Variable Selection with the Knockoffs: Composite Null Hypotheses

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Abstract

The Fixed-X knockoff filter is a flexible framework for variable selection with false discovery rate (FDR) control in linear models with arbitrary (non-singular) design matrices and it allows for finite-sample selective inference via the LASSO estimates. In this paper, we extend the theory of the knockoff procedure to tests with composite null hypotheses, which are usually more relevant to real-world problems. The main technical challenge lies in handling composite nulls in tandem with dependent features from arbitrary designs. We develop two methods for composite inference with the knockoffs, namely, shifted ordinary least-squares (S-OLS) and feature-response product perturbation (FRPP), building on new structural properties of test statistics under composite nulls. We also propose two heuristic variants of S-OLS method that outperform the celebrated Benjamini-Hochberg (BH) procedure for composite nulls, which serves as a heuristic baseline under dependent test statistics. Finally, we analyze the loss in FDR when the original knockoff procedure is naively applied on composite tests.

Keywords: Selective inference, composite hypothesis testing, FDR control, knockoff procedure, Benjamini-Hochberg procedure.

1. Introduction

Selecting variables from a large collection of potential explanatory variables that are associated with responses of interest is a fundamental problem in many fields of science including genome-wide association study (GWAS), geophysics, and economics. In this paper, we focus on the classical linear
regression model,

\[ y = X\beta + w, \quad w \sim N(0, \sigma^2 I_n), \quad (1) \]

where \( y \) and \( w \) are \( n \)-dimensional random vectors with elements denoting response and error variables, respectively, \( X = [X_1, ..., X_p] \in \mathbb{R}^{n \times p} \) denotes a fixed design matrix containing \( n \) samples of \( p \) explanatory features/variables, and \( \beta = [\beta_1, ..., \beta_p]^T \in \mathbb{R}^p \) is the vector of unknown fixed coefficients relating \( X \) and \( \mathbb{E}(y) \). For the following \( p \) hypotheses,

\[
\begin{align*}
H_{0,i} & : \beta_i = 0 \\
H_{1,i} & : \beta_i \neq 0, \quad 1 \leq i \leq p
\end{align*}
\]

the problem of interest is to test these hypotheses while controlling a simultaneous measure of type I error called the \textit{false discovery rate (FDR)}, defined by Benjamini and Hochberg (1995) as \( \text{FDR} = \mathbb{E} \left( \text{FDP} \right) \) with

\[
\text{FDP} = \frac{|\hat{R} \cap H_0|}{|\hat{R}| \lor 1}, \quad (2)
\]

where \( H_0 = \{1 \leq i \leq p : \beta_i = 0\} \) denotes the set of variables for which the null hypothesis is true and \( \hat{R} = \{i : H_{0,i} \text{ rejected}\} \) the selected variables by some variable selection procedure, and \( | \cdot | \) the cardinality of the sets. A selection rule controls the FDR at level \( q \) if its corresponding FDR is guaranteed to be at most \( q \) for some predetermined \( q \in [0, 1] \).

Recently, Barber and Candès (2015) proposed the (Fixed-X) knockoff filter procedure, a data-dependent selection rule that controls the FDR in finite sample settings and under arbitrary designs. In this procedure, a test statistic is computed for each feature through constructing a knockoff variable and a feature is selected by (data-dependent) thresholding the statistics according to the target FDR. The knockoff construction allows for correlated features and this framework has higher statistical power in comparison with the Benjamini-Hochberg (BH) procedure introduced in Benjamini and Hochberg (1995) (see Benjamini and Yekutieli (2001); Storey et al. (2004); Efron et al. (2001) for extensions and variants) in a range of settings. The knockoff filter has inspired various formulations such as the model-X knockoffs and deep learning based knockoffs among others (see Barber and Candès (2019); Candès et al. (2018); Barber et al. (2020); Romano et al. (2019); Jordon et al. (2018); Lu et al. (2018); Fan et al. (2019); Pournaderi and Xiang (2021)).
The original fixed-X knockoff filter is focused on the simple nulls ($\beta_i = 0$). However, in practice we are often interested in composite hypotheses rather than simple ones. The multiple testing of composite null hypotheses using (mutually) independent $p$-values has been studied in Benjamini and Yekutieli (2001); Sun and McLain (2012); Dickhaus (2013); Cabras (2010). Given that the knockoff selection framework deals with the dependencies between statistics inherently, a natural question is whether one can extend this to handle composite nulls, namely,

$$
\begin{align*}
    H_{0,i}^\prime & : |\beta_i| \leq \delta \\
    H_{1,i}^\prime & : |\beta_i| > \delta ,
\end{align*}
$$

for some given $\delta \geq 0$. In this paper, we provide an affirmative answer to the above question by developing two methods: shifted ordinary least-squares (S-OLS) and feature-response product perturbation (FRPP). We show that both methods achieve FDR control in finite sample settings under arbitrary designs, leveraging new structural properties for test statistics under composite nulls. The main technical difficulty is to handle composite nulls in tandem with dependent features. This is highly nontrivial and, to the best of our knowledge, the closest solution to this is the BH procedure for composite nulls but with independent test statistics (Benjamini and Yekutieli, 2001, Theorem 5.2) referred to as the composite BH in this paper. We use the composite BH as a heuristic baseline in our simulations, as the theoretical guarantees no longer hold for composite nulls with dependent test statistics. Our S-OLS method motivates two LASSO-based heuristic variants that outperform the composite BH in power. Furthermore, we quantify the loss in FDR when one uses the original fixed-X knockoff filter for composite nulls, and the result reduces to the exact FDR control for simple nulls.

The paper is organized as follows. In Section 2 we briefly present the knockoff filter framework by introducing the main steps to set the stage for our analysis. In Section 3 we present our main results and theoretical guarantees, along with two heuristic methods, with all the proofs deferred to Appendices. We report our experimental results in Section 4 for a range of composite nulls, amplitude of alternatives, and correlation coefficients.

2. Background: Fixed-X Knockoff Filter

The knockoff variable selection procedure Barber and Candès (2015) consists of two main steps: (I) computing an statistic $W_j$ for each variable in the
model, and (II) selecting $\hat{R}_{ko} = \{j : W_j \geq T(q, W)\}$, where the threshold $T \geq 0$ depends on the target FDR $q$ and the set of computed statistics, i.e., $W = \{W_1, \ldots, W_p\}$. In this section we look at this procedure in more details.

2.1. Knockoff Design

The knockoff methodology for detecting non-null variables involves creating a control (or knockoff) design that mimic the correlation structure of $X$ but break down the relationship between $X$ and $y$.

**Assumption 1.** $\Sigma = X^\top X$ is invertible.

Specifically, if $n \geq 2p$, Barber and Candès (2015) proposes the following construction to produce knockoff designs

$$\tilde{X}(s) = X(I_p - \Sigma^{-1}\text{diag}\{s\}) + \tilde{U}C,$$

(3)

where $s \in \mathbb{R}^p_+$ is a free vector of parameters as long as it satisfies $G := [X \tilde{X}]^\top [X \tilde{X}] \succeq 0$, $C$ is obtained by Cholesky decomposition of the Schur complement of $G$, and $\tilde{U}^{n \times p}$ is an orthonormal matrix that satisfies $\tilde{U}^\top X = 0$ (see Barber and Candès (2015) for details). Therefore, knockoff matrices are not unique and they are constructed according to the original design matrix. Using (3), the following relation can be easily verified.

$$G = \begin{bmatrix} \Sigma & \Sigma - \text{diag}\{s\} \\ \Sigma - \text{diag}\{s\} & \Sigma \end{bmatrix}.$$  

(4)

In fact, this construction not only preserves the correlation structure of $X$, but also has another subtle yet important geometrical implication: $X_i$ (i-th column of $X$) and $\tilde{X}_i$ are second-order “exchangable” in a deterministic sense, i.e., swapping $X_i$ and $\tilde{X}_i$ does not change the inner product structure (Gram matrix) of the augmented design. This property makes $\tilde{X}$ an appropriate tool for FDR control. It should be noted that the detection power highly depends on the parameter $s$ as it determines the angle between a feature and its corresponding knockoff. In other words, $s_i$ (i-th element of $s$) controls how different (or orthogonal) $X_i$ and $\tilde{X}_i$ would be. Assuming the columns of $X$ are normalized by the Euclidean norm, one way to choose $s$ is to solve the following convex problem,

$$\text{minimize} \quad \sum_{i=1}^p |1 - s_i|$$

subject to  

$$s_i \geq 0, \quad \text{diag}\{s\} \leq 2 \Sigma.$$  

(5)
This semi-definite programming minimizes the average correlation between variables and their corresponding knockoff variable.

