A Pseudo Knockoff Filter for Correlated Features

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Abstract

In [3], the authors introduce a new variable selection procedure called the knockoff filter to control the false discovery rate (FDR) and prove that this method achieves exact FDR control. Inspired by the work of [3], we propose and analyze a pseudo-knockoff filter that inherits some advantages of the original knockoff filter and has more flexibility in constructing its knockoff matrix. Although we have not been able to obtain exact FDR control of the pseudo knockoff filter, we show that it satisfies an expectation inequality that offers some insight into FDR control. Moreover, we provide some partial analysis of the pseudo knockoff filter for the half Lasso and the least squares statistics. Our analysis indicates that the inverse of the covariance matrix of the feature matrix plays an important role in designing and analyzing the pseudo knockoff filter. Our preliminary numerical experiments show that the pseudo knockoff filter with the half Lasso statistic has FDR control. Moreover, our numerical experiments show that the pseudo-knockoff filter could offer more power than the original knockoff filter with the OMP or Lasso Path statistic when the features are correlated and non-sparse.

1 Introduction

In many applications, we need to study a statistical model that consists of a response variable and a large number of potential explanatory variables and determine which variables are truly associated with the response. In [3], Barber and Candès introduce the knockoff filter to control the FDR in a statistical linear model. More specifically, the knockoff filter constructs knockoff variables that mimic the correlation structure of the true feature variables to obtain exact FDR control in finite sample settings. It has been demonstrated that this method has more power than existing selection rules when the proportion of null variables is high.

1.1 A brief review of the knockoff filter

Consider the following linear regression model

$$y = X\beta + \epsilon,$$

where the feature matrix $X$ is a $n \times p$ ( $n \geq p$) matrix with full rank, its columns have been normalized to be unit vectors in the $l^2$ norm, and $\epsilon$ is a Gaussian noise $N(0, \sigma^2 I_n)$. The knockoff filter begins with the construction of a knockoff matrix $\tilde{X}$ that obeys

$$\tilde{X}^T\tilde{X} = X^TX, \quad \tilde{X}^TX = X^TX - \text{diag}(s),$$

(1)

where $s_i \in [0, 1], i = 1, 2, ..., p$. The positive definiteness of the Gram matrix $[X\tilde{X}]^T[X\tilde{X}]$ requires

$$\text{diag}(s) \preceq 2X^TX.$$  

(2)
The first condition in (1) ensures that $\tilde{X}$ has the same covariance structure as the original feature matrix $X$. The second condition in (1) guarantees that the correlations between distinct original and knockoff variables are the same as those between the original variables. To ensure that the method has good statistical power to detect signals, we should choose $s_j$ as large as possible to maximize the difference between $X_j$ and its knockoff $\tilde{X}_j$. These two conditions are crucial in establishing the exchangeability condition [3], which in turn gives exact FDR control. After constructing the knockoff matrix, one needs to calculate a statistic, $W_j$, for each pair of $X_j$ and $\tilde{X}_j$. One of the knockoff statistics considered in [3] is the Lasso path statistic, which is defined as $W_j = \max(Z_j, \tilde{Z}_j) \cdot \text{sign}(Z_j - \tilde{Z}_j)$, where $Z_j$ and $\tilde{Z}_j$ are the solutions of the Lasso path problem given below:

\[
(\hat{\beta}(\lambda), \tilde{\beta}(\lambda)) = \arg\min_{(b, \tilde{b})} \left\{ \frac{1}{2} \| y - Xb - \tilde{X}\tilde{b} \|_2^2 + \lambda (\|b\|_1 + \|\tilde{b}\|_1) \right\},
\]

\[Z_j = \sup\{\lambda : \hat{\beta}_j(\lambda) \neq 0\}, \quad \tilde{Z}_j = \sup\{\lambda : \tilde{\beta}_j(\lambda) \neq 0\}.
\]

The final step is to run the knockoff+ selection procedure at level $q$

\[
T \triangleq \min \left\{ t > 0 : \frac{1 + \#\{j : W_j \leq -t\}}{\#\{j : W_j \geq t\} \vee 1} \leq q \right\}, \quad \hat{S} \triangleq \{j : W_j \geq T\}.
\]

The main result in [3] is that such procedure controls exact FDR

\[FDR \triangleq E \left[ \frac{\#\{j \in \hat{S} : \beta_j = 0\}}{\#\{j \in \hat{S}\} \vee 1} \right] \leq q, \quad \forall q \in (0, 1).
\]

A knockoff filter for high-dimensional selective inference and model free knockoffs have been recently established in [4,5]. This research has inspired a number of follow-up works, such as [6,7,9,14–16].

The power (the proportion of true discoveries) of the knockoff filter depends critically on the value of $s_i$. In [6], we perform some analysis and numerical experiments on the knockoff filter to understand how (1) and (2) impose a constraint on $s_i$ when the features are correlated. Our analysis shows that $s_i$ could be small for strongly correlated features. On the other hand, for strongly correlated features with a finite sample size, we simply do not have enough resolution in the data to tell which variables are responsible for the response. In this case, it is more appropriate to define clusters of these correlated variables and ask whether there is any signal in those clusters rather than trying to decide which variable within the cluster is truly significant.

We note that a prototype knockoff filter based on group clustering of correlated data has been proposed in [14], and a group knockoff filter has been also proposed by Dai and Barber in [7] with exact FDR control. In [6], we also propose a PCA prototype group selection filter that achieves exact FDR control. Our PCA prototype group selection filter has the advantage of being more efficient and has higher power for correlated features. A localized knockoff filter has been proposed by Xu et al [16]. There are several other feature selection methods that offer some level of FDR control (e.g. [1,2,8,10,13]). We refer to [3] for a thorough comparison between the knockoff filter and these other approaches.

### 1.2 Three classes of pseudo knockoff filters

In this paper, we propose several pseudo-knockoff filters that inherit some advantages of the original knockoff filter and have greater flexibility in constructing their pseudo-knockoff matrix. In the pseudo knockoff filter, we seek to establish a weaker version of the exchangeability condition by relaxing the second condition in (1). The first condition that we impose on the pseudo knockoff filter is the following orthogonality condition:

\[(X + \tilde{X})^T(X - \tilde{X}) = 0.
\]
It can be shown that this condition is equivalent to \(X^TX = \hat{X}^T\hat{X}, X^T\hat{X} = \hat{X}^TX\). In a linear model \(y = X\beta + \epsilon, \epsilon \sim N(0, \sigma^2 I_n)\), this orthogonality condition implies that the projection of \(\epsilon\) onto \(\text{span}(X + \hat{X})\) and \(\text{span}(X - \hat{X})\) are independent.

In this paper, we consider three classes of pseudo knockoffs. For the first class of pseudo knockoff filters, the pseudo knockoff matrix \(\hat{X}\) is chosen to be orthogonal to \(X\), i.e. \(X^T\hat{X} = \hat{X}^TX = 0\). We call this pseudo knockoff the orthogonal pseudo knockoff. It maximizes the difference between the pseudo knockoff matrix \(\hat{X}\) and its original design matrix \(X\). Due to this orthogonality condition, we can always distinguish the original \(X_j\) and its pseudo knockoff \(\hat{X}_j\), independent of the correlation structure of \(X\).

The second class of pseudo knockoff filters is called the block diagonal pseudo knockoff. We begin by constructing a block diagonal matrix \(B\) that satisfies the property \(B \succeq \Sigma^{-1}\). We can then solve for \(\hat{X}\) from the relationship \(B = 4[(X - \hat{X})^T(X - \hat{X})]^{-1}\). More specifically, we consider a block diagonal matrix \(B = 2\text{diag}(S_{11}^{-1}, S_{22}^{-1}, \ldots, S_{kk}^{-1})\), where \(S_{ii}\)'s are invertible matrices. It can be shown that the condition (4) and the constraint \(B \succeq \Sigma^{-1}\) imply that

\[
X^TX = \hat{X}^T\hat{X}, \quad X^T\hat{X} - X^TX = \text{diag}(S_{11}, S_{22}, \ldots, S_{kk}). \tag{5}
\]

It is interesting to note that the pseudo knockoff matrix, \(\hat{X}\), in (5) is exactly a group knockoff matrix of \(X\) in [7]. Moreover, if we further impose \(S_{ii}\) to be a diagonal matrix for \(i = 1, 2, \ldots, k\), then \(\hat{X}\) is a knockoff matrix of \(X\) [3]. In this sense, we can consider the block diagonal pseudo knockoff filter as a generalization of the knockoff filter. We note that the group knockoff filter is designed for group selection while the block diagonal pseudo knockoff filter is designed for feature selection.

The third class of the pseudo knockoff filter is called the banded knockoff filter by imposing \(B\) to be a banded matrix. The construction is similar to the case when \(B\) is a block diagonal matrix.

### 1.3 A half Lasso statistic

We propose to use a half penalized method to construct our pseudo knockoff filter. More specifically, the pseudo knockoff statistic is based on the solution of the following half penalized optimization problem

\[
\min_{\beta, \hat{\beta}} \frac{1}{2}||y - X\hat{\beta} - \hat{X}\hat{\beta}||_2^2 + P(\hat{\beta} + \beta), \tag{6}
\]

where \(P(x)\) is an even non-negative and non-decreasing function in each coordinate of \(x\). An important consequence of the orthogonality condition (4) is that we can reformulate the half penalized problem into two sub-problems, i.e the minimization problem (6) is equivalent to the following minimization problem:

\[
\min_{\beta, \hat{\beta}} \left\{ \frac{1}{2}||X + \hat{X}((\beta^{ls} + \hat{\beta}^{ls} - \beta - \hat{\beta})||_2^2 + P(\hat{\beta} + \beta) \right\} + \min_{\beta, \hat{\beta}} \left\{ \frac{1}{2}||X - \hat{X}((\beta^{ls} - \hat{\beta}^{ls} - (\beta - \hat{\beta}))||_2^2 \right\},
\]

where \(\beta^{ls}\) and \(\hat{\beta}^{ls}\) are the least squares coefficients by regressing \(y\) on the augmented feature matrix \([X, \hat{X}]\). If we choose \(P \equiv 0\), we recover the least squares method. If we choose \(P = \lambda ||\cdot||_2\), we obtain a half Lasso method, which we introduce in [6]. Once we solve the half penalized problem, we can construct the pseudo knockoff statistic as follows

\[
W_j = (\hat{\beta}_j + \beta_j) \cdot \text{sign}(\hat{\beta}_j - \beta_j) \quad \text{or} \quad W_j = \max(|\hat{\beta}_j|, |\beta_j|) \cdot \text{sign}(|\hat{\beta}_j| - |\beta_j|). \tag{7}
\]

We can show the following symmetry property of the pseudo knockoff filter. Conditional on some \(\sigma\)-field, we have for any threshold \(t\) that

\[
\#\{j : \beta_j = 0 \text{ and } W_j \geq t\} \overset{d}{=} \#\{j : \beta_j = 0 \text{ and } W_j \leq -t\}. \tag{8}
\]
1.4 Partial analysis of the pseudo knockoff filter

The construction of our pseudo knockoff filter does not satisfy the exchangeability property, which is crucial for the knockoff filter in establishing exact FDR control by using a supermartingale argument [3]. In this paper, we provide some partial analysis for the pseudo knockoff filter by trying to establish the following expectation inequality:

$$E \left[ \frac{\# \{ j : W_j \geq t, \beta_j = 0 \}}{\# \{ j : W_j \leq -t, \beta_j = 0 \} + m} \right] \leq 1$$

(9)

for any fixed threshold $t > 0$ and some $m \in \mathbb{N}_+$ that depends on the pseudo knockoff matrix $\tilde{X}$. This inequality can be considered as an approximation to the corresponding expectation inequality for the knockoff filter:

$$E \left[ \frac{\# \{ j : W_j \geq T, \beta_j = 0 \}}{\# \{ j : W_j \leq -T, \beta_j = 0 \} + 1} \right] \leq 1,$$

(10)

for an adaptive threshold $T$.

