ and $(D_2 \setminus D_1)_x = (D_2)_x \setminus (D_1)_x$, and hence

$$h(x, (D_2 \setminus D_1)_x) = h(x, (D_2)_x) - h(x, (D_1)_x).$$

Observe that the RHS of the equality above is measurable since the subtraction of measurable functions is still measurable. Next, if $D_1 \in L$ and $D_1 \subset D_{i+1}$, by the continuity of measure, we have that for each $x \in \mathbb{R}^{k_1}$, $\lim_{i \to \infty} h(x, (\cup_{i=1}^\infty D_i)_x) = h(x, (\cup_{i=1}^\infty D_i)_x)$. Thus, $h(x, (\cup_{i=1}^\infty D_i)_x)$ is a measurable function of $x$, and we have $\cup_{i=1}^\infty D_i \in L$. This shows that $L$ is a $\lambda$-system containing the set of all the rectangles. Hence, by Lemma 8 in Section B.12, we see that $L$ contains the $\sigma$-algebra generated by the set, which concludes the proof for part 2) of Lemma 2.

Finally, let us show part 3). Note that the RHS of the assertion is well-defined due to part 2) of Lemma 2. By the definition of the conditional expectation, the change of variables formula, and the fact that for each $x \in \mathbb{R}^{k_1}$, $A \in \mathcal{R}^{k_1}$, $B \in \mathcal{R}^{k_2}$,

$$1_{\{x \in A\}} h(x, B) = h(x, (A \times B)_x),$$

we can deduce that

$$\mathbb{P}((X^T, Y^T) \in A \times B) = \int_\Omega 1_{\{X \in A\}} \mathbb{P}(Y \in B \mid X) d\mathbb{P}$$

$$= \int_\Omega 1_{\{X \in A\}} h(X, B) d\mathbb{P}$$

$$= \int_{\mathbb{R}^{k_1}} \mu_X(dx) 1_{\{x \in A\}} h(x, B)$$

$$= \int_{\mathbb{R}^{k_1}} \mu_X(dx) h(x, (A \times B)_x),$$

where $\Omega$ represents the underlying probability space.

Denote by $L$ the collection of sets in $\mathcal{R}^{k_1+k_2}$ satisfying the required condition; that is, for each $D \in L$, it holds that $\mathbb{P}((X^T, Y^T) \in D) = \int_{\mathbb{R}^{k_1}} \mu_X(dx) h(x, (D)_x)$. In view of (A.89), $L$ contains all the rectangles in $\mathbb{R}^{k_1+k_2}$. In addition, we will make use of the following two facts.
a) If \( \mathcal{D}_1, \mathcal{D}_2 \in L \) and \( \mathcal{D}_1 \subset \mathcal{D}_2 \), then an application of similar arguments to those in the proof for part 2) of Lemma 2 leads to

\[
\mathbb{P}( (X^T, Y^T) \in \mathcal{D}_2 \setminus \mathcal{D}_1 ) = \mathbb{P}( (X^T, Y^T) \in \mathcal{D}_2 ) - \mathbb{P}( (X^T, Y^T) \in \mathcal{D}_1 ) \\
= \int_{\mathbb{R}^k} \mu_X(dx) \left( h(x, (\mathcal{D}_2)_x) - h(x, (\mathcal{D}_1)_x) \right) \\
= \int_{\mathbb{R}^k} \mu_X(dx) h(x, (\mathcal{D}_2)_x) \setminus (\mathcal{D}_1)_x) \\
= \int_{\mathbb{R}^k} \mu_X(dx) h(x, (\mathcal{D}_2 \setminus \mathcal{D}_1)_x),
\]

which shows that \( \mathcal{D}_2 \setminus \mathcal{D}_1 \in L \).

b) Assume that \( \mathcal{D}_i \in L \) for each \( n \) and \( \mathcal{D}_i \subset \mathcal{D}_{i+1} \). Then it follows from the continuity of measure, the definition of \( L \), and the monotone convergence theorem that

\[
\mathbb{P}( (X^T, Y^T) \in \bigcup_{i=1}^{\infty} \mathcal{D}_i ) = \lim_{n \to \infty} \mathbb{P}( (X^T, Y^T) \in \mathcal{D}_n ) \\
= \lim_{n \to \infty} \int_{\mathbb{R}^k} \mu_X(dx) h(x, (\mathcal{D}_n)_x) \\
= \int_{\mathbb{R}^k} \mu_X(dx) \lim_{n \to \infty} h(x, (\mathcal{D}_n)_x) \\
= \int_{\mathbb{R}^k} \mu_X(dx) h(x, (\bigcup_{i=1}^{\infty} \mathcal{D}_i)_x),
\]

which shows that \( \bigcup_{i=1}^{\infty} \mathcal{D}_i \in L \).