**Remark 1.** Since a column-wise normalization of the design matrix is natural for variable selection purpose and essential in terms of statistical power, throughout this paper, we always assume \( X \) is normalized by \( \ell_2 \) norm of columns.

### 2.2. Statistics

Using the knockoff features, we now compute a vector of anti-symmetric statistics \( W = (W_1, W_2, \ldots, W_p)\top \) by regression over the augmented design \([X \, \tilde{X}]\). Let \( \hat{\theta}_i \) and \( \hat{\theta}'_i \) denote some estimated parameters corresponding to the variables \( X_i \) and \( \tilde{X}_i \). In this case, one can define an statistic as follows

\[
W_i = |\hat{\theta}_i| - |\hat{\theta}'_i|, \quad 1 \leq i \leq p.
\]

We can also define the statistics differently,

\[
W_i = \operatorname{sgn}(|\hat{\theta}_i| - |\hat{\theta}'_i|) \max(|\hat{\theta}_i|, |\hat{\theta}'_i|).
\]

To be more precise, the term anti-symmetric here means that swapping the estimates \( \hat{\theta}_i \) and \( \hat{\theta}'_i \) for any subset of indices \( F \subseteq \{1, 2, \ldots, p\} \) has the effect of switching the signs of \( \{W_i : i \in F\} \). Specifically, the knockoff framework guarantees the FDR control when the (anti-symmetric) statistics are computed based on estimators that depend on the data through the following form,

\[
\begin{pmatrix}
\hat{\theta}_{p \times 1} \\
\hat{\theta}'_{p \times 1}
\end{pmatrix} = \mathcal{E}(G, [X \, \tilde{X}]\top y),
\]

where \( \mathcal{E} \) is a deterministic operator and, swapping \( X_i \) and \( \tilde{X}_i \) will result in swapping \( \hat{\theta}_i \) and \( \hat{\theta}'_i \). For instance, the LASSO [Tibshirani (1996)](9) regression estimates \( \hat{\beta}_{\text{LAS}} \) given by

\[
\hat{\beta}_{\text{LAS}} := \arg\min_{b \in \mathbb{R}^{2p}} \left\{ \|y - [X \, \tilde{X}]b\|_2^2 + \lambda\|b\|_1 \right\}, \quad \lambda \geq 0,
\]

can be considered as an example of estimators satisfying (8).
2.3. FDR Control

In this subsection, we briefly discuss the existing approaches to show the FDR control in the knockoff procedure. Let \( P_F \) denote the \( 2p \times 2p \) permutation matrix corresponding to swapping \( X_i \) and \( \tilde{X}_i \) for all \( i \in F \), then by the structure of knockoff matrix we have,

\[
P_F^\top G P_F = G, \quad F \subseteq \{1, \ldots, p\}.
\]

(10)

Also, according to (1) we get

\[
P_F^\top [X \tilde{X}]^\top y \overset{d}{=} [X \tilde{X}]^\top y, \quad F \subseteq H_0.
\]

(11)

The identities (10) and (11) immediately imply an interesting property of the estimates \( \hat{\theta} \) and \( \hat{\theta}' \): the estimated parameters for null variables and their corresponding knockoff variables are exchangeable. This property along with the anti-symmetric structure of the statistics are the main ingredients of the FDR control proof in the original paper. In fact, under the simple null hypotheses, these properties lead to the so-called i.i.d. sign property of the nulls, i.e., the signs of null statistics (signs of \( W_0 = \{W_j : \beta_j = 0\} \)) are independent of the magnitudes and have i.i.d. Rademacher distribution (i.e., \( \mathbb{P}(+1) = \mathbb{P}(-1) = 1/2 \)). In this case, using the martingale theory, it is shown that rejecting \( \{j : W_j \geq T\} \) with the following threshold \( T \) controls the FDR at level \( q \),

\[
T = \inf \left\{ t \in \Phi : \hat{\text{FDP}}(t) \leq q \right\},
\]

(12)

\[
\hat{\text{FDP}}(t) := \frac{1 + \#\{j : W_j \leq -t\}}{\#\{j : W_j \geq t\} \lor 1},
\]

(13)

where \( \Phi = \{\{|W_i| : i = 1, 2, \ldots, p\} \setminus \{0\} \). Although this approach is elegant, we shall not follow it in development of composite tests as in this situation (11) fails to hold immediately. On the other hand, Barber et al. (2020) provides another proof for FDR control which requires weaker conditions on the statistics (Barber et al., 2020, equation (16)). Specifically, it suggests that if the null statistics (\( j \in H_0 \)) satisfy

\[
\mathbb{P}\left\{W_j > 0 \mid |W_j|, W_{-j}\right\} \leq C \cdot \mathbb{P}\left\{W_j < 0 \mid |W_j|, W_{-j}\right\}.
\]

(14)

\[1\]The results in Barber et al. (2020) concern robustness of the Model-X knockoff framework (where \( X \) is random) but the FDR control proof works for the Fixed-X setting as well, since they only rely on antisymmetry of the statistics and (14).
(almost surely) for some \( C > 0 \), then the knockoff procedure with the target FDR \( q/C \) controls the FDR at level \( q \). It is straightforward to verify that in the case of simple nulls, this condition holds with \( C \geq 1 \) according to the i.i.d. sign property of the null statistics, resulting in FDR control.

### 3. Main Results

In case of a single composite test of the form \( |\beta_i| \leq \delta \), the common approach is to compute super uniform p-values under the null (i.e., \( P(P \leq t) \leq t \)) which clearly controls the probability of type I error by definition. The super uniformity usually happens when the p-value is computed according to the distribution corresponding to a parameter on the boundary of the null region. However, for composite multiple testing problems under the FDR control constraint, this argument gets more complicated as the dependencies between the statistics should be considered. The composite BH procedure [Benjamini and Yekutieli, 2001, Theorem 5.2] guarantees the FDR control when the null p-values are super uniform, but it is only valid for independent p-values. On the other hand, the knockoff filter is designed to utilize the model and covariates structure for computing one-bit p-values that handle the dependencies naturally. It turns out that we can actually maintain this property of the knockoff procedure when developing composite tests. To show the FDR control we rely on manipulating the estimates so that the statistics satisfy the following inequality for some \( B < \infty \),

\[
P\left\{ W_j > 0 \mid |W_j|, W_{-j} \right\} \leq B \cdot P\left\{ W_j < 0 \mid |W_j|, W_{-j} \right\} \text{ a.s., all } j \in \mathcal{H}_0,
\]

which is equivalent to

\[
R := \max_{j \in \mathcal{H}_0} \sup_{\omega : W_j \neq 0} \frac{P\left\{ W_j > 0 \mid |W_j|, W_{-j} \right\}}{P\left\{ W_j < 0 \mid |W_j|, W_{-j} \right\}} \leq B. \quad (15)
\]

It is known from [Barber et al., 2020, Theorem 2 with \( E_j = 0 \)] that having this bound leads to rigorous FDR control at level \( q \cdot B \). In fact, showing \( R \leq 1 \) in the knockoff procedure framework means that the procedure overestimates FDP(t) and therefore, can be interpreted as an equivalent for super uniformity of null p-values in terms of BH procedure. However, for bounds \( R \leq B \) where \( B > 1 \), we need to correct the test size by a factor of \( 1/B \), i.e., \( q' = q/B \). In
cases where \( R = \infty \), we use a generalization of this argument which leads to tighter bounds. We bound the following quantity.

\[
R' := \max_{j \in H_0} \sup_{\omega : W_j \neq 0} \frac{\Pr\{W_j > 0, A_j \mid |W_j|, W_{-j}\}}{\Pr\{W_j < 0 \mid |W_j|, W_{-j}\}},
\]

where \( A_j \) is some event regarding the \( j \)-th variable.