In this paper, we establish the expectation inequality (9) for the block diagonal and the banded pseudo knockoff filters. For the orthogonal pseudo knockoff filter, we use a probabilistic argument to obtain a relatively tight upper bound to the expectation in (9) for $t = 0$ when $\Sigma^{-1}$ is diagonally dominated or when $\Sigma^{-1}$ has some special structure. Interestingly, our analysis reveals that the decaying property of $\Sigma^{-1}$ plays an important role in determining the performance of the pseudo knockoff filter and the knockoff filter.

We also carry out a number of numerical experiments to test the performance of the three classes of pseudo knockoff filters and compare their performance with that of the knockoff filter. In the examples that we consider in this paper, we find that the three classes of pseudo knockoff filters with the half Lasso statistic have FDR control. The orthogonal pseudo knockoff filter seems to offer the most power among all other pseudo knockoff filters. In the case when the features are highly correlated and non-sparse (e.g., about 20% non-null features), the orthogonal pseudo knockoff filter offers more power than the knockoff filter with the OMP or Lasso Path statistic. In the extreme case when $\Sigma^{-1}$ decays very slowly away from its main diagonal, the knockoff filter with the OMP or the Lasso Path statistic tends to lose considerable power. The orthogonal pseudo knockoff filter still offers reasonably high power in this case.

The rest of the paper is organized as follows. In Section 2, we introduce the three classes of pseudo-knockoff filters and discuss some essential properties of the pseudo knockoff filters. In Section 3, we present a number of numerical experiments to demonstrate the effectiveness of the proposed methods. In Section 4, we provide some partial analysis of the pseudo knockoff filters and present additional numerical experiments to compare the performance of the pseudo knockoff filters with the knockoff filter using the OMP and the Lasso Path statistics.

2 A pseudo knockoff filter

2.1 An expectation inequality

In the knockoff filter, the exchangeability property is essential [3]. This important property allows one to apply a supermartingale argument to obtain the following expectation inequality:

$$E \left[ \frac{\# \{ j : W_j \geq T, \beta_j = 0 \}}{\# \{ j : W_j \leq -T, \beta_j = 0 \} + 1} \right] \leq 1,$$

(11)

for an adaptive threshold $T$. The above estimate plays a crucial role in establishing exact FDR control of the knockoff filter [3]. Our motivation is to relax the second constraint in (11) in a way such that (11) is still approximately valid. In particular, we consider a modified version of (11)
for any fixed threshold \( t > 0 \) and some \( m \in \mathbb{N}_+ \) that depends on the pseudo knockoff matrix \( \hat{X} \).

To see how (12) relates to FDR control, we first define the pseudo knockoff+ adaptive threshold \( T \) as follows
\[
T_m \triangleq \min \left\{ t : \frac{\# \{ j : W_j \leq -t \} + m}{\# \{ j : W_j \geq t \} + 1} \leq q \right\}.
\]

(13)

By the definition of \( T_m \), we have
\[
FDR \triangleq E \left[ \frac{\# \{ j \in S_0 : W_j \geq T \}}{\# \{ j : W_j \geq T \} \lor 1} \right] = E \left[ \frac{\# \{ j \in S_0 : W_j \geq T \}}{\# \{ j : W_j \leq -T \} + m} \right] \cdot \frac{\# \{ j \in S_0 : W_j \leq -T \} + m}{\# \{ j : W_j \geq T \} \lor 1}
\]
\[
\leq q \cdot E \left[ \frac{\# \{ j : W_j \geq T, \beta_j = 0 \}}{\# \{ j : W_j \leq -T, \beta_j = 0 \} + m} \right],
\]

(14)

where \( S_0 = \{ j : \beta_j = 0 \} \). For \( m = 1 \), (11) and (13) establish FDR control of the knockoff filter.

One may consider (12) as an approximation of (11). Our numerical study shows that when (12) is valid, (11) is approximately valid and we have FDR control for the pseudo knockoff filter. However, (12) alone does not give exact FDR control since \( T_m \) is a random variable.

2.2 The Basic Constraint and a Symmetry Property

The basic constraint of the pseudo knockoff matrix is given by
\[
\hat{X}^T \hat{X} = X^T X, \quad X^T \hat{X} = \hat{X}^T X.
\]

The correlation structure and the commutativity imply
\[
(X + \hat{X})^T (X - \hat{X}) = X^T X + \hat{X}^T X - X^T \hat{X} - \hat{X}^T \hat{X} = 0.
\]

(15)

(16)

We can prove that (15) and (16) are equivalent. If (16) holds, we have \( X^T X - \hat{X}^T \hat{X} = X^T \hat{X} - \hat{X}^T X \).

Note that the right hand side is a symmetric matrix, while the left hand side is a skew-symmetric matrix. It follows that \( X^T X - \hat{X}^T \hat{X} \) is symmetric and skew-symmetric. Thus we must have \( X^T X - \hat{X}^T \hat{X} = X^T \hat{X} - \hat{X}^T X = 0 \). These two equations establish (15).

The orthogonality condition (16) is the foundation of the pseudo knockoff filter and leads to a symmetry property of the pseudo knockoff filter.

Least squares coefficients

Consider the least squares coefficients of regressing \( y \) on the augmented design matrix \([X \bar{X}]\)
\[
y \sim X \hat{\beta}^{ls} + \bar{X} \tilde{\beta}^{ls} = \frac{X + \bar{X}}{2} (\hat{\beta}^{ls} + \bar{\beta}^{ls}) + \frac{X - \bar{X}}{2} (\hat{\beta}^{ls} - \bar{\beta}^{ls}).
\]

Using \( y = X \beta + \epsilon \) and the orthogonality condition (16), we have a simple expression of the least squares coefficients,
\[
\begin{pmatrix}
\hat{\beta}^{ls} + \bar{\beta}^{ls} - \beta \\
\hat{\beta}^{ls} - \bar{\beta}^{ls} - \beta
\end{pmatrix} = \begin{pmatrix}
\frac{X + \bar{X}}{2}, & \frac{X - \bar{X}}{2}
\end{pmatrix}^T \begin{pmatrix}
\frac{X + \bar{X}}{2}, & \frac{X - \bar{X}}{2}
\end{pmatrix}^{-1} \begin{pmatrix}
(X + \bar{X})^T \epsilon \\
(X - \bar{X})^T \epsilon
\end{pmatrix}
\]
\[
= \begin{pmatrix}
\frac{X + \bar{X}}{2}, & \frac{X - \bar{X}}{2}
\end{pmatrix}^{-1} \begin{pmatrix}
(X + \bar{X})^T \epsilon \\
(X - \bar{X})^T \epsilon
\end{pmatrix} \triangleq \begin{pmatrix}
\epsilon^{(1)} \\
\epsilon^{(2)}
\end{pmatrix}.
\]

(17)
Using the orthogonality condition (\(X\)) we can exclude the residue \(\tilde{r}\). From the orthogonality property (16), we know that (2) \((X^\top \tilde{X})^T \epsilon\) and \((X^\top \tilde{X})^T \epsilon\) have independent multivariate normal distributions. Using (17), we know that (1) \(\epsilon\) and (2), \(\eta = \hat{\beta}^{ls} + \tilde{\beta}^{ls}\) and \(\xi = \hat{\beta}^{ls} - \tilde{\beta}^{ls}\) are also independent.

**The Pseudo Knockoff Statistic** Similar to the knockoff filter process, we construct a pseudo knockoff statistic for each pair of the original feature \(X_j\) and its pseudo knockoff \(\tilde{X}_j\).

Consider a half penalized optimization problem

\[
\min_{\hat{\beta}, \tilde{\beta}} \frac{1}{2} ||y - X\hat{\beta} - \tilde{X}\hat{\beta}||_2^2 + P(\hat{\beta} + \tilde{\beta}).
\]  

(19)

Denote by \(r\) the residue of regressing \(y\) onto the augmented design matrix \([X\tilde{X}]\), i.e. \(r = y - X\hat{\beta}^{ls} - \tilde{X}\tilde{\beta}^{ls}\). The geometric property of the least squares method implies \(r \perp X, \tilde{X}\), which leads to

\[
||y - X\hat{\beta} - \tilde{X}\hat{\beta}||_2^2 = ||r + X\hat{\beta}^{ls} + \tilde{X}\tilde{\beta}^{ls} - X\hat{\beta} - \tilde{X}\hat{\beta}||_2^2 = ||r||_2^2 + ||X\hat{\beta}^{ls} + \tilde{X}\tilde{\beta}^{ls} - X\hat{\beta} - \tilde{X}\hat{\beta}||_2^2.
\]

Using the orthogonality condition \((X + \tilde{X})^T (X - \tilde{X}) = 0\) and the fact that \(r\) is independent of \(\hat{\beta}, \tilde{\beta}\), we can exclude the residue \(r\) from the optimization problem (19) and reformulate it as follows

\[
\min_{\hat{\beta}, \tilde{\beta}} \frac{1}{2} ||X\hat{\beta}^{ls} + \tilde{X}\tilde{\beta}^{ls} - X\hat{\beta} - \tilde{X}\hat{\beta}||_2^2 + P(\hat{\beta} + \tilde{\beta})
\]

\[
\iff \min_{\hat{\beta}, \tilde{\beta}} \frac{1}{2} ||X\hat{\beta}^{ls} + \tilde{X}\tilde{\beta}^{ls} - X\hat{\beta} - \tilde{X}\hat{\beta}||_2^2 + P(\hat{\beta} + \tilde{\beta})
\]

\[
= \min_{\hat{\beta}, \tilde{\beta}} \left\{ \frac{1}{2} \left| \frac{X + \tilde{X}}{2} (\hat{\beta}^{ls} + \tilde{\beta}^{ls} - \hat{\beta} - \tilde{\beta}) \right|_2^2 + P(\hat{\beta} + \tilde{\beta}) \right\} + \left\{ \frac{1}{2} \left| \frac{X - \tilde{X}}{2} (\hat{\beta}^{ls} - \tilde{\beta}^{ls} - (\hat{\beta} - \tilde{\beta})) \right|_2^2 \right\} + \min_{\beta - \tilde{\beta}} \left\{ \frac{1}{2} \left| \frac{X - \tilde{X}}{2} (\hat{\beta}^{ls} - \tilde{\beta}^{ls} - (\hat{\beta} - \tilde{\beta})) \right|_2^2 \right\},
\]

(20)

where \(\hat{\beta}^{ls}\) and \(\tilde{\beta}^{ls}\) are the least squares coefficients given in (17). It is easy to derive that the solution of these problems can be expressed as

\[
\hat{\beta} + \tilde{\beta} = f(\hat{\beta}^{ls} + \tilde{\beta}^{ls}) = f(\eta), \quad \hat{\beta} - \tilde{\beta} = \hat{\beta}^{ls} - \tilde{\beta}^{ls} = \xi,
\]

(21)

for some function \(f : \mathbb{R}^p \rightarrow \mathbb{R}^p\). We construct the pseudo knockoff statistic as follows

\[
W_j \triangleq (\hat{\beta}_j + \tilde{\beta}_j) \cdot \text{sign}(\hat{\beta}_j - \tilde{\beta}_j) \text{ or } W_j = \max(\|\hat{\beta}_j\|, \|\tilde{\beta}_j\|) \cdot \text{sign}(\|\hat{\beta}_j\| - \|\tilde{\beta}_j\|).
\]

(22)

The pseudo knockoff statistic satisfies the following two properties.