Therefore, using the aforementioned facts, an application of Lemma 8 leads to the conclusion in part 3) of Lemma 2. This completes the proof of of Lemma 2.

**B.5 Lemma 3 and its proof**

**Lemma 3.** Let \( X_1, X_2, \) and \( X_3 \) be \( k_1 \)-dimensional, \( k_2 \)-dimensional, and \( k_3 \)-dimensional random vectors, respectively, such that for each \( \mathcal{D} \in \mathcal{R}^{k_3} \),

\[
\mathbb{P}(X_3 \in \mathcal{D} \mid X_2) = \mathbb{P}(X_3 \in \mathcal{D} \mid X_2, X_1).
\]

We define a transition kernel \( h : \mathcal{R}^{k_2} \times \mathcal{R}^{k_3} \rightarrow [0, 1] \) such that for each \( \mathcal{D} \in \mathcal{R}^{k_3} \), \( h(X_2, \mathcal{D}) \) is a version of \( \mathbb{P}(X_3 \in \mathcal{D} \mid X_2) \). Then it holds that

1) For each \( \mathcal{D} \in \mathcal{R}^{k_1}, h(X_2, \mathcal{D}) \) is a version of \( \mathbb{P}(X_3 \in \mathcal{D} \mid X_2, X_1) \).

2) For each \( \mathcal{D} \in \mathcal{R}^{k_1+k_2+k_3}, h(X_2, \mathcal{D}(X_1, X_2)) \) is a version of \( \mathbb{P}((X_1, X_2, X_3) \in \mathcal{D} \mid X_2, X_1) \).

**Proof.** We first show part 1). Since \( h(X_2, \mathcal{D}) \) is a version of \( \mathbb{P}(X_3 \in \mathcal{D} \mid X_2) \), \( h(X_2, \mathcal{D}) \) is \( \sigma(X_2) \)-measurable, and hence \( \sigma(X_1, X_2) \)-measurable. In conjunction with (A.90) and the definition of conditional expectation, we see that \( h(X_2, \mathcal{D}) \) a version of \( \mathbb{P}(X_3 \in \mathcal{D} \mid X_2, X_1) \). This yields the conclusion in part 1) of Lemma 3. We then establish part 2). Let us first
verify that \( h(X_2, D_{X_1}, x_2) \) is \( \sigma(X_1, X_2) \)-measurable for each \( D \in \mathcal{R}^{k_1+k_2+k_3} \). We start with an observation that for each \( D_1 \in \mathcal{R}^{k_1}, D_2 \in \mathcal{R}^{k_2}, D_3 \in \mathcal{R}^{k_3}, \) it holds that

\[
h(X_2, (D_1 \times D_2 \times D_3) x_1, x_2) = h(X_2, D_3) 1_{\{x_1 \in D_1\}} 1_{\{x_2 \in D_2\}},
\]

which is \( \sigma(X_1, X_2) \)-measurable. This shows that for each Borel rectangle \( D \), \( h(X_2, D_{X_1}, x_2) \) is \( \sigma(X_1, X_2) \)-measurable. In conjunction with similar arguments to those in the proof of Lemma 2 in Section B.4, the desired result follows.

Let \( D \in \mathcal{R}^{k_1+k_2+k_3} \) be given. Then we will show that for each \( B \in \mathcal{R}^{k_1+k_2} \),

\[
\int h(X_2, D_{X_1}, x_2) 1_{\{(x_1, x_2) \in B\}} d\mathbb{P} = \int \mathbb{P}((X_1, X_2, X_3) \in D \mid X_2, X_1) 1_{\{(x_1, x_2) \in B\}} d\mathbb{P}. \tag{A.91}
\]