**Theorem 1** (Barber et al. (2020), Theorem 2). If \( R' \leq B' \), we get \( \text{FDR} \leq q \cdot B' + \Pr(\bigcup_{j \in H_0} A_c^j) \).

In the following subsection we present composite selective inference methods that allow for theoretical FDR control.

### 3.1. Composite Testing with FDR Control

The following theorem concerns the composite knockoff procedure based on the ordinary least-squares.\(^2\) We consider both one-sided and two-sided null hypothesis, i.e., \( \beta_j \leq \delta \) and \( |\beta_j| \leq \delta \), respectively. We show that shifting the estimates corresponding to the knockoff variables by \( \delta \) will result in exact FDR control for one-sided test (i.e., we prove \( R \leq 1 \) in this case). Regarding the two-sided test, we derive a bound for the FDR of the knockoff procedure (i.e., \( R = \infty \) and we show \( R' \leq 1 \)).

**Theorem 2** (S-OLS). Consider the knockoff procedure (target FDR=\( q \)) and based on the estimates \( \hat{\beta}_{S-OLS} = \hat{\beta}_{OLS} + \left(0_{p \times 1}^\top \delta_{p \times 1}\right) \) with some \( \delta_i \geq \delta \) for all \( 1 \leq i \leq p \). Let \( \hat{\beta}_j \) and \( \hat{\beta}'_j \) denote the \( j \)-th and \((j + p)\)-th elements of \( \hat{\beta}_{S-OLS} \).

**I** Consider testing \( H_{0,j} : \beta_j \leq \delta \) for \( 1 \leq j \leq p \). If \( W_j = \hat{\beta}_j - \hat{\beta}'_j \), then the procedure controls the FDR at level \( q \).

**II** Consider testing \( H_{0,j} : |\beta_j| \leq \delta \) for \( 1 \leq j \leq p \). If \( |W_j| \) depends on the estimator \( \hat{\beta}_{S-OLS} \) through the unordered pair \( \{\hat{\beta}_j, \hat{\beta}'_j\} \) and \( \text{sgn}(W_j) = \text{sgn}(|\hat{\beta}_j| - |\hat{\beta}'_j|) \), then

\[
\text{FDR} \leq q + \Pr\left\{ \min_{j \in H_0} (\hat{\beta}_j + \hat{\beta}'_j) < 0 \right\}. 
\]

\(^2\)Note that performing the knockoff procedure using the OLS estimator requires that \( \mathbf{G} \) is invertible. In Lemma \( \blacksquare \) we show that this is the case if \( \max_{1 \leq i \leq p} s_i < 2\lambda_{\min}(\Sigma) \).
**Remark 2.** We note that \((\hat{\beta}_j + \hat{\beta}'_j) \sim \mathcal{N}(\beta_j + \delta'_j, \phi \sigma^2)\) with \(\phi\) determined by Lemma 2. This evidences how larger shifts \(\delta'\) will help the theoretical FDR control.

**Corollary 1 (Alternative method for Theorem 2 (II)).** Fix \(\delta'_j \leq -\delta\). Under the same setting as Theorem 2 (II) we get,

\[
\text{FDR} \leq q + \mathbb{P}\left\{\max_{j \in \mathcal{H}_0} (\hat{\beta}_j + \hat{\beta}'_j) > 0\right\}.
\]

The next method generalizes the knockoff framework in the sense that composite inference is allowed but it is not limited to any particular estimator. In this situation, the shifted estimates are no longer feasible to analyze. Therefore, in order to perform composite inference in such a general setting, we propose to introduce artificial randomness to the procedure. Specifically, we perturb the feature-response products \([X \tilde{X}]^\top y\) by noise generated from Laplace distribution. In this case, we will be able to show that \(R \leq e^\epsilon\) with \(\epsilon\) being determined by the noise variance.

**Theorem 3 (FRPP).** Fix some \(\epsilon > 0\). Define the null variables \(\mathcal{H}_0 = \{i : |\beta_i| \leq \delta\}\) and let \(\Delta_i \overset{i.i.d.}{\sim} \text{Lap}(2s_i \delta / \epsilon)\) where \(s_i = 1 - X_i^\top \tilde{X}_i\), \(1 \leq i \leq p\). The knockoff procedure with the target FDR \(q/\epsilon\), and using (antisymmetric) statistics based on any estimator of the form \(\tilde{\theta} = \mathcal{E}(G, [X \tilde{X}]^\top y + \Delta)\) controls the FDR at level \(q\).

**Remark 3.** As we discussed in the previous section, the original knockoff framework focuses on the estimators of the form \(\tilde{\theta} = \mathcal{E}(G, P_i[X \tilde{X}]^\top y)\) where \(P_i\) is the (symmetric) permutation matrix swapping \(i\)-th and \((i + p)\)-th elements. We also keep assuming this property as we refer to general estimators, e.g., we assume \(P_i \tilde{\theta} = \mathcal{E}(G, P_i([X \tilde{X}]^\top y + \Delta))\). Observe that this is a very mild assumption (since \(P_i GP_i = G\)) and is satisfied by almost every estimators of linear models.

We note that Theorem 3 gives an stochastic generalization of the knockoff procedure, i.e., if \(\delta = 0\) the FRPP method reduces to the original method without any additional assumptions.

### 3.2. Heuristic Methods

Motivated by our results that show the shifting argument is theoretically valid in case of using the OLS estimator, we propose the following two methods based on shifting the LASSO estimates.
Method S-LAS1: This method shifts the LASSO estimates just as the S-OLS method. Namely, we use the following formulae to compute the statistics.

\[
\hat{\beta}_{S-LAS1} = \hat{\beta}_{LAS}(\lambda) + \begin{pmatrix} 0 \\ \delta \end{pmatrix}
\]

Method S-LAS2: This method estimate the coefficients by solving the following LASSO problem.

\[
\hat{\beta}_{S-LAS2} := \arg \min_{b \in \mathbb{R}^p} \left\{ \left\| y - [X \tilde{X}] \left( b + \begin{pmatrix} 0 \\ \delta \end{pmatrix} \right) \right\|_2^2 + \lambda \|b\|_1 \right\},
\]

where \( \lambda \geq 0 \).

Remark 4. We note that both methods reduce to the S-OLS method if \( \lambda = 0 \).

3.3. FDR Bound for Naive Selection

Theorem 4. Naive application of the (fixed) knockoff procedure (with target FDR \( q \)) on composite null hypotheses \( \mathcal{H}_0 = \{ i : |\beta_i| \leq \delta \} \) and using (antisymmetric) statistics based on any estimator of the form \( \mathcal{E}(G, [X \tilde{X}]^\top y) \),

will result in FDR bounded as follows.

\[
FDR \leq \min_{\epsilon \geq 0} \left\{ q . e^\epsilon + \mathbb{P} \left( \frac{\delta}{\sigma^2} \max_{j \in \mathcal{H}_0} |\gamma_j - \gamma_j'| > \epsilon \right) \right\},
\]

where \( \begin{pmatrix} \gamma_{p \times 1} \\ \gamma'_{p \times 1} \end{pmatrix} = [X \tilde{X}]^\top y \).

Remark 5. We note that the bound \((17)\) will reduce to \( q \) in the case of simple nulls, i.e., \( \delta = 0 \).

4. Simulations

In this section we present simulation results on synthetic data sets for all methods. We set the sample size and dimension to be \( n = 2000 \) and \( p = 800 \), respectively. The samples (rows of \( X \)) are generated i.i.d. according to \( \mathcal{N}(0, S_p) \) where \( S_{ij} = \rho^{|i-j|}, \ |\rho| < 1 \) and we normalize the columns of \( X \) by the \( \ell_2 \)-norm. The responses \( y \) are generated according to the linear model \((11)\) with noise variance \( \sigma^2 = 1 \) and the number of true alternatives is
$k = 100$. The composite null boundary is set to be $\delta = 1$, and we consider two distributions for generating coefficients corresponding to null variables:

(a) $\beta_0 \sim U[-1, 1]$ which is presented in the left column of the figures. We consider this setting as a practical case.

(b) $\beta_0 \sim$ Rademacher, which is presented in the right column of the figures. This setting tries to examine the methods in the hardest situation (worst case scenario) for FDR control.