**Amplitude Property** The amplitude of \(W\) is decided by \(\hat{\beta} + \tilde{\beta} = f(\eta)\) and \(|\hat{\beta} - \tilde{\beta}| = |\xi|\).

In fact, using the definition of \(W\) and (21), we have

\[
|W| = |\hat{\beta} + \tilde{\beta}| = |f(\eta)| \quad \text{or} \quad |W| = |\hat{\beta}| \vee |\tilde{\beta}| = \frac{1}{2} (|\hat{\beta} + \tilde{\beta}| + |\hat{\beta} - \tilde{\beta}|) \vee |\hat{\beta} + \tilde{\beta} - |\hat{\beta} - \tilde{\beta}||).
\]

**Sign Property** The sign of \(W\) is determined by \(\text{sign}(\hat{\beta} + \tilde{\beta})\) and \(\text{sign}(\hat{\beta} - \tilde{\beta})\). Since \(\text{sign}(\|\hat{\beta}\| - |\tilde{\beta}|) = \text{sign}(|\tilde{\beta}^2 - |\hat{\beta}|^2|)\), we have

\[
\text{sign}(W) = \text{sign}(\hat{\beta} + \tilde{\beta}) \cdot \text{sign}(\hat{\beta} - \tilde{\beta}) = \text{sign}(f(\eta)) \cdot \text{sign}(\xi),
\]

for both definitions of \(W\).

Now we show that the pseudo knockoff statistic satisfies a symmetry property.
Proposition 2.1. (The Symmetry Property of the Pseudo Knockoff Statistic) Conditional on $\eta$, we have for any threshold $t$ that

$$\#\{j : \beta_j = 0 \text{ and } W_j \geq t\} \overset{d}{=} \#\{j : \beta_j = 0 \text{ and } W_j \leq -t\},$$

(23)

where the pseudo knockoff statistic $W_j$ determined by a projection is generated by $(\hat{\beta}_j, \tilde{\beta}_j)$. Hence, conditional on $\eta$, we get

$$\lambda \min_{\hat{\beta}, \tilde{\beta}} \frac{1}{2} ||y - X\hat{\beta} - \tilde{X}\tilde{\beta}||^2_2 + \lambda ||\hat{\beta} + \tilde{\beta}||_1.$$  

(26)

From (24) and (25), we have

$$\hat{\beta}_\text{new} + \tilde{\beta}_\text{new} = f(\eta) = \hat{\beta} + \tilde{\beta}, \quad \hat{\beta}_\text{new} - \tilde{\beta}_\text{new} = \beta - \epsilon(2).$$

(25)

Recall that $W_S$ is generated by $\epsilon(1), \epsilon(2)$ and that $\epsilon(1), \epsilon(2)$ have independent multivariate normal distributions with zero mean. Conditional on $\eta$ (or equivalently $\epsilon(1)$), we have

$$\epsilon(1), \epsilon(2) \overset{d}{=} (\epsilon(1), -\epsilon(2)) \implies W_{S_0} \overset{d}{=} W_{S_0} = -W_{S_0}.$$  

(27)

As a result, conditional on $\eta$, we get

$$\#\{j : \beta_j = 0 \text{ and } W_j \geq t\} \overset{d}{=} \#\{j : \beta_j = 0 \text{ and } W_j \leq -t\},$$

for any threshold $t > 0$.

Pseudo knockoff least squares and half Lasso statistics We give two examples of the pseudo knockoff statistics.

The least squares statistic Let $P \equiv 0$ in (20). The half penalized problem becomes the least squares problem of the response $y$ and the augmented design matrix $[\tilde{X} \tilde{X}]$.

A half Lasso statistic In [6], we introduce a half penalized method for the knockoff filter. The derivation in (20) implies that we can also apply this idea to the pseudo knockoff filter. Specifically, we choose $P(x) = \lambda ||x||_1$ in (20) to obtain a half Lasso statistic:

$$\min_{\hat{\beta}, \tilde{\beta}} \frac{1}{2} ||y - X\hat{\beta} - \tilde{X}\tilde{\beta}||_2^2 + \lambda ||\hat{\beta} + \tilde{\beta}||_1.$$  

Let $\hat{\beta}, \tilde{\beta}$ be the solution of the least squares or the half Lasso problem and we define the pseudo knockoff statistic $W_j = |\hat{\beta}_j + \tilde{\beta}_j| \text{sign}(\hat{\beta} - \tilde{\beta})$ or $W_j \overset{d}{=} \text{max}(|\hat{\beta}_j|, |\tilde{\beta}_j|) \cdot \text{sign}(|\hat{\beta}_j| - |\tilde{\beta}_j|)$. The symmetry property (23) of these statistics is guaranteed by Proposition 2.1. The tuning parameter $\lambda$ can be determined by a projection

$$\lambda = \mu \cdot \frac{1}{\sqrt{n - 2p}} ||U^Ty||_2,$$

where $U \in R^{n \times (n - 2p)}$ is an orthonormal matrix such that $[\tilde{X} \tilde{X}]^TU = 0$ and $\mu$ is a parameter that we can choose empirically. In fact, $U^Ty$ is exactly the residue of regressing $y$ onto $[\tilde{X} \tilde{X}]$. One can verify the symmetry property of the pseudo knockoff statistic with this tuning parameter using a similar argument.
2.3 Three Classes of the Pseudo Knockoff Matrix

We have proposed the basic constraint \((15)\) for the pseudo knockoff matrix in the last section. In this section, we impose an additional constraint on \(\tilde{X}\) so that we can establish an additional property on the pseudo knockoff statistic. In particular, we are interested in three classes of pseudo knockoff matrices, namely the orthogonal, the block diagonal, and the banded pseudo knockoff matrices.

2.3.1 An Orthogonal Construction

In this special pseudo knockoff filter, we impose an orthogonal constraint on the second condition of \((15)\)

\[
X^T X = \tilde{X}^T \tilde{X}, \quad X^T \tilde{X} = \tilde{X}^T X = 0
\]

(28)

to yield the orthogonal pseudo knockoff matrix.

To construct an orthogonal pseudo knockoff matrix \(\tilde{X}\), we first find the SVD of \(X \in R^{n \times p}: X = UDV^T, U \in \text{Orth}^{n \times p}, D = \text{diag} (\sigma_1, ..., \sigma_p) \) and \(V \in \text{Orth}^{p \times p}. \) We then choose any orthonormal matrix \(W \in R^{n \times p}\), whose column space is orthogonal to that of \(X\) (i.e. \(X^T W = 0\)), and construct the pseudo knockoff matrix \(\tilde{X}\) as \(\tilde{X} = WDV^T\). It is easy to verify that \(\tilde{X}\) satisfies the pseudo knockoff matrix condition \((28)\).

2.3.2 A Block Diagonal Construction

It follows from \((17)\) and \((18)\) that the covariance matrix of \(\epsilon^{(2)}\), or equivalently \(\xi\), is given by

\[
B \triangleq 4[(X - \tilde{X})^T (X - \tilde{X})]^{-1}.
\]

(29)

We can design \(B\) to yield a special correlation structure on \(\xi\). Due to the existing constraint \((15)\) or \((16)\), the covariance matrix \(B\) cannot be chosen arbitrarily. Below we give a necessary and sufficient condition on \(B\) to find \(\tilde{X}\) that satisfies \((16)\) and \((29)\).

**Necessary Condition on \(B\)** Assume that there exists some \(\tilde{X}\) that satisfies \((16)\) and \((29)\) and \(X - \tilde{X}\) has full rank. Performing SVD on \((X - \tilde{X})/2\), we have \((X - \tilde{X})/2 = PM^{-1}\) for some orthonormal matrix \(P \in R^{n \times p}\) and some invertible matrix \(M \in R^{p \times p}\). As a result, we get \(B = [\text{det}(PM^{-1})^{-1}]^{-1} = MM^T\). Substituting the last equation into the orthogonal condition \((X + \tilde{X})^T (X - \tilde{X}) = 0\) \((16)\), we obtain

\[
4(X - PM^{-1})^T PM^{-1} = 0 \iff M^{-T}M^{-1} = M^{-T}P^TX
\]

Since \(P \in R^{n \times p}\) is orthonormal, we have

\[
X^T PP^TX \preceq X^T LX = X^T X = \Sigma \implies B = (X^T PP^TX)^{-1} \succeq \Sigma^{-1}.
\]

(30)

**Sufficiency** We prove that the condition \((30)\) on \(B\) is sufficient to find a \(\tilde{X}\) that satisfies \((16)\) or \((15)\). To see this, we construct \(\tilde{X}\) as follows

\[
\tilde{X} = X(I - 2\Sigma^{-1}B^{-1}) + 2UCB^{-1}
\]

(31)

where \(C \in R^{p \times p}\) satisfies \(C^T C = B - \Sigma^{-1}\) and \(U \in R^{n \times p}\) is an orthonormal matrix with \(U^T X = 0\). We can verify that \(\tilde{X}\) constructed from \((31)\) satisfies \((16)\) and \((29)\) in the Appendix.

**A Block Diagonal Construction** Consider a block diagonal matrix \(B = 2\text{diag}(S_{11}^{-1}, S_{22}^{-1}, ..., S_{kk}^{-1})\), where \(S_{ii}\)'s are invertible matrices. The constraint on \(B\) is equivalent to

\[
2B^{-1} = \text{diag}(S_{11}, S_{22}, ..., S_{kk}) \succeq 2\Sigma.
\]

(32)

Hence \((X - \tilde{X})^T (X - \tilde{X}) = 4B^{-1} = 2\text{diag}(S_{11}, S_{22}, ..., S_{kk})\). Using this relationship together with the basic constraint \((15)\), i.e. \(X^T X = \tilde{X}^T \tilde{X}, X^T \tilde{X} = \tilde{X}^T X\), we obtain

\[
X^T X = \tilde{X}^T \tilde{X}, \quad X^T X - X^T \tilde{X} = \text{diag}(S_{11}, S_{22}, ..., S_{kk}).
\]

(33)
Construction. Assume that $X$ can be clustered into $(X_{G_1}, X_{G_2}, \ldots, X_{G_k})$, $|G_i| = g_i$. Inspired by the group knockoff construction in [3], we first choose $S_{ii}$ as

$$S_{ii} \triangleq \gamma \Sigma_{G_i, G_i} = \gamma X_{G_i}^T X_{G_i}, \quad i = 1, 2, \ldots, k.$$  

The constraint (32) implies $\gamma \cdot \text{diag}(\Sigma_{G_i, G_i}, \Sigma_{G_2, G_2}, \ldots, \Sigma_{G_k, G_k}) \leq 2\Sigma$. In order to maximize the difference between $X$ and $\tilde{X}$, $\gamma$ should be chosen as large as possible: $\gamma \leq \min\{1, 2 \cdot \lambda_{\min}(D\Sigma D)\}$, where $D = \text{diag}(\Sigma^{-1/2}_{G_1, G_1}, \Sigma^{-1/2}_{G_2, G_2}, \ldots, \Sigma^{-1/2}_{G_k, G_k})$. To ensure that the matrix $(X + \tilde{X})^T (X + \tilde{X})$ is nonsingular, we choose $\gamma = \min\{1, 2 \cdot \lambda_{\min}(D\Sigma D)\}$ in our numerical experiments. Once we construct $B$, we can generate the pseudo knockoff matrix via the procedure described earlier.