The left-hand side of (A.91) is well-defined since \( h(X_2, D_{X_1}, x_2) \) is measurable. To show (A.91), we again apply similar arguments to those in the proof of Lemma 2. Specifically, let \( L \) be the collection of sets in \( \mathcal{R}^{k_1+k_2+k_3} \) such that (A.91) holds. Since for each \( D_1 \in \mathcal{R}^{k_1}, D_2 \in \mathcal{R}^{k_2}, D_3 \in \mathcal{R}^{k_3}, \) we have

\[
\mathbb{P}((X_1, X_2, X_3) \in (D_1 \times D_2 \times D_3) \mid X_2, X_1) = \mathbb{P}(X_3 \in D_3 \mid X_2, X_1) 1_{\{x_1 \in D_1\}} 1_{\{x_2 \in D_2\}} = h(X_2, D_3) 1_{\{x_1 \in D_1\}} 1_{\{x_2 \in D_2\}} = h(X_2, (D_1 \times D_2 \times D_3) x_1, x_2),
\]

it holds that \( L \) contains all Borel rectangles \( D \in \mathcal{R}^{k_1+k_2+k_3} \). The remaining arguments follow those in the proof of Lemma 2. Finally, since \( h(X_2, D_{X_1}, x_2) \) is \( \sigma(X_1, X_2) \)-measurable, by (A.91) and the definition of conditional expectation, we can obtain the conclusion in part 2) of Lemma 3. This concludes the proof of Lemma 3.

**B.6 Lemma 4 and its proof**

**Lemma 4.** Let \( \{U_i\} \) and \( \{V_i\} \) be sequences of \( k_1 \)-dimensional and \( k_2 \)-dimensional random vectors, respectively. Assume that \( \{U_i, V_i\} \)'s are identically distributed. Then there exists a transition kernel \( g : \mathbb{R}^{k_1} \times \mathbb{R}^{k_2} \to [0, 1] \) such that for each \( i \) and \( D \in \mathcal{R}^{k_2}, \) \( g(U_i, D) \) is a version of \( \mathbb{P}(V_i \in D \mid U_i) \).

**Proof.** For each \( \{U_i, V_i\} \), there exists a transition kernel \( g_i : \mathbb{R}^{k_1} \times \mathbb{R}^{k_2} \to [0, 1] \) such that for each \( D \in \mathcal{R}^{k_2}, \) \( g_i(U_i, D) \) is a version of \( \mathbb{P}(V_i \in D \mid U_i) \); see, for example, Theorem 4.1.18 of [16]. By this and the fact that \( \mu U_i = \mu U_1 \) for each \( i \), we have that for each \( A \in \mathcal{R}^{k_1} \) and
\[ B \in \mathcal{R}^{k_2}, \]

\[
\mathbb{P}((U_i, V_i) \in \mathcal{A} \times \mathcal{B}) = \int_{\Omega} 1_{\{U_i \in \mathcal{A}\}} \mathbb{P}(V_i \in \mathcal{B} | U_i) d\mathbb{P} \\
= \int_{\Omega} 1_{\{U_i \in \mathcal{A}\}} g_i(U_i, \mathcal{B}) d\mathbb{P} \\
= \int_{\mathbb{R}^{k_1}} \mu_{U_i}(dx) 1_{\{x \in \mathcal{A}\}} g_i(x, \mathcal{B}) \\
= \int_{\mathbb{R}^{k_1}} \mu_{U_i}(dx) 1_{\{x \in \mathcal{A}\}} g_i(x, \mathcal{B}) \\
= \int_{\mathbb{R}^{k_1}} \mu_{U_i}(dx) 1_{\{x \in \mathcal{A}\}} g_i(x, \mathcal{B}) \\
= \int_{\Omega} 1_{\{U_i \in \mathcal{A}\}} g_i(U_i, \mathcal{B}) d\mathbb{P},
\]

where \( \Omega \) represents the underlying probability space, the third and last equalities above follow from the change of variables formula, and the fourth and fifth equalities above are due to the assumption of identical distributions. Therefore, it follows from (A.92) and the definition of conditional expectation that \( g_1(U_i, D) \) is a version of \( \mathbb{P}(V_i \in D | U_i) \) for each \( i \) and \( D \in \mathcal{R}^{k_2} \). This completes the proof of Lemma 4.

**B.7 Lemma 5 and its proof**

Intuitively, Lemma 5 below extracts the total variation distance from a difference of two integrals. The results are natural but the arguments are somewhat delicate. We note that if the density functions \( f_X \) and \( f_Y \) exist, then it holds that

\[
\sup_{D \in \mathbb{R}^{K}} \left| \int_{D} f_X(z)dz - \int_{D} f_Y(z)dz \right| = \sup_{D \in \mathbb{R}^{K}} \int_{D} |f_X(z) - f_Y(z)|dz \\
= \frac{1}{2} \| \mu_X - \mu_Y \|_{TV}.
\]

However, the same calculation does not apply directly to distributions because the integral \( \int |\mu_X(dz) - \mu_Y(dz)| \) is not well-defined due to the two \( dz \)'s inside the integration. Lemma 5 provides valid arguments in such situations.