The super uniform $p$-values for the composite BH procedure are computed according to $P_j = 2 \mathbb{P}(N(\delta, 1) \geq |\hat{\beta}_j|)$. We adopt the equicorrelated knockoffs and set the elements of $s$ (the vector used in creating the knockoff matrices) to be $\min(1.8\lambda_{\min}(\Sigma), 1)$, $\min(\lambda_{\min}(\Sigma), 1)$, and $\min(2\lambda_{\min}(\Sigma), 1)$ for the S-OLS, FRPP, and heuristic methods (S-LAS1 and S-LAS2), respectively. We adopt the structure (7) to construct the coefficient signed max statistics and use the LASSO estimator (9) with $\lambda = 1$. The target FDR is $q = 0.2$ and the plots are based on averaging 200 trials. The power is defined as follows,

$$\text{Power} := \frac{1}{k} \mathbb{E} \left| \hat{R} \cap \mathcal{H}_0^c \right| . \tag{18}$$

**Remark 6.** In [Barber and Candès (2015)](2015), it is suggested to set $s_i = \min(2\lambda_{\min}(\Sigma), 1)$ for equicorrelated knockoffs. However, this is not possible in case of using OLS estimator as it would result in a singular augmented design if $2\lambda_{\min}(\Sigma) \leq 1$ (See Lemma 7). Regarding the FRPP method, note that unlike the deterministic methods larger values of $s_i$ does not result in higher detection power necessarily, because the variance of the additive Laplacian noise is proportional to $s_i^2$. In our experiments it turns out that for $\rho = 0$ (no correlation) case, the procedure reaches to its highest power when $s_i = \min(\lambda_{\min}(\Sigma), 1)$. However this is not the case for high correlations and $\lambda_{\min}(\Sigma)$ would be too small. In this case, the maximum power is reached when $s_i = \min(2\lambda_{\min}(\Sigma), 1)$.

5. Discussion

Fixed-X knockoff procedure is an elegant method for selective inference in general linear models with FDR control guarantee. However, the composite extension of this method has not been developed yet. In this paper, we have investigated the Fixed-X knockoff filter approach to the variable selection problem with composite nulls and under arbitrary dependencies among
Figure 1: FDR and power vs Amplitude of the true alternatives. In this experiment the correlation coefficient is set to be $\rho = 0$ and all of the true alternatives have the same underlying coefficient. It can be observed that both heuristic methods outperform the composite BH procedure.

statistics. The knockoff inference procedure handles the dependencies between variables very naturally by computing model-based statistics. We have shown that this structure is still useful under the composite nulls and allows for development of methods with theoretical FDR control guarantee. We have derived a full stochastic generalization of the knockoff procedure which has reasonable statistical power. We have shown that if we restrict ourselves to the ordinary least-squares estimates, the intuitive (and deterministic) method of shifting the estimate would be theoretically valid. We have also derived a general bound on the FDR for cases where the original knockoff procedure is applied on a composite problem, without any additional assumptions.
Figure 2: FDR and power vs Correlation coefficient $\rho$. In this experiment the coefficients corresponding to the true alternatives is set to be $\beta_a = 8$. Although both heuristic methods outperform the BH procedure in high correlations, it can be observed that the second heuristic method fails to control the FDR.

Appendix A. Technical Lemmas

Lemma 1. If $\max_{1 \leq i \leq p} s_i < 2\lambda_{\min}(\Sigma)$, then G is invertible.

Proof. Recall,
$$
G = \begin{bmatrix}
\Sigma & \Sigma - \text{diag}(s) \\
\Sigma - \text{diag}(s) & \Sigma
\end{bmatrix},
$$
where $s \in \mathbb{R}_+^p$. We note,
$$
\begin{bmatrix}
I & -I \\
O & I
\end{bmatrix}
\begin{bmatrix}
A & B \\
B & A
\end{bmatrix}
\begin{bmatrix}
I & I \\
O & I
\end{bmatrix}
= 
\begin{bmatrix}
A - B & O \\
B & A + B
\end{bmatrix}.
$$

Therefore, $\det(G - \lambda I) = \det \left( \text{diag}(s) - \lambda I \right) \det \left( 2\Sigma - \text{diag}(s) - \lambda I \right)$ and as a result, the set of eigenvalues of $G$ is the union of the eigenvalues of $\text{diag}(s)$
and $2\Sigma - \text{diag}(s)$. If $\max_{1 \leq i \leq p} s_i < 2\lambda_{\min}(\Sigma)$ holds, then $\lambda_{\min}(2\Sigma - \text{diag}(s)) > 0$ which implies that $G$ is positive definite and therefore, invertible. \hfill ■

**Lemma 2.** Let $G = [X \tilde{X}]^\top [X \tilde{X}]$ and $\Sigma = X^\top X$. If $G$ is invertible, $G^{-1}$ has the following structure.

$$G^{-1} = \begin{bmatrix} A & A - D \\ A - D & A \end{bmatrix},$$

where $D$ is a diagonal matrix.

**Proof.** From (4) recall,

$$G = \begin{bmatrix} \Sigma & \Sigma - D^* \\ \Sigma - D^* & \Sigma \end{bmatrix}, \quad (A.2)$$

with some diagonal $D^*$. From the inverse of $2 \times 2$ block matrices we have

$$G^{-1} = \begin{bmatrix} J & -J(I_p - D^*\Sigma^{-1}) \\ -J(I_p - D^*\Sigma^{-1}) & J \end{bmatrix},$$

where $J = (2D^* - D^*\Sigma^{-1}D^*)^{-1}$. We observe,

$$J - (-J(I_p - D^*\Sigma^{-1})) = D^*^{-1}. \quad (A.3)$$

Therefore, $A = (2D^* - D^*\Sigma^{-1}D^*)^{-1}$ and $D = D^*^{-1}$. \hfill ■

**Lemma 3.** Let $\begin{pmatrix} \gamma_p \gamma' \end{pmatrix} = [X \tilde{X}]^\top y$. It holds that $|\mathbb{E}(\gamma_j - \gamma'_j)| \leq s_j \delta$ for all $j \in \mathcal{H}_0$.

**Proof.** We observe $\mathbb{E}(\gamma) = G \begin{pmatrix} \beta \\ 0_{p \times 1} \end{pmatrix}$. According to the structure of $G$ (A.2), we get

$$|\mathbb{E}(\gamma_j - \gamma'_j)| = \left| (G_{(j)} - G_{(j+p)}) \begin{pmatrix} \beta \\ 0 \end{pmatrix} \right|$$
$$= \left| \left( \Sigma_{(j)} - (\Sigma_{(j)} - D^*_{(j)}) \right) \beta \right|$$
$$= s_j |\beta_j| \leq s_j \delta,$$

where the index $(j)$ denotes the $j$-th row of the matrices and the inequality holds according to the definition of $\mathcal{H}_{0,j}'$. \hfill ■
Appendix B. Proof of Theorem 4

Lemma 4. Let \( \left( \gamma_p \times 1 \right) = [X \ 	ilde{X}]^T y \). For fixed \( X \), any anti-symmetric \( \hat{W} = W([X \ 	ilde{X}]^T [X \ 	ilde{X}], [X \ 	ilde{X}]^T y) \) satisfies the following properties.

(I) For all \( j \in H_0 \),

\[
\mathbb{P}\left\{ W_j > 0 \mid \{\gamma_j, \gamma'_j\}, (\gamma_{-j}, \gamma'_{-j}) \right\} \leq \exp\left( \frac{\delta}{\sigma^2} |\gamma_j - \gamma'_j| \right) \mathbb{P}\left\{ W_j < 0 \mid \{\gamma_j, \gamma'_j\}, (\gamma_{-j}, \gamma'_{-j}) \right\} \text{ a.s.,}
\]

where \( \{\cdot, \cdot\} \) denotes an unordered pair.

(II) For all \( 1 \leq j \leq p \) we have,

\[
\text{sgn}(W_j) \perp \perp \text{sgn}(W_{-j}) \mid \{\gamma, \gamma'\}_V ,
\]

where \( \{\cdot, \cdot\}_V \) denotes a vector of unordered pairs and \( \text{sgn}(\cdot) \) operates coordinate-wise.