Connection between the pseudo knockoff filter and the knockoff filter. By comparing our block diagonal pseudo knockoff construction with the group knockoff filter in [3], we can see that the pseudo knockoff filter, $\tilde{X}$, in (33) is actually a group knockoff matrix of $X$. Moreover, if $S_{ii}$ is a diagonal matrix for $i = 1, 2, \ldots, k$, then $\tilde{X}$ is a knockoff matrix of $X$ [3]. Recall that the second constraint in (11) in the original knockoff filter requires that $X^T X - X^T \tilde{X}$ be a diagonal matrix. In the block diagonal pseudo knockoff filter, we only require that $X^T X - X^T \tilde{X}$ be a block diagonal matrix. In this sense, we can consider the block diagonal construction of the pseudo knockoff filter as a generalization of the group knockoff matrix proposed by Dai-Barber in [7]. The group knockoff filter is originally designed for group selection with group FDR control while our block diagonal pseudo knockoff filter is designed for feature selection. We will show that the pseudo knockoff filter with the block diagonal construction satisfies (12) and provide some partial analysis of this method later on. Our numerical experiments seem to suggest that this method works reasonably well.

2.3.3 A Banded Matrix Construction

Consider a banded matrix $B$ with band width $m$, i.e. $B_{ij} = 0$ if $|i - j| > m$. We are mostly interested in $m = 2$. The other cases can be handled similarly. There are many approaches to construct $B$ that satisfy $B \succeq \Sigma^{-1}$. We propose one of these approaches and outline the main steps as follows.

Step 1: Extraction. Extract the tri-diagonal elements of $\Sigma^{-1}$, i.e.

$$D \triangleq \begin{bmatrix} (\Sigma^{-1})_{11} & (\Sigma^{-1})_{12} \\ (\Sigma^{-1})_{21} & \ddots & \ddots \\ \cdots & \ddots & (\Sigma^{-1})_{p-1,p} \\ (\Sigma^{-1})_{p,p-1} & (\Sigma^{-1})_{pp} \end{bmatrix}.$$  

In general, $D$ is not a positive definite matrix. We need to modify the diagonal elements of $D$ to get a positive definite matrix.

Step 2: Modification of $D$. We consider the following modification of $D$:

$$\tilde{D}_{ii} = D_{ii} + \frac{D_{i,i+1}^2}{D_{i+1,i+1}}, \quad i = 1, 2, \ldots, p-1, \quad \tilde{D}_{pp} = D_{pp}, \quad \tilde{D}_{ij} = D_{ij}, \quad \forall i \neq j.$$  

To see that $\tilde{D}$ is positive definite, we consider $v^T \tilde{D} v$ for an arbitrary vector $v \neq 0 \in R^p$.

$$v^T \tilde{D} v = \sum_{i=1}^{p-1} \left( D_{ii} + \frac{D_{i,i+1}^2}{D_{i+1,i+1}} \right) v_i^2 + 2 \sum_{i=1}^{p-1} D_{i,i+1} v_i v_{i+1} + D_{pp} v_p^2$$

$$= \sum_{i=1}^{p-1} \left( D_{i+1,i+1} v_i^2 + \frac{D_{i,i+1}^2}{D_{i+1,i+1}} v_i^2 + 2 D_{i,i+1} v_i v_{i+1} \right) + D_{11} v_1^2$$

$$= \sum_{i=1}^{p-1} \sum_{j=i}^{p-1} \frac{D_{i,j}^2}{D_{j+1,j+1}} v_i v_j + 2 \sum_{i=1}^{p-1} D_{i,i+1} v_i v_{i+1} + D_{pp} v_p^2.$$  

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\[
= \sum_{i=1}^{p-1} \frac{1}{D_{i+1,i+1}} (D_{i,i+1}v_i + D_{i+1,i+1}v_{i+1})^2 + D_{11}v_1^2 > 0, \quad \forall v \neq 0.
\]

**Step 3: Construction of B**  Since $\tilde{D}$ is positive definite, we take
\[
B \triangleq \tau \lambda_{\text{max}}(\tilde{D}^{-1/2} \Sigma^{-1} \tilde{D}^{-1/2}) \cdot \tilde{D},
\]
where $\tau \geq 1$ is a parameter. Since $\lambda_{\text{max}}(\tilde{D}^{-1/2} \Sigma^{-1} \tilde{D}^{-1/2}) \geq \tilde{D}^{-1/2} \Sigma^{-1} \tilde{D}^{-1/2}$, we have
\[
B = \tau \tilde{D}^{1/2} \cdot \lambda_{\text{max}}(\tilde{D}^{-1/2} \Sigma^{-1} \tilde{D}^{-1/2}) \cdot \tilde{D}^{1/2} \geq \tilde{D}^{1/2} \cdot \tilde{D}^{-1/2} \Sigma^{-1} \tilde{D}^{-1/2} \cdot \tilde{D}^{1/2} = \Sigma^{-1}.
\]

In our numerical experiments, we choose $\tau = 1.2$ to ensure that $(X + \tilde{X})^T(X + \tilde{X})$ is nonsingular.

**Remark 1.** For some design matrices with a special correlation structure, we can use a different construction of $B$ or $\tilde{B}$. Since the covariance matrix of $\xi = \hat{\beta}_{\text{ls}} - \tilde{\beta}_{\text{ls}}$ is $B$, we can divide $\xi, 1 \leq i \leq p$ into $m$ groups $C_1, C_2, \ldots, C_m$ such that the random variables in the same group are mutually independent.

For the block diagonal construction, $C_i$ consists of the $i$-th element in each block if there exists such an element. For the banded construction, $C_i \triangleq \{ j : j \equiv i (\text{mod } m), 1 \leq j \leq p \}$. It is easy to verify that the random variables within each group are independent.

### 2.4 A theoretical result for the expectation inequality

In this section, we prove (12) for the pseudo knockoff statistic that is constructed using either a block diagonal or a banded matrix construction.

**Theorem 2.2.** Assume that the pseudo knockoff matrix is generated via a block diagonal or a banded construction and the pseudo knockoff statistic is defined as $W \triangleq (\hat{\beta} + \tilde{\beta}) \cdot \text{sign}(\hat{\beta} - \tilde{\beta})$. For any $t > 0$, we have
\[
E \left[ \frac{\# \{ j \in S_0 : W_j \geq t \}}{\# \{ j \in S_0 : W_j \leq -t \} + m} \right] \leq 1,
\]
where $m$ is the largest group size in the block diagonal construction or the band width in the banded construction. When $m = 1$, (34) replicates a result similar to (11).

**Proof.** Let $\mathcal{F}$ be the $\sigma$-field generated by $\eta$. Since $|W| = |f(\eta)|$ by our choice of $W$, conditional on $\eta$, we can determine $|W|$ and $N_t \triangleq \{ j \in S_0 : |W_j| \geq t \}$. We will show that the conditional expectation satisfies
\[
E \left[ \frac{\# \{ j \in S_0 : W_j \geq t \}}{\# \{ j \in S_0 : W_j \leq -t \} + m} \mid \mathcal{F} \right] \leq 1.
\]
(35)

Once we obtain (35), we can integrate both sides to obtain (34). From our previous discussion, we can divide $N_t$ into $m$ groups $C_1, C_2, \ldots, C_m$ ($C_i \subset S_0$) such that the elements of $\xi_{C_i}$ are mutually independent. Obviously, $|N_t| = \sum_{i=1}^{m} |C_i|$. Using the following Cauchy-Schwarz inequality
\[
\sum_{i=1}^{m} \frac{a_i^2}{b_i} \sum_{i=1}^{m} b_i \geq (\sum_{i=1}^{m} a_i)^2 \iff \frac{1}{\sum_{i=1}^{m} a_i} \sum_{i=1}^{m} \frac{a_i^2}{b_i} \geq \frac{\sum_{i=1}^{m} a_i}{\sum_{i=1}^{m} b_i}, \quad a_i, b_i > 0,
\]
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with \( a_i = |C_i| + 1 \), \( b_i = \#\{j \in C_i : W_j \leq -t\} + 1 \), we obtain

\[
E \left[ \frac{\#\{j \in S_0 : W_j \geq t\}}{\#\{j \in S_0 : W_j \leq -t\} + m} \right] = E \left[ \frac{|N_t| + m}{\sum_{i=1}^{m} (\#\{j \in C_i : W_j \leq -t\} + 1)} \right] - 1
\]

\[
\leq E \left[ \frac{1}{|N_t| + m} \sum_{i=1}^{m} \frac{(|C_i| + 1)^2}{\#\{j \in C_i : W_j \leq -t\} + 1} \right] - 1
\]

\[
= \sum_{i=1}^{m} \frac{|C_i| + 1}{|N_t| + m} \left\{ 1 + E \left[ \frac{\#\{j \in C_i : W_j \geq t\}}{\#\{j \in C_i : W_j \leq -t\} + 1} \right] \right\} - 1.
\]

(36)

Here, we use \( \#\{j \in C_i : W_j \leq -t\} + 1 + \#\{j \in C_i : W_j \geq t\} = |C_i| + 1 \) to obtain the first and the last equality, and use the fact that \( |N_t|, |C_i| \) are measurable w.r.t \( \mathcal{F} \) to yield the second equality.

Note that \( \xi \) and \( \eta \) are independent, \( \text{sign}(\xi) \), \( j \in C_i \) are mutually independent, and \( \xi_{S_0} \) have mean zero multivariate normal distributions. Conditional on \( \mathcal{F} \), \( \text{sign}(W_j) = \text{sign}(f(\eta))_{ij} \text{sign}(\xi) \), \( j \in C_i \) are independent and thus \( \text{sign}(W_j), j \in C_i \) obeys a binomial distribution. We yield

\[
E \left[ \frac{\#\{j \in C_i : W_j \geq t\}}{\#\{j \in C_i : W_j \leq -t\} + 1} \right] = E \left[ \frac{\#\{j \in C_i : W_j > 0\}}{\#\{j \in C_i : W_j < 0\} + 1} \right] \leq 1.
\]

Therefore, the last line in (36) is bounded by

\[
-1 + \frac{1}{|N_t| + m} \sum_{i=1}^{m} 2(|C_i| + 1) = -1 + \frac{2}{|N_t| + m} (|N_t| + m) = 1.
\]

(38)

Combining (36) with (38) yields (35). Finally, we integrate both sides of (35) to conclude the proof. \( \square \)

Remark 2. In order to control the expectation in (33) by 1, we consider the conditional expectation (35) and add the maximal group size \( m \) (or the band width in the banded construction) in the denominator. We show that this is optimal.