**Lemma 5.** 1) Let \( \mu \) and \( \nu \) be two probability measures and \( f : \mathbb{R}^{K} \rightarrow \mathbb{R} \) a measurable function with \( 0 \leq f \leq 1 \). Then it holds that

\[
\sup_{D \in \mathbb{R}^{K}} \left| \int_{D} f(x)\mu(dx) - \int_{D} f(x)\nu(dx) \right| \leq \frac{1}{2} \| \mu - \nu \|_{TV}.
\]

2) Let \( p(\cdot, \cdot) : \mathbb{R}^{K_1} \times \mathbb{R}^{K_2} \rightarrow [0, 1] \) be a transition kernel and \( \mu \) a probability measure on \( \mathbb{R}^{K_2} \) such that for each \( x \in \mathbb{R}^{K_1} \), \( p(x, \cdot) \) is dominated by \( \mu \). Further let \( \nu \) be a probability
measure on $\mathbb{R}^{K_1}$ and $0 \leq f \leq 1$ a measurable function on $\mathbb{R}^{K_2}$. Then it holds that

$$\sup_{D \in \mathbb{R}^{K_1+K_2}} \left| \int_D \nu(dx_1)p(x_1, dx_2)f(x_2) - \int_D \nu(dx_1)\mu(dx_2)f(x_2) \right| \leq \frac{1}{2} \int_{\mathbb{R}^{K_1}} \nu(dx_1)\|p(x_1, \cdot) - \mu(\cdot)\|_{TV}.$$  \hfill (A.93)

**Proof.** We start with proving the first assertion. By the definition of the total variation distance, we can show that there exists some set $A \in \mathbb{R}^{K}$ such that

$$\int_{A} \mu(dx) - \int_{A} \nu(dx) = \frac{1}{2}\|\mu - \nu\|_{TV}.$$  

Further it holds that for each $B \in \mathbb{R}^{K}$ with $B \subset A$,

$$\int_{B} \mu(dx) - \int_{B} \nu(dx) \geq 0.$$  

Let us define $D_j := A \cap \left\{ x : \frac{j-1}{M} \leq f(x) < \frac{j}{M} \right\}$ for $j = 1, \ldots, M + 1$ with $M$ some positive integer. Denote by $\bar{f}$ a step function such that on $D_j$, it holds that $\bar{f} = \frac{j}{M}$. Then we can deduce that

$$\left| \int_{\cup_j D_j} f(x)\mu(dx) - \int_{\cup_j D_j} f(x)\nu(dx) - \left( \int_{\cup_j D_j} \bar{f}(x)\mu(dx) - \int_{\cup_j D_j} \bar{f}(x)\nu(dx) \right) \right| \leq \int_{\cup_j D_j} |f(x) - \bar{f}(x)|\mu(dx) + \int_{\cup_j D_j} |f(x) - \bar{f}(x)|\nu(dx) \leq \frac{1}{M} \left( \int_{\cup_j D_j} \mu(dx) + \int_{\cup_j D_j} \nu(dx) \right) \leq \frac{2}{M}.$$  \hfill (A.94)

In light of the construction of $D_j$’s and $\bar{f}$ above, we have that

$$\int_{\cup_j D_j} \bar{f}(x)\mu(dx) - \int_{\cup_j D_j} \bar{f}(x)\nu(dx) = \sum_j \int_{D_j} \bar{f}(x)\mu(dx) - \int_{D_j} \bar{f}(x)\nu(dx) = \sum_j \frac{j}{M} \left( \int_{D_j} \mu(dx) - \int_{D_j} \nu(dx) \right) \leq \sum_j \left( \int_{D_j} \mu(dx) - \int_{D_j} \nu(dx) \right) = \frac{1}{2}\|\mu - \nu\|_{TV}.$$  \hfill (A.95)

Then it follows from $A = \cup_j D_j$, (A.94), (A.95), and the fact that the positive integer $M$ can be arbitrarily large that

$$\left| \int_{A} f(x)\mu(dx) - \int_{A} f(x)\nu(dx) \right| \leq \frac{1}{2}\|\mu - \nu\|_{TV}. \hfill (A.96)$$
Using similar arguments as above, we can show that
\[
\sup_{D \in \mathbb{R}^K} \left| \int_{D} f(x) \mu(dx) - \int_{D} f(x) \nu(dx) \right| = \left| \int_{A} f(x) \mu(dx) - \int_{A} f(x) \nu(dx) \right|.
\] (A.97)

Therefore, combining (A.96) and (A.97) results in the desired conclusion in part 1) of Lemma 5.