Proof. (I) We compute the conditional distribution \( (\gamma_j, \gamma'_j) \mid (\gamma_{-j}, \gamma'_{-j}) \). We note that \( \left( \begin{array}{c} \gamma' \\ \gamma' \end{array} \right) \sim \mathcal{N}\left( \left( \begin{array}{c} \tilde{\gamma} \\ \tilde{\gamma}' \end{array} \right), \sigma^2 G \right) \) where \( \left( \begin{array}{c} \tilde{\gamma} \\ \tilde{\gamma}' \end{array} \right) = G \left( \begin{array}{c} \beta \\ 0_{p \times 1} \end{array} \right) \) according to (II). Therefore we have,

\[
\left( (\gamma_j, \gamma'_j) \mid (\gamma_{-j}, \gamma'_{-j}) = (a, b) \right) \sim \mathcal{N}(\eta^{(j)}, \sigma^2 R^{(j)}) ,
\]

where

\[
\eta^{(j)} = \left( \begin{array}{c} \tilde{\gamma}_j \\ \tilde{\gamma}'_j \end{array} \right) + [X_j \ 	ilde{X}_j]^T [X_{-j} \ 	ilde{X}_{-j}] \left( [X_{-j} \ 	ilde{X}_{-j}]^T [X_{-j} \ 	ilde{X}_{-j}] \right)^{-1} \left[ \begin{array}{c} a \\ b \end{array} \right] - \left( \begin{array}{c} \tilde{\gamma}_j \\ \tilde{\gamma}'_j \end{array} \right),
\]

and

\[
R^{(j)} = [X_j \ 	ilde{X}_j]^T [X_j \ 	ilde{X}_j] - [X_j \ 	ilde{X}_j]^T [X_{-j} \ 	ilde{X}_{-j}] \left( [X_{-j} \ 	ilde{X}_{-j}]^T [X_{-j} \ 	ilde{X}_{-j}] \right)^{-1} [X_{-j} \ 	ilde{X}_{-j}]^T [X_j \ 	ilde{X}_j] .
\]
From the definition of the knockoff variables we have \( [X_j X_j^\top] [X_{-j} X_{-j}^\top] = [z_j z_j^\top] \) with some \( z_j \in \mathbb{R}^{p-1} \) and according to Lemma 2 and eigenvalue interlacing theorem we have

\[
\left( [X_{-j} X_{-j}^\top] [X_{-j} X_{-j}^\top] \right)^{-1} = \left[ \begin{array}{cc} A' & A' - D' \\ A' - D' & A' \end{array} \right],
\]

with some symmetric positive-definite \( A' \in \mathbb{R}^{(p-1) \times (p-1)} \) and diagonal \( D' \). Therefore we get

\[
[X_j X_j^\top] [X_{-j} X_{-j}^\top] \left( [X_{-j} X_{-j}^\top] [X_{-j} X_{-j}^\top] \right)^{-1} = [c_j c_j^\top],
\]

with some \( c_j \in \mathbb{R}^{p-1} \). Hence,

\[
\eta^{(j)} = \begin{pmatrix} \eta_j \\ \eta_j' \end{pmatrix} = \begin{pmatrix} \tilde{\gamma}_j \\ \tilde{\gamma}_j' \end{pmatrix} + \begin{pmatrix} c_j \\ c_j \end{pmatrix} \left( \begin{array}{cc} a - \tilde{\gamma}_j \\ b - \tilde{\gamma}_j' \end{array} \right) = \begin{pmatrix} \tilde{\gamma}_j + c_j (a + b - \tilde{\gamma}_j - \tilde{\gamma}_j') \\ \tilde{\gamma}_j' + c_j (a + b - \tilde{\gamma}_j - \tilde{\gamma}_j') \end{pmatrix} = \begin{pmatrix} \tilde{\gamma}_j + d_j \\ \tilde{\gamma}_j' + d_j \end{pmatrix}.
\]

Similarly, for the covariance matrix \( R \) we have,

\[
R^{(j)} = \begin{pmatrix} e_j \\ e_j \end{pmatrix} \left( \begin{array}{cc} e_j \\ e_j \end{array} \right) = \begin{pmatrix} e_j e_j \\ e_j e_j \end{pmatrix},
\]

where \( e_j \in \mathbb{R} \) does not depend on \( a \) or \( b \). We note that the desired inequality holds trivially for \( \{ \omega : W_j = 0 \} \). Also, \( \mathbb{P} \left\{ W_j < 0 \middle| \{ \gamma_j, \gamma_j' \}, (\gamma_{-j}, \gamma_{-j}') \right\} > 0 \) for \( \{ \omega : W_j \neq 0 \} \). Therefore, it is sufficient to prove

\[
\frac{\mathbb{P} \left\{ W_j > 0 \middle| \{ \gamma_j, \gamma_j' \}, (\gamma_{-j}, \gamma_{-j}') \right\}}{\mathbb{P} \left\{ W_j < 0 \middle| \{ \gamma_j, \gamma_j' \}, (\gamma_{-j}, \gamma_{-j}') \right\}} \leq \exp \left\{ \frac{\delta}{\sigma^2} |\gamma_j - \gamma_j'| \right\},
\]

almost everywhere on \( \{ \omega : W_j \neq 0 \} \) and all \( j \in \mathcal{H}_0 \). Let \( h(\cdot, \cdot) \) denote \( h_{(\gamma_j, \gamma_j')} \mid (\gamma_{-j}, \gamma_{-j}') \overset{\text{pdf}}{\sim} N(\eta^{(j)}, \sigma^2 R^{(j)}) \). Notice that on \( \{ \omega : W_j \neq 0 \} \), swapping
\( \gamma_j \) and \( \gamma'_j \) would switch the sign of \( W_j \). Hence, we get
\[
\mathbb{P}\{W_j > 0 \mid \{\gamma_j, \gamma'_j\} = \{u, v\}, (\gamma_j, \gamma'_j)\} = \mathbb{P}\{W_j < 0 \mid \{\gamma_j, \gamma'_j\} = \{u, v\}, (\gamma_j, \gamma'_j)\}
\]
\[
\leq \max \left\{ \frac{h(u,v)}{h(v,u)+h(v,u)}, \frac{h(v,u)}{h(u,v)+h(v,u)} \right\}
\]
\[
= \max \left\{ \frac{h(u,v)}{h(v,u)}, \frac{h(v,u)}{h(u,v)} \right\}, \quad (B.5)
\]
almost everywhere on \( \{(u,v,\omega) : W_j \neq 0\} \). By a \( \frac{\pi}{4} \) counter-clockwise rotation of \( h \) we get
\[
\frac{h(u,v)}{h(v,u)} = \frac{h_1}{h_1} \left( \frac{1}{\sqrt{2}} (u-v) \right) \frac{h_2}{h_2} \left( \frac{1}{\sqrt{2}} (u+v) \right)
\]
\[
= \frac{h_1}{h_1} \left( \frac{1}{\sqrt{2}} (u-v) \right), \quad (B.6)
\]
where,
\[
h_1 \overset{\text{pdf}}{\sim} \mathcal{N} \left( \frac{1}{\sqrt{2}} (\eta_j - \eta'_j), \sigma^2 \left( R^{(j)}_{11} - R^{(j)}_{12} \right) \right),
\]
\[
h_2 \overset{\text{pdf}}{\sim} \mathcal{N} \left( \frac{1}{\sqrt{2}} (\eta_j + \eta'_j), \sigma^2 \left( R^{(j)}_{11} + R^{(j)}_{12} \right) \right).
\]
According to (B.3) and (B.4), we have
\[
\mathcal{N} \left( \frac{1}{\sqrt{2}} (\eta_j - \eta'_j), \sigma^2 \left( R^{(j)}_{11} - R^{(j)}_{12} \right) \right) = \mathcal{N} \left( \frac{1}{\sqrt{2}} \left( \gamma_j - \gamma'_j \right), \sigma^2 \right), \quad (B.7)
\]
where \( \sigma^2 = s_j \sigma^2 \) and \( s_j = 1 - \mathbf{X}_j^\top \tilde{\mathbf{X}}_j \) since the columns of \( \mathbf{X} \) are normalized. Therefore, \( h_1 \) is free of the given values for \( (\gamma_j, \gamma'_j) \), which also means
\[
\left( \gamma_j - \gamma'_j \mid \gamma_j, \gamma'_j \right) \overset{d}{=} \left( \gamma_j - \gamma'_j \right), \quad (B.8)
\]
and hence \( (\gamma_j - \gamma'_j) \perp \perp (\gamma_j, \gamma'_j) \). We now use (B.6) and (B.7) to bound
the RHS of (B.5) under $H'_{0,j}$,