Let us consider the block diagonal construction with \( \beta = 0 \) (no signal). Recall that the covariance matrix of \( \xi \) is block diagonal, i.e. \( B = \text{diag}(D_{11}, D_{22}, \ldots, D_{kk}) \). Assume that the size of each block is \( m \) and the off-diagonal elements of \( D_{ii} \) are close to the diagonal elements. Accordingly, \( \xi_i, \xi_j \) are strongly correlated if \( i, j \) are in the same block or are independent if \( i, j \) come from different blocks. Let \( t = 0 \) in (35). Conditional on \( \eta \), we have \( \text{sign}(W_j) = \text{sign}(f(\eta))_{ij} \text{sign}(\xi) \). If \( \text{sign}(f(\eta))_{ij} \)'s are the same in each block, i.e. \( \text{sign}(f(\eta))_{ij} = \text{sign}(f(\eta))_{ij,1} \), we yield

\[
Z_1 \triangleq \sum_{i=1}^{p} \sum_{j=1}^{m} \mathbf{1}_{W_{i,j} > 0} = \sum_{i=1}^{k} \sum_{j=1}^{m} \mathbf{1}_{W_{i,j} > 0} \geq \sum_{i=1}^{k} \sum_{j=1}^{m} \mathbf{1}_{\xi_{i,j}, (f(\eta))_{i,j} > 0} \geq m \sum_{i=1}^{k} \mathbf{1}_{\xi_{i,1}, (f(\eta))_{i,1} > 0} = m \sum_{i=1}^{k} \mathbf{1}_{W_{i,1} > 0}.
\]

Here, \( \xi_{i,j} \) and \( W_{i,j} \) are the \( j \)-th element in block \( i \). In the above derivation, we have used that \( \xi_i, \xi_j \) are strongly correlated if \( i, j \) are in the same block. Similar analysis can be applied to \( Z_2 \triangleq \sum_{i=1}^{p} \mathbf{1}_{W_{i} < 0} \). Plugging these estimates into the expectation, we obtain

\[
E \left( \frac{Z_1}{Z_2 + m} \right) \approx E \left[ \frac{\sum_{i=1}^{k} \mathbf{1}_{W_{i,1} > 0}}{m + m \sum_{i=1}^{k} \mathbf{1}_{W_{i,1} < 0}} \right] = E \left[ \frac{\sum_{i=1}^{k} \mathbf{1}_{W_{i,1} > 0}}{1 + \sum_{i=1}^{k} \mathbf{1}_{W_{i,1} < 0}} \right].
\]

Since \( \xi_{i,1} \) are mutually independent with mean 0, \( \mathbf{1}_{W_{i,1} > 0} \) are i.i.d and obeys a binomial distribution. Thus, the expectation on the right hand side is \( 1 - 2^{-k} \). Consequently, for any \( \tilde{m} < m \), it is likely that the expectation \( E(Z_1/(Z_2 + \tilde{m})) \) exceeds 1.
In the above analysis, we rely on the fact that the amplitude of \( W_{S_0} \) and \( \text{sign}(W_{S_0}) \) are controlled by independent random variables \( \eta, \xi \). In our numerical experiments, we find that the signed max statistic, i.e., \( W = |\hat{\beta}| \lor |\tilde{\beta}| \cdot \text{sign}(|\hat{\beta}| - |\tilde{\beta}|) \), is more powerful than the statistic in (34). To establish (34) for the signed max statistic, we cannot apply the same argument since the amplitude of \( W_{S_0} \) depends on \( \eta \) and \( |\xi_{S_0}| \). If the pseudo knockoff matrix is generated by the block diagonal construction, we have the following result.

**Theorem 2.3.** Assume that the pseudo knockoff matrix is generated by the block diagonal construction. For any \( t > 0 \), (34) is true for the signed max statistic.

**Proof.** From the amplitude property of the signed max statistic, \( |W_{S_0}| \) depends on \( \eta, |\xi_{S_0}| \). Let \( \mathcal{F} \) be the \( \sigma \)-field generated by \( \eta \) and \( |\xi_{S_0}| \). In the following, we will use the same notations \( N_t, C_i (C_i \subset S_0) \) as in the proof of Theorem 2.2. Note that (35) does not rely on the independence of \( \xi_{C_i} \). Based on the previous proof, we only need to verify (37).

For the block diagonal construction, the elements of \( C_i \) come from different blocks. Note that \( \text{Var}(\xi) = B = \text{diag}(S_{11}, S_{22}, \ldots, S_{kk}) \) and \( \xi_{S_0} = \xi_{S_0}^{(2)} \) (see (18)). We can change the sign of \( \xi_{S_0}^{(2)} \) in any block \( S_{i_1 i_2}, S_{i_2 i_3}, \ldots, S_{i_j i_2} \), without changing \( |\xi_{S_0}| \) and the joint distribution of \( \xi_{S_0}^{(2)} \). Consequently, conditional on \( \mathcal{F} \), the elements of \( \text{sign}(\xi_{C_i}) \) are mutually independent. Using the independence of \( \text{sign}(\xi_{C_i}) \) together with the sign property of \( W \), we conclude that the elements of \( \text{sign}(W_{C_i}) \) are i.i.d random variables satisfying

\[
P(\text{sign}(W_{C_i,j}) = 1) = P(\text{sign}(W_{C_i,j}) = -1) = 1/2.
\]

Finally, conditional on \( \mathcal{F} \), \( \{j \in C_i : W_j \geq t\} \sim \text{Binomial}(|C_i|, 1/2) \) and \( \{j \in C_i : W_j \leq -t\} = |C_i| - \{j \in C_i : W_j \geq t\} \) imply (37).

**Variance of the numerator.** We show that the variance of the numerator in (34) for \( t = 0+ \) is \( O(mp) \). Denote \( N_0 \triangleq \{j \in S_0 : (f(\eta))_j \neq 0\} \). By definition, \( N_0 \) is determined by \( \eta \). Based on the sign property of \( W \) and the fact that \( \xi \) is a multi-normal random variable, conditional on \( \eta \), \( N_0 = \{j \in S_0 : W_j \neq 0\} \) and \( \{j \in S_0 : W_j > 0\} = \{j \in N_0 : W_j > 0\} \) almost surely. For the block diagonal or banded pseudo knockoff, we can divide \( N_0 \) into \( m \) groups \( C_1, C_2, \ldots, C_m (C_i \subset S_0) \) such that the elements of \( \xi_{C_i} \) are mutually independent. Applying the Cauchy-Schwarz inequality yields

\[
\text{Var}(\{j \in S_0 : W_j > 0\}|\eta) = \text{Var}(\sum_{i=1}^{m} \{\{j \in C_i : W_j > 0\}|\eta) \leq m \sum_{i=1}^{m} \text{Var}(\{j \in C_i : W_j > 0\}|\eta) = m \sum_{i=1}^{m} \left( \sum_{j \in C_i} \text{Var}(1_{W_j > 0}|\eta) \right) = m \sum_{i=1}^{m} \left( \sum_{j \in C_i} \frac{1}{4} \right) = \frac{m|N_0|}{4} = O(mp).
\]

To obtain the second and the third equality, we apply a property of \( W_j \) in the proof of Theorem 2.2 and Theorem 2.3 that \( \text{sign}(W_j), j \in C_i \) are i.i.d conditional on \( \eta \) with \( P(\text{sign}(W_j) = 1|\eta) = P(\text{sign}(W_j) = -1|\eta) = 1/2 \).

It is interesting to perform a similar variance estimate for the knockoff filter. Since the knockoff statistic \( W \) has the property that \( \text{sign}(W_j), j \in S_0 \) are i.i.d conditional on \( |W| \) with \( P(\text{sign}(W_j) = 1|\mathcal{F}) = P(\text{sign}(W_j) = -1|\mathcal{F}) = 1/2 \), we obtain \( \text{Var}(\{j \in S_0 : W_j > 0\}|\mathcal{F}) = |S_0|/4 = O(p) \), where \( \mathcal{F} \) is the \( \sigma \)-field generated by \( |W| \).

### 3 Numerical results for the pseudo knockoff filter

In this section, we perform a number of numerical experiments to test the robustness of the pseudo knockoff filter and study the performance of various methods.

**Default Setting**
Notations. \( \beta_i \overset{i.i.d.}{\sim} \{ \pm A \} \) means that \( \beta_i \) takes value \( A \) or \( -A \) independently with equal probability \( 1/2 \). We denote the orthogonal pseudo knockoff, the pseudo knockoff with the block diagonal construction, and the pseudo knockoff with the banded construction as orthogonal, block diagonal and banded.

Data. Throughout all simulations, the noise \( \epsilon \in \mathbb{R}^n \) is a standard Gaussian, i.e. \( \epsilon \sim N(0, I_n) \). Given some covariance matrix \( \Sigma \), we first draw the rows of the design matrix \( X \in \mathbb{R}^{n \times p} \) from a multivariate normal distribution \( N(0, \Sigma) \), and then normalize the columns of \( X \). The pseudo knockoff matrix (orthogonal, block diagonal or banded) is generated according to Section 2.3; the knockoff matrix is generated by the standard SDP construction in \([3]\). To generate the signal strength \( \beta \in \mathbb{R}^p \), we choose \( k \) coefficients \( \beta_{i_1}, \beta_{i_2}, \ldots, \beta_{i_k} \) randomly and set \( \beta_{j} \overset{i.i.d.}{\sim} \{ \pm A \} \). Finally, the response variable \( y \in \mathbb{R}^n \) is generated from \( y = X\beta + \epsilon \). Without specification, the sample size is \( p = 500 \), \( n = 1500 \), the sparsity is \( k = 30 \), the signal amplitude is \( A = 3.5 \) and the covariance matrix is \( \Sigma = I_p \).

Pseudo Knockoff+ Threshold. We introduce the pseudo knockoff+ adaptive threshold \( T_m \) in \([13]\) and discuss how \([13]\) and \([12]\) contribute to the FDR control. In Remark 2, we argue that the inequality \([12]\) is tight in some extreme case. In general, adding \( m \) to the denominator is an over-estimate. Our numerical study indicates that we can replace \( m \) by 1 and the associated expectation is still close to 1 in the numerical examples that we consider in this paper. In the following numerical experiments, we choose \( T_1 \) as the adaptive threshold to select features. We note that this criterion is exactly the same as the original knockoff+ adaptive threshold. The nominal FDR level in the definition of \( T_1 \) is \( q = 20\% \).

Metrics. We use the following metrics to study the robustness of various methods: the \( FDR \) (the mean false discovery proportion), the \( power \) (the proportion of true discoveries) and the \( expectation \), which is defined as the mean of

\[
\frac{\# \{ j : W_j \geq T_1 \& \beta_j = 0 \}}{\# \{ j : W_j \leq -T_1 \& \beta_j = 0 \} + 1}.
\] (40)

Methods. The methods that we focus on include the orthogonal, the block diagonal, the banded pseudo knockoff filters with the half Lasso statistic (\( \lambda = 0.75 \)), and the knockoff filter with the orthogonal matching pursuit (OMP) statistic \([3]\). The reason we choose the OMP statistic for the knockoff filter is because the OMP statistic seems to give the most robust performance among other knockoff statistics from our numerical study in this paper and in \([6]\). For the banded pseudo knockoff filter, we construct \( W_j = (\hat{\beta}_j + \tilde{\beta}_j) \cdot \text{sign}(\hat{\beta}_j - \tilde{\beta}_j) \); for the other methods, we use the signed max statistic, i.e. \( W_j = |\hat{\beta}_j| \lor |\tilde{\beta}_j| \cdot \text{sign}(|\hat{\beta}_j| - |\tilde{\beta}_j|) \).