We now proceed with showing the second assertion. Since \( \|p(x_1, \cdot) - \mu(\cdot)\|_{TV} \) is a measurable function in \( x_1 \), the RHS of (A.93) is well defined. Such claim can be established using similar arguments to those in Theorem 5.2.2 of Durrett [16]; for simplicity, we omit the details. By the assumptions, let \( f_1(x_1, x_2) \) be the Radon–Nikodym derivative such that for each \( x_1 \in \mathbb{R}^{K_1} \) and \( D \in \mathbb{R}^{K_2} \),
\[
\int_{D} p(x_1, dx_2) = \int_{D} f_1(x_1, x_2) \mu(dx_2).
\]

If \( \mu \) is the Lebesgue measure and for each \( D \in \mathbb{R}^{K_2} \), \( p(X, D) \) is a version of \( \mathbb{P}(Y \in D|X) \) for some random mappings \( Y \) and \( X \) dominated by the Lebesgue measure, such a Radon–Nikodym derivative is usually referred to as the conditional (on the density function of \( X \)) probability density function; for this, see also Example 4.1.6 in [16]. Thus, for each \( D \in \mathbb{R}^{K_1+K_2} \), we have that
\[
\left| \int_{D} \nu(dx_1)p(x_1, dx_2)f(x_2) - \int_{D} \nu(dx_1)\mu(dx_2)f(x_2) \right| = \left| \int_{D} \nu(dx_1)(f_1(x_1, x_2) - 1)\mu(dx_2)f(x_2) \right|.
\] (A.98)

Next let us define \( D^* \) as
\[
D^* := \arg \sup_{D \in \mathbb{R}^{K_1+K_2}} \int_{D} \nu(dx_1)(f_1(x_1, x_2) - 1)\mu(dx_2)f(x_2)
\] (A.99)
such that for each \( A \subset D^* \), the integration of (A.99) over \( A \) is nonnegative. Then by (A.98), (A.99), and the assumption of \( 0 \leq f \leq 1 \), it holds that
\[
\sup_{D \in \mathbb{R}^{K_1+K_2}} \left| \int_{D} \nu(dx_1)p(x_1, dx_2)f(x_2) - \int_{D} \nu(dx_1)\mu(dx_2)f(x_2) \right| \leq \int_{D^*} \nu(dx_1)(f_1(x_1, x_2) - 1)\mu(dx_2).
\] (A.100)

Thus, it follows from the definition of \( f_1 \), Lemma 2, and the definition of the total variation norm that
\[
\int_{D^*} \nu(dx_1)(f_1(x_1, x_2) - 1)\mu(dx_2)
\]
\[
= \int_{\mathbb{R}^{K_1}} \nu(dx_1)(p(x_1, (D^*)_{x_1}) - \mu((D^*)_{x_1}))
\] (A.101)
\[
\leq \int_{\mathbb{R}^{K_1}} \nu(dx_1) \frac{1}{2} \|p(x_1, \cdot) - \mu(\cdot)\|_{TV}.
\]
Since \((Y_i^T, X_i^T)\) and \((V_i^T, U_i^T)\) with \(i \geq 1\) are identically distributed, by Lemma 4 in Section B.6, there exists a transition kernel \(h_1 : \mathbb{R}^{Kk_1} \times \mathbb{R}^{Kk_2} \rightarrow [0, 1]\) such that for each \(i\) and \(D \in \mathbb{R}^{k_2}\), \(h_1(Y_i, D)\) and \(h_1(V_i, D)\) are versions of \(\mathbb{P}(X_i \in D \mid Y_i)\) and \(\mathbb{P}(U_i \in D \mid V_i)\), respectively.