$$
\max \left\{ \frac{h(u,v)}{h(v,u)} \cdot \frac{h(v,u)}{h(u,v)} \right\} = \max \left\{ \frac{h_1 \left( \frac{1}{\sqrt{2}} (u-v) \right)}{h_1 \left( \frac{-1}{\sqrt{2}} (u-v) \right)} \cdot \frac{h_1 \left( \frac{-1}{\sqrt{2}} (u-v) \right)}{h_1 \left( \frac{1}{\sqrt{2}} (u-v) \right)} \right\}
\leq \exp \left\{ -\frac{1}{4\sigma_j^2} \left( |\bar{\gamma}_j - \bar{\gamma}'_j| - |u-v| \right)^2 \right\}
\leq \exp \left\{ -\frac{1}{4\sigma_j^2} \left( |\bar{\gamma}_j - \bar{\gamma}'_j| + |u-v| \right)^2 \right\}
= \exp \left\{ \frac{1}{\sigma_j^2} |\bar{\gamma}_j - \bar{\gamma}'_j| |u-v| \right\}
\leq \exp \left\{ \frac{s_j \delta}{\sigma_j^2} |u-v| \right\} = \exp \left\{ \frac{\delta}{\sigma^2} |u-v| \right\},
$$

where the second inequality is a consequence of $|\bar{\gamma}_j - \bar{\gamma}'_j| \leq s_j \delta$ under $H'_{0,j}$ (Lemma 3).

(II) According to (B.3) and (B.4), the conditional distribution (B.2) only depends on $a + b$ (through $\eta_j$). Hence, we have

$$
\left( \gamma_j, \gamma'_j \left| \gamma_{-j}, \gamma'_{-j} \right. \right) \overset{d}{=} \left( \gamma_j, \gamma'_j \left| \{ \gamma_{-j}, \gamma'_{-j} \} \right. \right)_{V},
$$

We observe that the unordered pair $\{ \gamma_j, \gamma'_j \}$ is a function of $(\gamma_j, \gamma'_j)$. Therefore, by conditioning on it we get,

$$
\left( \gamma_j, \gamma'_j \left| \{ \gamma_{-j}, \gamma'_{-j} \}, \{ \gamma_j, \gamma'_j \} \right. \right) \overset{d}{=} \left( \gamma_j, \gamma'_j \left| \{ \gamma, \gamma' \} \right. \right)_{V}.
$$

Therefore,

$$
\left( \text{sgn}(W_j) \left| \text{sgn}(W_{-j}), \{ \gamma, \gamma' \} \right. \right) \overset{d}{=} \left( \text{sgn}(W_j) \left| \{ \gamma, \gamma' \} \right. \right)_{V},
$$

which implies (B.1) immediately.

Lemma 5. For all $j \in \mathcal{H}_0$ we have

$$
P \left\{ W_j > 0, \frac{\delta}{\sigma^2} |\gamma_j - \gamma'_j| \leq \epsilon \left| |W_j|, W_{-j} \right. \right\} \leq e^\epsilon P \left\{ W_j < 0 \left| |W_j|, W_{-j} \right. \right\},
$$

almost surely.
Proof.

\[
\mathbb{P}\{W_j > 0, \frac{\delta}{\sigma^2} |\gamma_j - \gamma'_j| \leq \epsilon \mid |W_j|, W_{-j}\} = \mathbb{E}\left\{\mathbb{P}(W_j > 0, \frac{\delta}{\sigma^2} |\gamma_j - \gamma'_j| \leq \epsilon \mid \{\gamma_j, \gamma'_j\}, (\gamma_{-j}, \gamma'_{-j}) \mid |W_j|, W_{-j}\}\right\}
\]

\[
= \mathbb{E}\left\{1\left\{\frac{\delta}{\sigma^2} |\gamma_j - \gamma'_j| \leq \epsilon\right\} \mathbb{P}(W_j > 0 \mid \{\gamma_j, \gamma'_j\}, (\gamma_{-j}, \gamma'_{-j}) \mid |W_j|, W_{-j}\}\right\}
\]

\[
\leq \mathbb{E}\left\{1\left\{\frac{\delta}{\sigma^2} |\gamma_j - \gamma'_j| \leq \epsilon\right\} \exp\left(\frac{\delta}{\sigma^2} |\gamma_j - \gamma'_j|\right) \mathbb{P}(W_j < 0 \mid \{\gamma_j, \gamma'_j\}, (\gamma_{-j}, \gamma'_{-j}) \mid |W_j|, W_{-j}\}\right\}
\]

\[
\leq e^\epsilon \mathbb{E}\left\{\mathbb{P}(W_j < 0 \mid \{\gamma_j, \gamma'_j\}, (\gamma_{-j}, \gamma'_{-j}) \mid |W_j|, W_{-j}\}\right\} = e^\epsilon \mathbb{P}\{W_j < 0 \mid |W_j|, W_{-j}\} \quad \text{a.s.,}
\]

where \{\cdot, \cdot\} denotes an unordered pair, the first inequality holds according to Lemma 4 (I), and we used the tower property since \((|W_j|, W_{-j})\) is a function of \((\{\gamma_j, \gamma'_j\}, (\gamma_{-j}, \gamma'_{-j}))\). □

Hence (17) holds according to Theorem 1.

Appendix C. Proof of Theorem 2

Lemma 6. If we use estimates with distribution \(\left(\hat{\beta}, \hat{\beta}'\right) \sim \mathcal{N}\left(\left(\bar{\beta}, \bar{\beta}'\right), \sigma^2 G^{-1}\right)\) to compute the statistics, then, the following properties hold for any \(1 \leq j \leq p\).

(I) If \(W_j\) depends on the estimator only through \(\hat{\beta}_j\) and \(\hat{\beta}'_j\), and \(\text{sgn}(W_j) = \text{sgn}(|\hat{\beta}_j| - |\hat{\beta}'_j|)\), then

\[
\text{sgn}(W_j) \perp \perp W_{-j} \mid \{\hat{\beta}_j, \hat{\beta}'_j\},
\]

where \{\cdot, \cdot\} denotes an unordered pair.

(II) If \(W_j = \hat{\beta}_j - \hat{\beta}'_j\), then

\[
W_j \perp \perp W_{-j}.
\]
Proof. (I) We compute the conditional distribution,

\[
\left( \hat{\beta}_{-j}, \hat{\beta}'_{-j} \right | (\hat{\beta}_j, \hat{\beta}'_j) = (a, b) \sim \mathcal{N} \left( \xi^{(-j)}, C^{(-j)} \right)
\]

Let \( K = \sigma^2 G^{-1} \). We note that according to Lemma 2, \( G \) and \( G^{-1} \) have the same structure. Therefore, similar calculations as in the proof of Lemma 4 gives,

\[
\xi^{(-j)} = \left( \hat{\beta}_{-j}, \hat{\beta}'_{-j} \right) \rightarrow \left( \hat{\beta}_j, \hat{\beta}'_j \right)
\]

\[
C^{(-j)} = K_{-j} - \begin{bmatrix} Q & Q \\ Q & Q \end{bmatrix}
\]

with some \( c \in \mathbb{R}^{p-1} \) and symmetric \( Q \in \mathbb{R}^{(p-1) \times (p-1)} \) that does not depend on \( a \) and \( b \). We note that the conditional distribution depends on the pair \((a, b)\) only through their sum \( a + b \), so it is free of the order of the pair. Thus, we get

\[
\left( \hat{\beta}_{-j}, \hat{\beta}'_{-j} \right | \hat{\beta}_j, \hat{\beta}'_j \) = \left( \hat{\beta}_j, \hat{\beta}'_j \right)
\]

Therefore,

\[
\left( W_{-j} | \text{sgn}(W_j), \{ \hat{\beta}_j, \hat{\beta}'_j \} \right) \rightarrow \left( W_{-j} | \{ \hat{\beta}_j, \hat{\beta}'_j \} \right)
\]

which implies (C.1) immediately.