3.1 Numerical evidence of FDR control for the pseudo knockoff filter

In this subsection, we perform extensive numerical experiments to test whether the pseudo knockoff filter has FDR control. For this purpose, we apply it to select features in the linear model \( y = X\beta + \epsilon \) with different design matrices under various extreme conditions.

The default simulated data is discussed at the beginning of Section 3 and we vary one of the default settings in each experiment as follows (one setting is varied while keeping the others unchanged).

(a) \( \text{Sparsity} \): \( k \) varies from 10, 20, 30, ..., 90, 100.

(b) \( \text{Signal amplitude} \): \( A \) varies from 2.8, 2.9, ..., 4.2.

(c) \( \text{Correlation Structure} \): We use the covariance matrix \( \Sigma \in \mathbb{R}^{500 \times 500} \), \( \Sigma_{ij} = \rho^{\lfloor i-j \rfloor} \) and vary the correlation level \( \rho = 0, 0.1, ..., 0.9 \).

(d) \( \text{The sample size} \): We vary the sample size \( n = 150l \), \( p = 50l \) and sparsity \( k = 10l \) with \( l \in \{2, 3, ..., 12\} \).
**Group Structure:** We consider a design matrix \( X \in \mathbb{R}^{1500 \times 500} \) with a group structure. Specifically, we assume that the features \( X_j \) can be clustered into 100 groups with 5 features in each group. To generate a different group structure, we choose the covariance matrix \( \Sigma_{ii} = 1, \Sigma_{ij} = \rho \) for \( i \neq j \) in the same group and \( \Sigma_{ij} = \gamma \cdot \rho \) for \( i \neq j \) in different groups and generate the design matrix \( X \) as in the previous discussion.

(e) The within-group correlation: \( \gamma = 0 \) is fixed and \( \rho \) varies from 0, 0.1, 0.2, ..., 0.9.

(f) The between-group correlation: \( \rho = 0.5 \) is fixed and \( \gamma \) varies from 0, 0.1, 0.2, ..., 0.9.

We test the orthogonal, banded, and block diagonal pseudo knockoff filters and pay particular attention to the FDR control, the power and the expectation (mean of the ratio defined in (40)). Each experiment is repeated 200 times to calculate the mean FDR, the mean power, and the expectation. The design matrix \( X \) and the pseudo knockoff matrices \( \tilde{X} \) are fixed over these trials.

---

**Figure 1:** Testing the orthogonal, the banded, and the block diagonal pseudo knockoff+ at a nominal FDR \( q = 20\% \) by varying sparsity, the signal amplitude, or the feature correlation.

**Figure 2:** Testing the orthogonal, the banded, and the block diagonal pseudo knockoff+ at a nominal FDR \( q = 20\% \) by varying one of the following: the number of features \( p \), the within-group correlation, and the between-group correlation.

The dotted line in Figure 1 and Figure 2 represents the prescribed FDR \( q \) or constant 1 as a
reference. In all figures, we observe that the FDR is controlled by the nominal level \( q = 20\% \). From the results of the expectation, we observe that all of them are close to or less than 1, which can be explained by Theorem 2.2, though the definition of this expectation (averaged ratio defined in (40)) is different from that in (34). Meanwhile, the orthogonal pseudo knockoff+ offers more power than the banded and the block diagonal pseudo knockoff filters.

We have also applied the least squares statistic in these experiments. For the banded and the block diagonal pseudo knockoff+, we observe that the least squares statistic controls FDR. For the orthogonal pseudo knockoff, if \( \xi_i \) are strongly correlated (covariance matrix is \( 2(X^TX)^{-1} \)), the least squares statistic is not robust and cannot control FDR. By adding a half penalized term in (19), the performance of the half Lasso statistic is more robust than that of the least squares statistic. We will provide some partial analysis of the orthogonal pseudo knockoff later on.

### 3.2 The pseudo knockoff filter in some correlated scenarios

In the correlated case, the diagonal matrix \( \text{diag}(s) \) in the original knockoff filter constrained by (2) is small and leads to poor performance of the knockoff filter. A main advantage of the pseudo knockoff filter is that it relaxes the constraint of \( \tilde{X} \) in (15). In some correlated scenarios with a special structure, we can construct the pseudo knockoff matrix adapting to such structure and improve the power. To illustrate the effectiveness of the pseudo knockoff filter+, we perform a comparison between the knockoff filter and the pseudo knockoff filter.

**Methods** We use the representative statistics that give the most robust performance in both the knockoff filter and the pseudo knockoff filter based on our numerical experiments for the examples that we consider. Specifically, we compare the knockoff filter with the OMP statistic with the pseudo knockoff with the half Lasso statistic (\( \lambda = 0.75 \)).

**Group Structure** We consider a design matrix \( X \in \mathbb{R}^{1500 \times 500} \) with a group structure. In particular, we consider experiment (e) in Section 3.1. The within-group correlation factor \( \rho \) varies from \( 0.5, 0.55, 0.6, ..., 0.95 \) and the between-group correlation factor is \( \gamma = 0 \). We use a slightly larger signal amplitude \( A = 5 \) and consider two sparsity cases: \( k = 30 \) and \( k = 100 \). In all other settings, we use the default values. By taking advantage of the a priori knowledge of the correlation structure of \( X \), we use the block diagonal pseudo knockoff filter. We choose \( m = 5 \) in our construction of the block diagonal pseudo knockoff matrix. We also compare the orthogonal pseudo knockoff using the half Lasso statistic with the knockoff filter using the OMP statistic.

![Figure 3: Comparing the orthogonal, the block diagonal pseudo knockoff filter and the knockoff filter with the OMP statistic at nominal FDR \( q = 20\% \) by varying the within-group correlation.](image)

In both figures, the pseudo knockoff filter controls FDR successfully. In the very sparse case
Based on our analysis of the least squares statistic, we know that the half Lasso statistic favors the non-sparse case. We observe that it offers more power than the knockoff filter with the OMP statistic in the right figure where the sparsity is $k = 100$.

**Decaying Structure** We consider a design matrix $X \in \mathbb{R}^{1500 \times 500}$ with some decaying structure. Specifically, the design matrix $X$ is generated from $N(0, \Sigma)$ with $\Sigma_{ij} = \rho^{|i-j|}$, where $\rho$ varies from 0.5, 0.55, ..., 0.95. We use a slightly larger signal amplitude $A = 5$ and consider two sparsity cases: $k = 30$ and $k = 100$. Other settings use the default values. We know *a priori* that the off-diagonal elements of $\Sigma^{-1}$ decay rapidly, i.e. $|\Sigma_{ij}| \rightarrow 0$ as $|i-j|$ increases. Thus, it makes sense to apply the banded pseudo knockoff filter. In addition, we apply the orthogonal pseudo knockoff and the knockoff with the OMP statistic for comparison.

![Figure 4: Comparing the orthogonal, the banded pseudo knockoff filter and the knockoff filter with the OMP statistic at a nominal FDR $q = 20\%$ by varying the within-group correlation.](image)

From Figure 4, the pseudo knockoff filters control FDR in both cases. In the non-sparse case, the two pseudo knockoff filters offer more power than the knockoff filter with the OMP statistic.

In these correlated examples with a special correlation structure, we see that designing a special pseudo knockoff that adapts to the problem could increase the power of the pseudo knockoff filter. Moreover, we observe that the orthogonal pseudo knockoff filter offers more power than the other pseudo knockoff filters in each experiment.

**4 Partial analysis of the orthogonal pseudo knockoff**

From the previous numerical results, we observe that the orthogonal pseudo knockoff offers more power than other pseudo knockoff filters and still retains robust FDR control. In this section, we perform further numerical experiments to gain some insight and provide some partial analysis.

**4.1 Approximate monotonicity of the expectation of (34)**

The FDR control of the banded or the block diagonal pseudo knockoff relies on Theorem 2.2 and the expectation inequality (34). This result is based on the fact that $\xi_{S_0}$ can be classified into several groups such that the random variables in the same group are mutually independent. For the orthogonal pseudo knockoff, we have not made use of any special correlation structure of the design matrix. Thus, we cannot expect that (34) or a similar result holds.

We denote the expectation of the key ratio quantity in (34) with $m = 1$ as a function of $t$:

$$F(t) \triangleq E \left[ \frac{\#\{j : W_j \geq t, \beta_j = 0\}}{\#\{j : W_j \leq -t, \beta_j = 0\} + 1} \right].$$
Inspired by the supermartingale argument in [3], we investigate whether $F(t)$ decreases monotonically with respect to $t$. We use settings (a), (c), (e) and (f) in Section 3.1 respectively, to study numerically the behavior of $F(t)$ for a range of $t$ (averaged over 200 trials). Note that these settings correspond to different correlation structures of $X$. We apply the half Lasso signed max statistic ($\lambda = 0.75$) and plot the heat map of the expectation. The x-axis corresponds to the range of $t$ varying from 0, 0.2, 0.4, ..., 5 and the y-axis corresponds to the values of the sparsity or the correlation.

Figure 5: Computing the variance of $F(t)$ in different scenarios using the orthogonal pseudo knockoff filter. We vary one of the following default parameters in each sub figure: sparsity $k$, the correlation factor $\rho$ ($\Sigma_{ij} = \rho|j-j|$), the within-group correlation factor $\rho$ and the between-group correlation $\gamma$.

In each experiment, $F(t)$ varies slightly for small $t$ and decreases almost monotonically for large $t$. Based on these numerical observations, we focus on $F(0^+)$ in order to gain some insight on the behavior of $F(t)$.

4.2 Property of the Orthogonal Pseudo Knockoff

Symmetry Property (23) Since $X^T\tilde{X} = 0$ is symmetric, the symmetry property Proposition 2.1 holds for the orthogonal pseudo knockoff.

The identical distribution property From (17) and (18), the covariance matrix of $\eta$ and $\xi$ are $A = 4[(X + \tilde{X})^T(X + \tilde{X})]^{-1}$ and $B = 4[(X - \tilde{X})^T(X - \tilde{X})]^{-1}$, respectively. The orthogonality condition implies

$$A = 2(X^T X)^{-1} = 2\Sigma^{-1} = B.$$ 

Note that $E(\eta) = \beta = E(\xi)$ and that $\eta$ and $\xi$ are independent multivariate normal distributions. $\eta$ and $\xi$ are independent and identically distributed.

Control of the ratio We introduce the following notations, which will be used frequently later.

$$\Sigma = X^T X, \quad D = diag(\Sigma^{-1}) = diag(d_1, d_2, ..., d_p), \quad \Sigma^{-1} = D^{-1/2} \Sigma^{-1} D^{-1/2},$$

$$Z_1 \triangleq \# \{ j \in S_0 : W_j > 0 \}, \quad Z_2 \triangleq \# \{ j \in S_0 : W_j < 0 \}. \quad (41)$$

By definition, we have $(\Sigma^{-1})_{ii} = 1$. We have the following results.
Theorem 4.1. For any $\delta \in (0, 1)$, the orthogonal pseudo knockoff with the statistic defined in \cite{22} satisfies

\[
P\left(\frac{Z_1}{Z_2} \geq \frac{1 + \delta}{1 - \delta}\right) \leq \frac{1}{\delta^2|S_0|} \left(\frac{1 + 3\pi}{1 - \delta}\right),
\]

which is of order $O(1/((\delta^2|S_0|)) = O(\lambda_{\max}(\Sigma^{-1})/\delta^2p))$. Here, $d_i = (\Sigma^{-1})_{ii}$, $s_i$ is the knockoff factor in \cite{19} and $(s_i d_i)^{-\alpha} \triangleq |S_0|^{-1} \sum_{j \in S_0} (s_i d_i)_j^{-\alpha}$, $\alpha \in \{1, 2\}$.