Let us define \(h_2 : \mathbb{R}^{Kk_1} \times \mathbb{R}^{Kk_2} \rightarrow [0, 1]\) such that for each \(x = (x_1^T, \cdots, x_K^T) \in \mathbb{R}^{Kk_1}\), \(h_2(x, \cdot)\) is a probability measure such that for each \(D_i \in \mathbb{R}^{k_2}\) with \(i = 1, \cdots, K\),

\[
h_2(x, \bigotimes_{i=1}^K D_i) = \prod_{i=1}^K h_1(x, D_i). \tag{A.104}
\]

We make a useful claim below.
Claim 1. \( h_2 \) is a transition kernel satisfying (A.104).

The proof of Claim 1 is provided in Section B.10. Then it follows from (A.102), (A.103), and Claim 1 above that for each \( B_i \in \mathcal{R}^{k_2} \) with \( i = 1, \cdots, K \),

\[
\mathbb{P}((Y^T, X^T) \in A \times (\bigtimes_{i=1}^{K} B_i)) = \mathbb{E} \left[ 1_{\{Y \in A\}} \prod_{i=1}^{K} \mathbb{P} \left( X_i \in B_i \mid Y_i \right) \right] \\
= \mathbb{E} \left[ 1_{\{Y \in A\}} \prod_{i=1}^{K} h_1(Y_i, B_i) \right] \\
= \mathbb{E} \left[ 1_{\{Y \in A\}} h_2(Y, \bigtimes_{i=1}^{K} B_i) \right],
\]

and similarly,

\[
\mathbb{P}((V^T, U^T) \in A \times (\bigtimes_{i=1}^{K} B_i)) = \mathbb{E} \left[ 1_{\{V \in A\}} h_2(V, \bigtimes_{i=1}^{K} B_i) \right].
\]

By the construction of \( h_2 \), (A.105), (A.106), and Lemma 8 in Section B.12, it holds that for each \( A \in \mathcal{R}^{Kk_1} \) and \( B \in \mathcal{R}^{Kk_2} \),

\[
\mathbb{P}((Y^T, X^T) \in A \times B)) = \mathbb{E} \left[ 1_{\{Y \in A\}} h_2(Y, B) \right],
\]

\[
\mathbb{P}((V^T, U^T) \in A \times B)) = \mathbb{E} \left[ 1_{\{V \in A\}} h_2(V, B) \right].
\]

Since \( h_2 \) is a transition kernel, we see that for each \( B \in \mathcal{R}^{Kk_2} \), \( h_2(Y, B) \) is \( \sigma(Y) \)-measurable. Thus, in view of (A.107) we have that for each \( B \in \mathcal{R}^{Kk_2} \), \( h_2(Y, B) \) is a version of \( \mathbb{P}(X \in B \mid Y) \). A similar result for \( V \) and \( U \) can also be obtained, which leads to the first assertion.

Finally, by Lemma 2 and Lemma 5 in Sections B.4 and B.7, respectively, we can deduce that for each \( D \in \mathcal{R}^{K(k_1+k_2)} \),

\[
\left| \mathbb{P}((Y^T, X^T) \in D) - \mathbb{P}((V^T, U^T) \in D) \right| \\
= \left| \int_{\mathcal{R}^{Kk_1}} h_2(x, D)\mu_Y(dx) - \int_{\mathcal{R}^{Kk_1}} h_2(x, D)\mu_V(dx) \right| \\
\leq \frac{1}{2} \|\mu_Y - \mu_V\|_{TV},
\]

which yields the second assertion. This completes the proof of Lemma 6.

B.9 Lemma 7 and its proof

Let \( \widetilde{U} \) and \( \widetilde{V} \) be the knockoffs counterparts of \( r \times c \) design matrices \( U \) and \( V \), respectively. The corresponding response vectors are denoted as \( u \) and \( v \), respectively. Lemma 7 below ensures that the knockoffs matrix construction does not cause additional variation in distribution in terms of the total variation distance.

Lemma 7. Assume that 1) the rows of \((U, \widetilde{U})\) and \((V, \widetilde{V})\) are identically distributed, 2) the row vectors of \( \widetilde{U} \) are independent random vectors conditional on \( U \), 3) the \( i \)th row of \( \widetilde{U} \) is
independent of the other rows of \( U \) conditional on the \( i \)th row of \( U \), and 4) \( u \) is independent of \( \tilde{U} \) conditional on \( U \). In addition, we assume the same for \((v, V, \tilde{V})\). Then it holds that

\[
\sup_{\mathcal{D} \in \mathcal{R}^{r(1+2c)}} \left| P((u, U, \tilde{U}) \in \mathcal{D}) - P((v, V, \tilde{V}) \in \mathcal{D}) \right| \leq \frac{1}{2} \|\mu_u, U - \mu_v, V\|_{TV}
\]

and

\[
\sup_{\mathcal{D} \in \mathcal{R}^{rc}} \left| P((U, \tilde{U}) \in \mathcal{D}) - P((V, \tilde{V}) \in \mathcal{D}) \right| \leq \frac{1}{2} \|\mu_U - \mu_V\|_{TV}.
\]