(II) Again, since \( G \) and \( G^{-1} \) have the same structure (according to Lemma 2), the same argument that led to (B.8) applies and we get

\[
(\hat{\beta}_j - \hat{\beta}'_j) \perp (\hat{\beta}_{-j}, \hat{\beta}'_{-j})
\]

This would imply (C.2) since \( W_j \) and \( W_{-j} \) are functions of \((\hat{\beta}_j - \hat{\beta}'_j)\) and \((\hat{\beta}_{-j}, \hat{\beta}'_{-j})\), respectively.

Appendix C.1. One-sided Test:

Proof. According to (15), it is sufficient to show

\[
\text{ess sup}_{\omega: W_j \neq 0} \frac{P \left\{ W_j > 0 \ \middle\vert \ |W_j|, W_{-j} \right\}}{P \left\{ W_j < 0 \ \middle\vert \ |W_j|, W_{-j} \right\}} \leq 1, \quad \text{all } j \in \mathcal{H}_0.
\]

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Also since $|W_j|$ is a function of $W_j$, \((\text{C.2})\) yields
\[
\frac{\mathbb{P}\{W_j > 0 \mid |W_j|, W_{-j}\}}{\mathbb{P}\{W_j < 0 \mid |W_j|, W_{-j}\}} \leq \frac{\mathbb{P}\{W_j > 0 \mid |W_j|\}}{\mathbb{P}\{W_j < 0 \mid |W_j|\}} \quad \text{a.s.}
\]
Using the tower property we get,
\[
\frac{\mathbb{P}\{W_j > 0 \mid |W_j|\}}{\mathbb{P}\{W_j < 0 \mid |W_j|\}} = \frac{\mathbb{E}\left[\mathbb{P}(W_j > 0 \mid \hat{\beta}_j, \hat{\beta}'_j) \mid |W_j|\right]}{\mathbb{E}\left[\mathbb{P}(W_j < 0 \mid \hat{\beta}_j, \hat{\beta}'_j) \mid |W_j|\right]} = \frac{\mathbb{E}\left[\mathbb{P}(\hat{\beta}_j > \hat{\beta}'_j \mid \hat{\beta}_j, \hat{\beta}'_j) \mid |W_j|\right]}{\mathbb{E}\left[\mathbb{P}(\hat{\beta}_j < \hat{\beta}'_j \mid \hat{\beta}_j, \hat{\beta}'_j) \mid |W_j|\right]} \quad \text{a.s.}
\]
where $\{\cdot, \cdot\}$ denotes an unordered pair. Hence, it will be sufficient to prove,
\[
\operatorname{ess sup}_{\omega: \beta_j \neq \beta'_j} \frac{\mathbb{P}(\hat{\beta}_j > \hat{\beta}'_j \mid \hat{\beta}_j, \hat{\beta}'_j)}{\mathbb{P}(\hat{\beta}_j < \hat{\beta}'_j \mid \hat{\beta}_j, \hat{\beta}'_j)} \leq 1, \quad \text{all } j \in \mathcal{H}_0. \tag{\text{C.4}}
\]
Let $f(\cdot, \cdot)$ denote the probability density function for $(\hat{\beta}_j, \hat{\beta}'_j)^\top \sim \mathcal{N}((\beta_j, \delta'_j)^\top, K_j)$, where $K_j = \sigma^2_j \left[ \frac{1}{\rho'_j} \rho'_j \right]$ for some $\sigma^2_j > 0$ and $\rho'_j \in \mathbb{R}$ according to Lemma \ref{lemma:1}. Hence, we get
\[
\operatorname{ess sup}_{u \neq v} \frac{\mathbb{P}(\hat{\beta}_j > \hat{\beta}'_j \mid \hat{\beta}_j, \hat{\beta}'_j) = \{u, v\}}{\mathbb{P}(\hat{\beta}_j < \hat{\beta}'_j \mid \hat{\beta}_j, \hat{\beta}'_j) = \{u, v\}} \leq \operatorname{ess sup}_{u \neq v} \frac{f(u \lor v, u \land v)}{f(u, v) + f(u \lor v)} \leq 1 ,
\]
where the last inequality follows from $K_j = \sigma^2_j \left[ \frac{1}{\rho_j} \rho'_j \right]$ and $\mathbb{E}(\beta'_j) = \delta'_j \geq \delta \geq \mathbb{E}(\hat{\beta}_j)$ for all $j \in \mathcal{H}_0$. \hfill \blacksquare
Appendix C.2. Two-sided Test:

Proof. According to Theorem 1, it is sufficient to show

\[
\text{ess sup}_{\omega: W_j \neq 0} \frac{\mathbb{P}\left\{ W_j > 0, \hat{\beta}_j + \hat{\beta}'_j > 0 \mid |W_j|, W_{-j} \right\}}{\mathbb{P}\left\{ W_j < 0 \mid |W_j|, W_{-j} \right\}} \leq 1, \quad \text{all } j \in \mathcal{H}_0.
\]

By the tower property we have,

\[
\mathbb{P}\left\{ W_j > 0, \hat{\beta}_j + \hat{\beta}'_j > 0 \mid |W_j|, W_{-j} \right\} = \mathbb{E}\left\{ \mathbb{P}\left( W_j > 0, \hat{\beta}_j + \hat{\beta}'_j > 0 \mid W_{-j}, \{\hat{\beta}_j, \hat{\beta}'_j\} \right) \mid W_{-j}, |W_j| \right\} \mathbb{E}\left\{ \mathbb{P}\left( W_j < 0 \mid W_{-j}, \{\hat{\beta}_j, \hat{\beta}'_j\} \right) \mid W_{-j}, |W_j| \right\} \text{ a.s.},
\]

where \{·, ·\} denotes an unordered pair. Therefore, it is sufficient to prove,

\[
\text{ess sup}_{\omega: W_j \neq 0} \frac{\mathbb{P}\left( W_j > 0, \hat{\beta}_j + \hat{\beta}'_j > 0 \mid W_{-j}, \{\hat{\beta}_j, \hat{\beta}'_j\} \right)}{\mathbb{P}\left( W_j < 0 \mid W_{-j}, \{\hat{\beta}_j, \hat{\beta}'_j\} \right)} \leq 1, \quad \text{all } j \in \mathcal{H}_0.
\]

Since \(\hat{\beta}_j + \hat{\beta}'_j\) is a function of \(\{\hat{\beta}_j, \hat{\beta}'_j\}\), we have

\[
\frac{\mathbb{P}\left( W_j > 0, \hat{\beta}_j + \hat{\beta}'_j > 0 \mid W_{-j}, \{\hat{\beta}_j, \hat{\beta}'_j\} \right)}{\mathbb{P}\left( W_j < 0 \mid W_{-j}, \{\hat{\beta}_j, \hat{\beta}'_j\} \right)} = \frac{1\{\hat{\beta}_j + \hat{\beta}'_j > 0\}}{\mathbb{P}\left( W_j < 0 \mid W_{-j}, \{\hat{\beta}_j, \hat{\beta}'_j\} \right)} \mathbb{P}\left( W_j > 0 \mid W_{-j}, \{\hat{\beta}_j, \hat{\beta}'_j\} \right) \text{ a.s.},
\]

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where the last equality holds according to (C.1). Now we note,

\[
\text{ess sup}_{\omega: W_j \neq 0} \mathbb{1}\{\hat{\beta}_j + \hat{\beta}'_j > 0\} \frac{\mathbb{P}(W_j > 0 | \{\hat{\beta}_j, \hat{\beta}'_j\})}{\mathbb{P}(W_j < 0 | \{\hat{\beta}_j, \hat{\beta}'_j\})} \]

\[\equiv (\ast) \text{ess sup}_{\omega: W_j \neq 0} \mathbb{1}\{\hat{\beta}_j + \hat{\beta}'_j > 0\} \frac{\mathbb{P}(\hat{\beta}_j > \hat{\beta}'_j | \{\hat{\beta}_j, \hat{\beta}'_j\})}{\mathbb{P}(\hat{\beta}_j < \hat{\beta}'_j | \{\hat{\beta}_j, \hat{\beta}'_j\})}\]

\[\leq \text{ess sup}_{\omega: W_j \neq 0} \frac{\mathbb{P}(\hat{\beta}_j > \hat{\beta}'_j | \{\hat{\beta}_j, \hat{\beta}'_j\})}{\mathbb{P}(\hat{\beta}_j < \hat{\beta}'_j | \{\hat{\beta}_j, \hat{\beta}'_j\})}\]

\[\leq \text{ess sup}_{\omega: \hat{\beta}_j \neq \hat{\beta}'_j} \frac{\mathbb{P}(\hat{\beta}_j > \hat{\beta}'_j | \{\hat{\beta}_j, \hat{\beta}'_j\})}{\mathbb{P}(\hat{\beta}_j < \hat{\beta}'_j | \{\hat{\beta}_j, \hat{\beta}'_j\})} \leq 1, \quad \text{all } j \in \mathcal{H}_0.\]

where (\ast) holds since \(\hat{\beta}_j > \hat{\beta}'_j \iff |\hat{\beta}_j| > |\hat{\beta}'_j|\) when \(\hat{\beta}_j + \hat{\beta}'_j > 0\) and the last inequality holds according to (C.4).