Remark 3. \cite{22} controls the ratio $Z_1/Z_2$ in a probabilistic sense. By the definition of $F(t)$, $F(0+) = E(Z_1/(Z_2 + 1))$ and is bounded by $E(Z_1/Z_2)$. Note that the diagonal elements of $\Sigma^{-1}$ are all 1. From $p = Tr(\Sigma^{-1}) = \sum_{i=1}^p \lambda_i(\Sigma^{-1})$ and $\lambda_i(\Sigma^{-1}) > 0$, we have $\max(\Sigma^{-1}) < p$. We will demonstrate later that if the matrix $\Sigma^{-1}$ is well-conditioned and the number of null features $|S_0|$ is large enough, the ratio $Z_1/Z_2$ is bounded by a constant close to 1 with high probability.

We would like to draw a connection between the probabilistic upper bound (42) and the knockoff filter. Since the amplitude of $s_i$ is associated with the power of the knockoff filter, the right hand side relates to the power of the knockoff. Based on $\Sigma_{ii} = 1$ and $0 < \Sigma$, one can prove $d_i \geq 1$. To see this, we denote $\Sigma = \begin{bmatrix} 1 & v^T \\ v & E \end{bmatrix}$, $v \in R^{(p-1)}$, $0 < E \in R^{(p-1) \times (p-1)}$. The positive definiteness of $\Sigma$ guarantees $0 < 1 - v^T E^{-1} v \leq 1$. It follows $d_1 = (1 - v^T E^{-1} v)^{-1} \geq 1$. Similarly, we can prove $d_i \geq 1$. If $s_i$ is not small and is bounded from below (e.g. using the modified SDP construction in \cite{6}), then the quantity $s_i^{-1}$ cannot be too large. We can obtain a good control of $Z_1/Z_2$ in the probabilistic sense if $|S_0|$ is large enough.

4.3 The Mean-Variance Argument

From the sign property of $W$, we know $\text{sign}(W_{S_0}) = \text{sign}((f(\eta))_{S_0}) \cdot \text{sign}(\xi_{S_0})$. Denote $Y_i = 1_{W_i > 0}$. In order to estimate the variance of $Z_1, Z_2$, we first analyze the covariance of each pair $(Y_i, Y_j), i, j \in S_0$.

Lemma 4.2. Conditional on $\eta$, for any null variable i, j, we have

\[
\text{Cov}(Y_i, Y_j | \eta) \leq \frac{1}{2\pi} (\Sigma^{-1})_{ij} (1_{(f(\eta))_i > 0} - 1_{(f(\eta))_i < 0}) (1_{(f(\eta))_j > 0} - 1_{(f(\eta))_j < 0}) + \frac{3}{2} (\Sigma^{-1})_{ij}^2.
\]

where $(\Sigma^{-1})_{ij}$ is defined in (44).

We will defer the proof to the Appendix.

The Mean and Variance of $Z_i$ Denote $N_{\eta} \triangleq \{j \in S_0 : (f(\eta))_j \neq 0\}$. Obviously, $N_{\eta}$ is measurable with respect to the $\sigma$-field generated by $\eta$. Since $\xi = \beta^{ls} - \beta^{ls} \neq 0$ almost surely, we have $W_j = 0 \iff f(\eta)_j = 0$ almost surely and thus $N_{\eta} = \{j \in S_0 : W_j \neq 0\}$ almost surely.

The means of $Y_i$ and $Z_j$ are straight forward. For $i \in S_0$, we have

\[
E(Y_i | \eta) = 1_{(f(\eta))_i > 0} E(1_{\xi_i > 0} | \eta) + 1_{(f(\eta))_i < 0} E(1_{\xi_i < 0} | \eta) = 1_{(f(\eta))_i > 0} E(1_{\xi_i > 0}) + 1_{(f(\eta))_i < 0} E(1_{\xi_i < 0}),
\]

\[
E(Z_1 | \eta) = E(Z_2 | \eta) = \frac{|N_{\eta}|}{2}, \quad Z_1 + Z_2 = |N_{\eta}|,
\]

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where we use the fact that η and ξ are independent. Next, we show that

\[
\text{Var}(Z_1|\eta) \leq |N_\eta| \left( \frac{1}{2\pi} \min \left( \lambda_{\max}(\Sigma^{-1}), 2(s_i d_i)^{-1} \right) + \frac{3}{2} \min \left( \lambda_{\max}(\Sigma^{-1}), 4(s_i d_i)^{-2} \right) \right).
\]

Here \((s_i d_i)^{-\alpha} = |N_\eta|^{-1} \sum_{i \in N_\eta} (s_i d_i)^{-\alpha}\). Denote \(w_i \triangleq 1_{f_i(\eta)>0} - 1_{f_i(\eta)<0}\). Using (44), we have

\[
\text{Var}(Z_1|\eta) \leq \sum_{i,j \in N_\eta} \text{Cov}(Y_i, Y_j|\eta) \leq \sum_{i,j \in N_\eta} \frac{(\Sigma^{-1})_{ij}}{2\pi} w_i w_j + \frac{3}{2} \frac{(\Sigma^{-1})_{ij}}{2\pi} = \frac{w_{N_\eta}^T (\Sigma^{-1})_{N_\eta N_\eta} w_{N_\eta}}{2\pi} + \frac{3}{2} \text{Tr}((\Sigma^{-1})_{N_\eta N_\eta}^2)
\]

From \(\text{diag}(s) \preceq 2X^TX\) (42) and the definition of \(\Sigma^{-1}\) (41), we have \(\Sigma^{-1} \preceq 2D^{-1/2}(\text{diag}(s))^{-1}D^{-1/2}\). Meanwhile, \(\Sigma^{-1} \preceq \lambda_{\max}(\Sigma^{-1})I\). It follows

\[
w_{N_\eta}^T (\Sigma^{-1})_{N_\eta N_\eta} w_{N_\eta} \leq \min \left( w_{N_\eta}^T \lambda_{\max}(\Sigma^{-1}) I |N_\eta| w_{N_\eta}, 2w_{N_\eta}^T (D^{-1/2}(\text{diag}(s))^{-1}D^{-1/2})_{N_\eta N_\eta} w_{N_\eta} \right)
\]

\[
= |N_\eta| \min \left( \lambda_{\max}(\Sigma^{-1}), 2(s_i d_i)^{-1} \right)
\]

Here, we use the fact that \(\lambda_{\max}(\Sigma^{-1}) I, D^{-1/2}(\text{diag}(s))^{-1}D^{-1/2}\) are diagonal and \(|w_i| = 1\). \((s_i d_i)^{-1}\) is the average of \((s_i d_i)^{-1}\) over \(i \in N_\eta\). For any positive definite matrix \(0 < P \preceq Q\), we have

\[
\text{Tr}(Q^2 - P^2) = \text{Tr}((Q - P)(Q + P)) = \text{Tr}((Q - P)^{1/2}(Q - P)^{1/2}(Q + P)^{1/2}(Q + P)^{1/2}) = \text{Tr}((Q - P)^{1/2}(Q + P)^{1/2}(Q - P)^{1/2}) = \text{Tr}(R R^T) \geq 0, \quad R = (Q - P)^{1/2}(Q + P)^{1/2}
\]

Taking \(P = (\Sigma^{-1})_{N_\eta N_\eta}, Q = 2(D^{-1/2}(\text{diag}(s))^{-1}D^{-1/2})_{N_\eta N_\eta}\), we yield

\[
\text{Tr}((\Sigma^{-1})_{N_\eta N_\eta}^2) \leq 4 \text{Tr}((D^{-1/2}(\text{diag}(s))^{-1}D^{-1/2})_{N_\eta N_\eta}^2) = 4|N_\eta|(s_i d_i)^{-2}
\]

Note that for any \(0 \preceq A\), \(\text{Tr}(A^2) = \sum \lambda^2_i(A) \leq \lambda_{\max}(A) \text{Tr}(A)\) and \((\Sigma^{-1})_{ii} = 1\). We have

\[
\text{Tr}((\Sigma^{-1})_{N_\eta N_\eta}^2) \leq \lambda_{\max}(\Sigma^{-1}) \text{Tr}((\Sigma^{-1})_{N_\eta N_\eta}) = |N_\eta| \lambda_{\max}(\Sigma^{-1})
\]

Combining (48), (49), (50) and (51) yields (47).

**Proof of Theorem 4.1**

**Proof.** Conditional on \(\eta\), we apply \(E(Z_1|\eta) = E(Z_2|\eta) = |N_\eta|/2 = (Z_1 + Z_2)/2\) (46), (47), and the Chebyshev inequality to yield

\[
P(Z_2 \leq (1 - \delta)EZ_2|\eta) = P(Z_2 \geq (1 + \delta)EZ_2|\eta) \leq \frac{1}{2\delta^2} \text{Var}(Z_2|\eta) \leq \frac{1}{2\delta^2} \left( \frac{1}{|N_\eta|} \left( \frac{1}{\pi} \min \left( \lambda_{\max}(\Sigma^{-1}), 2(s_i d_i)^{-1} \right) + \frac{3}{2} \min \left( \lambda_{\max}(\Sigma^{-1}), 4(s_i d_i)^{-2} \right) \right) \right)
\]

\[
\leq \frac{1 + 3\pi|\lambda_{\max}(\Sigma^{-1})|}{\pi|N_\eta|}
\]

Here \((s_i d_i)^{-\alpha} = |N_\eta|^{-1} \sum_{i \in N_\eta} (s_i d_i)^{-\alpha}, \alpha = 1, 2\). The first identity holds since the symmetry property (23) implies that \(Z_2 \overset{d}{=} Z_1 = |N_\eta| - Z_2\). The estimate (42) follows from integrating the last inequality in (52). If \(W_i \neq 0 \forall i \in S_0\) almost surely, we have \(N_\eta = S_0\) almost surely. It follows \(|N_\eta| = |S_0|\) and \((s_i d_i)^{-\alpha} = |S_0|^{-1} \sum_{i \in S_0} (s_i d_i)^{-\alpha}\) almost surely. Consequently, we can integrate the second inequality in (52) to yield (44).

Next, we prove (43). Recall that conditional on \(\eta, Z_1 + Z_2 = |N_\eta| \triangleq n_\eta\). We know \(Z_1 \leq \frac{1 + \delta}{2} Z_2 \iff Z_2 \geq (1 - \delta) Z_2 \). Consequently, we obtain

\[
E \left( \frac{Z_1}{Z_2} | \frac{Z_1}{Z_2} \leq | \frac{Z_1}{Z_2} \leq \frac{1 + \delta}{2} \eta \right) = E \left( \frac{Z_1}{Z_2} | Z_2 \geq (1 - \delta) n_\eta / 2 \eta \right) \leq \frac{2E(Z_1 1_{Z_2 \geq (1 - \delta) n_\eta / 2 \eta})}{(1 - \delta) n_\eta} \leq \frac{2E(Z_1|\eta)}{(1 - \delta) n_\eta} = \frac{1}{1 - \delta}
\]

Integrating both sides yields the desired result (43).
4.4 Some Special Design Matrices

For some special design matrices, we can improve the estimate of $\text{Var}(Z_1)$ in (47) and get better control of $Z_1/Z_2$. In our simulations, we observe that the orthogonal pseudo knockoff filter offers robust FDR control and works better than other pseudo knockoff filters and the knockoff filter with the OMP statistic in these scenarios. We would like to offer a partial explanation of this phenomenon.