**Proof.** We start with showing the first assertion. Denote the \( i \)th rows of \( \tilde{U} \) and \( U \) by \( \tilde{U}_{i*} \) and \( U_{i*} \), respectively. Then for each \( \mathcal{D}_i \in \mathcal{R}^r \), we have that

\[
P(\cap_{i=1}^c \{ \tilde{U}_{i*} \in \mathcal{D}_i \}| \mathcal{U}) = \Pi_{i=1}^c P(\tilde{U}_{i*} \in \mathcal{D}_i| \mathcal{U})
\]

\[
= \Pi_{i=1}^c P(\tilde{U}_{i*} \in \mathcal{D}_i| U_{i*}),
\]

where the first equality follows from assumption 2) and the second one is due to assumption 3). By this, an application of Lemma 6 shows that there exists a transition kernel \( h : \mathcal{R}^{rc} \times \mathcal{R}^{rc} \rightarrow [0,1] \) such that for each \( \mathcal{D} \in \mathcal{R}^{rc} \), \( h(U, \mathcal{D}) \) and \( h(V, \mathcal{D}) \) are versions of \( P(\tilde{U} \in \mathcal{D} | U) \) and \( P(\tilde{V} \in \mathcal{D} | V) \), respectively.

We will make use of the claim below.

**Claim 2.** For each \( \mathcal{D} \in \mathcal{R}^{r(1+2c)} \), it holds that

\[
P((u, U, \tilde{U}) \in \mathcal{D}) = \int_{\mathcal{R}^{r(1+c)}} h(x_2, D_{x_1,x_2}) \mu_{u,U}(dx_1 \times dx_2),
\]

\[
P((v, V, \tilde{V}) \in \mathcal{D}) = \int_{\mathcal{R}^{r(1+c)}} h(x_2, D_{x_1,x_2}) \mu_{v,V}(dx_1 \times dx_2),
\]

where \( x_1 \) and \( x_2 \) denote \( r \)-dimensional and \( (rc) \)-dimensional vectors, respectively.

The proof of Claim 2 is presented in Section B.11. Then it follows from Claim 2 above, Lemma 5, and the fact of \( 0 \leq h \leq 1 \) that for each \( \mathcal{D} \in \mathcal{R}^{r(1+2c)} \),

\[
\left| P((u, U, \tilde{U}) \in \mathcal{D}) - P((v, V, \tilde{V}) \in \mathcal{D}) \right|
\]

\[
= \left| \int_{\mathcal{R}^{r(1+c)}} h(x_2, D_{x_1,x_2}) \mu_{u,U}(dx_1 \times dx_2) - \int_{\mathcal{R}^{r(1+c)}} h(x_2, D_{x_1,x_2}) \mu_{v,V}(dx_1 \times dx_2) \right|
\]

\[
\leq \frac{1}{2} \|\mu_u, U - \mu_v, V\|_{TV},
\]

which leads to the conclusion in the first assertion. Using similar arguments as above, we can establish the second assertion. This concludes the proof of Lemma 7.

**B.10 Proof of Claim 1**

Note that given \( x \), the existence of the probability measure \( h_2(x, \cdot) \) is guaranteed by an application of Theorem 1.7.1 in [16]. Let \( L \) be the collection of sets such that if \( \mathcal{D} \in L \), \( h_2(x, \mathcal{D}) \) is a measurable function of \( x \). We will make three observations due to the definition
of $h_2$. (i) $L$ contains all Borel rectangles since the product of measurable functions is still a measurable function. (ii) For $D_1, D_2 \in L$ with $D_1 \subset D_2$, it holds that $h_2(\cdot, D_2 \setminus D_1)$ is measurable and hence $D_2 \setminus D_1 \in L$. (iii) For $D_i \subset D_{i+1}, D_i \in L$, and $D := \bigcup_{i=1}^{\infty} D_i$, we have

$$h_2(\cdot, D) = \sup_i h_2(\cdot, D_i)$$

which is measurable, and thus $D \in L$. Therefore, it follows from these facts and Lemma 8 in Section B.12 that for each $D \in \mathcal{R}^{K_k^2}$, $h_2(\cdot, D)$ is measurable. This completes the proof of Claim 1.