\[\Box\]

**Appendix D. Proof of Theorem 3**

**Proof.** In this method, the Laplace noise \(\Delta_{2p \times 1}\) is added to the feature-response products,

\[
[X \tilde{X}]^\top y + \Delta = G\overline{\beta} + \Delta + [X \tilde{X}]^\top w,
\]

where \(\Delta_i \overset{\text{iid}}{\sim} \text{Lap}(2s_i \delta/\epsilon), s_i = 1 - X_i^\top \tilde{X}_i, \overline{\beta} = \begin{pmatrix} \beta \\ 0_{p \times 1} \end{pmatrix},\) and \(w\) is the model noise. For simplicity in notation we re-write the equation as follows,

\[
\begin{pmatrix} \kappa_{p \times 1} \\ \kappa'_{p \times 1} \end{pmatrix} = \begin{pmatrix} \theta \\ \theta' \end{pmatrix} + \begin{pmatrix} \alpha \\ \alpha' \end{pmatrix},
\]

where \(\begin{pmatrix} \theta \\ \theta' \end{pmatrix} = G\overline{\beta} + \Delta\) and \(\begin{pmatrix} \alpha \\ \alpha' \end{pmatrix} = [X \tilde{X}]^\top w.\) By Lemma 3 we have \(|\mathbb{E}(\theta_j - \theta'_j)| \leq s_j \delta\) for all \(j \in \mathcal{H}_0.\) Therefore, \(|\mathbb{E}(\theta_j - \theta'_j)| + |\mathbb{E}(\theta'_j - \theta_j)| \leq 2s_j \delta\)
and the following inequality holds for all \((x, y) \in \mathbb{R}^2\) and \(j \in \mathcal{H}_0\) according to the Laplace mechanism by Dwork et al. (2006, 2014).

\[
f_{(\theta, \theta')}^{(s)}(x, y) \leq e^\epsilon f_{(\theta, \theta')}^{(s)}(x, y),
\]

where \(f_{(\theta, \theta')}^{(s)}(x, y)\) denotes the probability density function.

In order to show the FDR control, according to (15), it will be sufficient to prove that

\[
\mathbb{P}\left\{ W_j > 0 \left| |W_j|, \mathbf{W}_{-j} \right. \right\} \leq e^\epsilon \mathbb{P}\left\{ W_j < 0 \left| |W_j|, \mathbf{W}_{-j} \right. \right\} \quad \text{a.s.,}
\]

for all \(j \in \mathcal{H}_0\). We note that \(|W_j|, \mathbf{W}_{-j}\) is a function of \(\{\kappa_j, \kappa'_j\}, \alpha_{-j}, \alpha'_{-j}, \theta_{-j}, \theta'_{-j}\)\), therefore, according to the tower property we get

\[
\mathbb{P}\left\{ W_j > 0 \left| |W_j|, \mathbf{W}_{-j} \right. \right\} = \mathbb{E}\left\{ \mathbb{P}\left( W_j > 0 \left| \kappa_j, \kappa'_j, \alpha_{-j}, \alpha'_{-j}, \theta_{-j}, \theta'_{-j} \right. \right. \right. \left| |W_j|, \mathbf{W}_{-j} \right. \right. \left. \right\} \quad \text{a.s.,}
\]

where \(\{\cdot, \cdot\}\) denotes an unordered pair. Therefore, it is sufficient to show

\[
\mathbb{P}\left( W_j > 0 \left| \kappa_j, \kappa'_j, \alpha_{-j}, \alpha'_{-j}, \theta_{-j}, \theta'_{-j} \right. \right) \leq e^\epsilon \mathbb{P}\left( W_j < 0 \left| \kappa_j, \kappa'_j, \alpha_{-j}, \alpha'_{-j}, \theta_{-j}, \theta'_{-j} \right. \right) \quad \text{a.s.,}
\]

We also note that \(\text{sgn}(W_j)\) is conditionally independent of \((\theta_{-j}, \theta'_{-j})\). Hence, we only need to show

\[
\text{ess sup}_{\omega: W_j \neq 0} \frac{\mathbb{P}\left( W_j > 0 \left| \kappa_j, \kappa'_j, \alpha_{-j}, \alpha'_{-j} \right. \right)}{\mathbb{P}\left( W_j < 0 \left| \kappa_j, \kappa'_j, \alpha_{-j}, \alpha'_{-j} \right. \right)} \leq e^\epsilon.
\]

We note

\[
\frac{\mathbb{P}\left( W_j > 0 \left| \kappa_j, \kappa'_j \right. \right. \left. \right)}{\mathbb{P}\left( W_j < 0 \left| \kappa_j, \kappa'_j \right. \right. \left. \right)} \leq \max \left\{ \frac{g(u, v)}{g(u, v) + g(v, u)}, \frac{g(v, u)}{g(u, v) + g(v, u)} \right\}
\]

\[
= \max \left\{ \frac{g(u, v)}{g(v, u) + g(u, v)}, \frac{g(v, u)}{g(u, v) + g(v, u)} \right\},
\]

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almost everywhere on \( \{(u, v, \omega) : W_j \neq 0\} \), with \( g(\cdot, \cdot) \) denoting the shorthand for the conditional probability density function \( g_{(\kappa, \kappa')|(\alpha_{-j}, \alpha'_{-j})} \). Now we note,

\[
g_{(\kappa, \kappa')|(\alpha_{-j}, \alpha'_{-j})}(u, v) = g_{(\theta_j + \alpha_j, \theta'_j + \alpha'_j)|(\alpha_{-j}, \alpha'_{-j})}(u, v)
\]

\[
= \mathbb{E}_{(\theta_j, \theta'_j)|(\alpha_{-j}, \alpha'_{-j})}\left\{ g_{(\theta_j, \theta'_j)|(\alpha_{-j}, \alpha'_{-j})}(u - \theta_j, v - \theta'_j) \right\}
\]

\[
= g_{(\theta_j + \alpha_j, \theta'_j + \alpha'_j)|(\alpha_{-j}, \alpha'_{-j})}(u, v)
\]

\[
= \mathbb{E}_{(\theta_j, \theta'_j)|(\alpha_{-j}, \alpha'_{-j})}\left\{ g_{(\theta_j, \theta'_j)|(\alpha, \alpha')}(u - \alpha_j', v - \alpha_j) \right\}
\]

\[
\leq e^\epsilon g_{(\theta'_j + \alpha'_j, \theta_j + \alpha_j)|(\alpha_{-j}, \alpha'_{-j})}(u, v) = e^\epsilon g_{(\kappa, \kappa')|(\alpha_{-j}, \alpha'_{-j})}(v, u),
\]

where \((*)\) holds according to the independence of \((\theta_j, \theta'_j)\) and \((\alpha, \alpha')\), and the fact that

\[
\left(\alpha_j', \alpha_j^\top, \alpha_j, \alpha_j'^\top\right) = \alpha_j \begin{pmatrix} X & \tilde{X} \end{pmatrix}^\top w \sim \mathcal{N}(0, \sigma^2 G).
\]

The inequality marked with \((**\) follows from the independence of \((\theta_j, \theta'_j)\) and \((\alpha, \alpha')\) and \((D.1)\). Therefore,

\[
\text{ess sup}_{u, v, \omega} \max \left\{ \frac{g(u, v)}{g(v, u)}, \frac{g(v, u)}{g(u, v)} \right\} \leq e^\epsilon,
\]

completing the proof. ■

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