**B.11 Proof of Claim 2**

Let us first show the first assertion. For each Borel rectangle $A_1 \times A_2 \times A_3 \in \mathcal{R}^r \times \mathcal{R}^{rc} \times \mathcal{R}^{rc}$, it holds that

$$\mathbb{P}((u, U, \tilde{U}) \in A_1 \times A_2 \times A_3) = \mathbb{E} \left[ 1_{ \{(u,U) \in A_1 \times A_2\} } \mathbb{P}(\tilde{U} \in A_3 \mid u, U) \right]$$

$$= \mathbb{E} \left[ 1_{ \{(u,U) \in A_1 \times A_2\} } \mathbb{P}(\tilde{U} \in A_3 \mid U) \right]$$

$$= \int_{\mathbb{R}^r(1+c)} h(x_2, (A_1 \times A_2 \times A_3)_{x_1,x_2}) \mu_{u,U}(dx_1 \times dx_2),$$

where the second equality is due to the assumption of Lemma 7 and the last equality is because of the definition of $h$. Let $L$ be a collection of sets in $\mathcal{R}^{r(1+2c)}$ such that if $D \in L$,

$$\mathbb{P}((u, U, \tilde{U}) \in D) = \int_{\mathbb{R}^r(1+c)} h(x_2, D_{x_1,x_2}) \mu_{u,U}(dx_1 \times dx_2).$$

Then we can see that $L$ contains all Borel rectangles which collection is a $\pi$-system.

Let us make a few observations below.

1) The set $L$ contains $\mathbb{R}^{r(1+2c)}$.

2) If $D_1, D_2 \in L$ and $D_1 \subset D_2$, then some basic measure and integration operations as well as the operation of $D_2$ give that

$$\mathbb{P}((u, U, \tilde{U}) \in D_2 \setminus D_1) = \mathbb{P}((u, U, \tilde{U}) \in D_2) - \mathbb{P}((u, U, \tilde{U}) \in D_1)$$

$$= \int_{\mathbb{R}^r(1+c)} \left( h(x_2, (D_2)_{x_1,x_2}) - h(x_2, (D_1)_{x_1,x_2}) \right) \mu_{u,U}(dx_1 \times dx_2)$$

$$= \int_{\mathbb{R}^r(1+c)} h(x_2, (D_2 \setminus D_1)_{x_1,x_2}) \mu_{u,U}(dx_1 \times dx_2),$$

which leads to $D_2 \setminus D_1 \in L$.

3) If $D_n \in L$ and $D_n \subset D_{n+1}$, then it follows from the continuity of measure and the
monotone convergence theorem that
\[
P((u, U, \tilde{U}) \in \cup_n \mathcal{D}_n) = \lim_n P((u, U, \tilde{U}) \in \mathcal{D}_n)
= \lim_n \int_{\mathbb{R}^{(1+c)}} h(x_2, (D_n)_{x_1,x_2}) \mu_{u,U}(dx_1 \times dx_2)
= \int_{\mathbb{R}^{(1+c)}} h(x_2, (\cup_n D_n)_{x_1,x_2}) \mu_{u,U}(dx_1 \times dx_2),
\]
which results in \( \cup_n \mathcal{D}_n \in L \).

Therefore, using the aforementioned facts, an application of Lemma 8 in Section B.12 yields the conclusion in the first assertion. The conclusion in the second assertion can be shown in a similar fashion, which concludes the proof of Claim 2.

### B.12 Lemma 8

**Definition** (\( \pi \)-system and \( \lambda \)-system). A collection of sets \( P \) is said to be a \( \pi \)-system if for any \( A, B \in P \), \( A \cap B \in P \). A collection \( L \) of sets in \( \Omega \) is said to be a \( \lambda \)-system if

1) \( \Omega \in L \);

2) If \( A \subset B \) and \( A, B \in L \), then \( B \setminus A \in L \);

3) If \( A_n \in L \) and \( A_n \subset A_{n+1} \), then \( \cup_n A_n \in L \).

**Lemma 8** (\( \pi - \lambda \) Theorem in [16]). If \( P \) is a \( \pi \)-system and \( L \) is a \( \lambda \)-system that contains \( P \), then the smallest \( \sigma \)-algebra containing \( P \) is also contained in \( L \).