A diagonally dominated case Let $X \in \mathbb{R}^{n \times p}$ and $\Sigma = XX^T$. We consider several classes of design matrices described below.

(a) For any $i \neq j$, $\langle X_i, X_j \rangle \equiv X_i^T X_j - \rho$, $\rho \in [0, 1)$.

(b) Assume that $X$ can be clustered into $k$ groups, $X = (X_{C_1}, X_{C_2}, \ldots, X_{C_k})$. The within-group correlation of group $i$ is $\rho_i$ for some $\rho_i \in [0, 1)$ and the between-group correlation is zero.

(c) The sizes of different groups are equal. The within-group correlation is $\rho$ and the between-group correlation is $\gamma \cdot \rho$.

Case (b) and (c) correspond to setting (e) and (f) in Section 3.1. Denote $E \equiv \Sigma^{-1}$ for convenience. From (41), $(\Sigma^{-1})_{ij} = E_{ij}/(E_{ii}^{1/2}E_{jj}^{1/2})$. For the design matrices described above, we can show that $\Sigma^{-1}$ is diagonally dominated, i.e., $\sum_{j \neq i} (\Sigma^{-1})_{ij} \leq \Sigma_{ii}^{-1}$. The proof is a bit technical and tedious. We will omit the proof here. From Lemma 4.2 we have

$$Cov(Y_i, Y_j|\eta) \leq \frac{1}{2\pi} (\Sigma_{ij}^{-1})w_i w_j + \frac{3}{2} (\Sigma_{ii}^{-1}) \leq c_0 |(\Sigma_{ij}^{-1})|, \quad c_0 = \frac{1}{2\pi} + \frac{3}{2} < 2 \quad (53)$$

Using the fact that $\Sigma^{-1}$ is diagonally dominated, we can improve the estimate of $\text{Var}(Z_1|\eta)$ in (47)

$$\text{Var}(Z_1|\eta) \leq \sum_{i,j \in N_{\eta}} c_0 |(\Sigma_{ij}^{-1})| = c_0 \sum_{i,j \in N_{\eta}} \frac{|E_{ij}|}{E_{ii}^{1/2}E_{jj}^{1/2}} \leq c_0 \left( \sum_{i,j \in N_{\eta}} \frac{|E_{ij}|}{E_{ii}} \right)^{1/2} \left( \sum_{i,j \in N_{\eta}} \frac{|E_{ij}|}{E_{jj}} \right)^{1/2} = c_0 \left( \sum_{i \in N_{\eta}} \frac{1}{E_{ii}} \sum_{j \in N_{\eta}} |E_{ij}| \right)^{1/2} \left( \sum_{j \in N_{\eta}} \frac{1}{E_{jj}} \sum_{i \in N_{\eta}} |E_{ij}| \right)^{1/2} \leq c_0 \left( \sum_{i \in N_{\eta}} \frac{2E_{ii}}{E_{ii}} \right)^{1/2} \left( \sum_{j \in N_{\eta}} \frac{2E_{jj}}{E_{jj}} \right)^{1/2} = 2c_0 |N_{\eta}|. $$

Here, we have used $E_{ij} = E_{ji}$ and the diagonal dominated assumption to yield $\sum_{j \in N_{\eta}} |E_{ij}| \leq \sum_{j=1}^{p} |E_{ij}| \leq 2E_{ii}$. Accordingly, the estimate of $Z_1/Z_2$ in Theorem 4.1 can be improved.

**Proposition 4.3.** Assume that $\Sigma^{-1} = (X^T X)^{-1}$ is diagonally dominated, the orthogonal pseudo knockoff satisfies

$$P \left( \frac{Z_1}{Z_2} \geq \frac{1+\delta}{1-\delta} \right) \leq 2 + \frac{6\pi}{\pi \delta^2} E \left[ \# \{ j \in S_0 : W_j \neq 0 \} \right]^{-1},$$

If $W_i \neq 0 \forall i \in S_0$ almost surely, the upper bound becomes $(2 + 6\pi)/(\pi \delta^2 |S_0|) = O((\delta^2 p)^{-1})$.

**Exponentially Decaying Class** Assume that $|\langle (\Sigma^{-1})_{ij} \rangle| \leq C |\rho^{i-j}|$ for $\rho \in [0, 1)$ and some constant $C$. The design matrix in setting (c) in Section 3.1 has a similar structure. One can prove that $(\Sigma^{-1})_{ii} \geq 1$ using the fact that $\Sigma_{ii} = 1$ and $\Sigma$ is positive definite. By our assumption, we have $|\langle (\Sigma^{-1})_{ij} \rangle| \leq |\langle (\Sigma^{-1})_{ij} \rangle| \leq C |\rho^{i-j}|$. Hence, we have $\lambda_{\max}(\Sigma^{-1}) \leq ||\Sigma^{-1}||_{1} \leq 2C/(1-\rho)$. Using (47) and Theorem 4.1 we yield

$$\text{Var}(Z_1|\eta) \leq c_0 \lambda_{\max}(\Sigma)^{-1} |N_{\eta}| \leq \frac{2c_0 C |N_{\eta}|}{1-\rho}, \quad P \left( \frac{Z_1}{Z_2} \geq \frac{1+\delta}{1-\delta} \right) \leq \frac{4c_0 C}{\delta^2 (1-\rho)} E |N_{\eta}|^{-1} \approx \frac{4c_0 C}{\delta^2 (1-\rho) |S_0|},$$

where $c_0 = (1+3\pi)/(2\pi)$. If $1-\rho \geq c_1$ for some positive constant $c_1$ not too small, this probabilistic upper bound is of the order $O((\delta^2 |S_0|)^{-1}) = O((\delta^2 p)^{-1})$.  

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Summary Let $\mathcal{F}_{kf}$ be the $\sigma$-field generated by all $|W_i|$ in the knockoff filter, $B = 4[(X - \tilde{X})^T(X - \tilde{X})]$, $N_0 \triangleq \# \{ i \in S_0 : |W_i| \neq 0 \}$, $m$ be the maximal group size or the band width, and $Z_1(t) \triangleq \# \{i \in S_0 : W_i \geq t\}$, $Z_2(t) \triangleq \# \{i \in S_0 : W_i \leq -t\}$ $\forall t > 0$. In particular, $Z_1(0) \triangleq \# \{ i \in S_0 : W_i > 0 \}$, $Z_2(0) \triangleq \# \{i \in S_0 : W_i < 0 \}$. We summarize the variance estimates for several classes of pseudo knockoff filters and the knockoff filter as follows. We note that $\tilde{X}$ in all filters satisfies $X^T X = \tilde{X}^T \tilde{X}$, and $B \geq \Sigma^{-1}$ being diagonal is equivalent to the second constraint in (1) and (2).

| Filter          | Constraint on X              | FDR Control                | Conditional Variance                      |
|-----------------|-------------------------------|----------------------------|-------------------------------------------|
| Knockoff        | $B \geq \Sigma^{-1}$ being diagonal | Exact. For adaptive $T$, $E(Z_1(T)) / (Z_2(T) + 1) \leq 1$ | $\text{Var}(Z_1(0)|\mathcal{F}_{kf}) = |N_0|/4$ |
| Block Diagonal  | $B \geq \Sigma^{-1}$ being block diagonal | Partial. For fixed $t > 0$, $E(Z_1(t))/(Z_2(t) + m) \leq 1$ | $\text{Var}(Z_1(0)|\eta) \leq |N_0|m/4$ |
| Banded          | $B \geq \Sigma^{-1}$ being banded | Partial. For fixed $t > 0$, $E(Z_1(t))/(Z_2(t) + m) \leq 1$ | $\text{Var}(Z_1(0)|\eta) \leq |N_0|m/4$ |
| Orthogonal      | $B = 2\Sigma^{-1}$ or $X^T \tilde{X} = 0$ | $P(Z_1(0)/Z_2(0) \geq (1 + \delta)/(1 - \delta)) \leq 2c_0(\delta)^{-2} E(\lambda_{\max}(\Sigma^{-1})^2)/|N_0| \leq c_0|N_0|\lambda_{\max}(\Sigma^{-1})$ |

We focus on the conditional variance of the pseudo knockoff. The estimate of $\text{Var}(Z_1(0)|\eta)$ of the block diagonal or the banded pseudo knockoff is given by $\lambda_{\max}(\Sigma^{-1})$ and $\text{Var}(Z_1(0)|\mathcal{F})$ of the knockoff is discussed in the paragraph after (39). For small $m$, $\text{Var}(Z_1(0)|\eta)$ of the block diagonal or the banded pseudo knockoff is of the same order as that of the knockoff. For the orthogonal pseudo knockoff, $\text{Var}(Z_1(0)|\eta)$ in the above table is $c_0|N_0|\lambda_{\max}(\Sigma^{-1})$ and $c_0 = (1 + 3\pi)/(2\pi)$. If $\Sigma^{-1}$ is well-conditioned, e.g. $\Sigma^{-1}$ is diagonally dominated or $X$ is one of the design matrices we discussed in this section, then $\lambda_{\max}(\Sigma^{-1})$ is small and $\text{Var}(Z_1(0)|\eta)$ is $O(|N_0|)$. Note that $E(Z_1|\eta) = E(Z_2|\eta) = |N_0|/2$. If $\text{Var}(Z_1(0)|\eta)$ is bounded by $C|N_0|^\alpha$ for $\alpha < 2$ and some universal constant $C$, the mean-variance argument provides a relatively tight upper bound (that is close to 1) for $Z_1(0)/Z_2(0)$ as $|N_0|$ tends to infinity. This preliminary analysis offers some insight as to why the pseudo knockoff filter may offer FDR control similar to that of the knockoff filter in the examples that we consider here. Based on the mean-variance argument, it is reasonable to conjecture that if $\text{Var}(Z_1(0)|\eta) \leq C|N_0|$ for some universal constant $C$, then the pseudo knockoff may have FDR control similar to that of the knockoff.

4.5 An extreme example

The banded or the block diagonal pseudo knockoff filters are constructed for those design matrices with some special correlation structure, i.e. either the off-diagonal elements of $(X^T X)^{-1}$ decay rapidly or $(X^T X)^{-1}$ can be approximated by a block diagonal matrix or a banded matrix. In this subsection, we consider a class of design matrices that violate these assumptions. Specifically, the covariance matrix $M$ to generate $X \in R^{1500 \times 500}$ ($X \sim N(0, M)$) satisfies $(M^{-1})_{ij} = \rho \ \forall i \neq j$ and $(M^{-1})_{ii} = 1$ for some $\rho \geq 0$. We need to normalize the columns of $X$ to be a unit vector. We focus on two sparsity levels with $k = 30$ and $k = 100$, and choose the signal amplitude to be $A = 5 (\beta_i \overset{i.i.d.}{\sim} \{\pm A\})$. We let $\rho$ vary from $0, 0.1, 0.2, ..., 0.9$. We construct the pseudo knockoff matrix according to Section 2.3 with $m = 2$ ($m$ is the largest block size or the band width)

In Figure 6, we can see that the orthogonal pseudo knockoff with the half Lasso statistic has FDR control and considerable power for varying $\rho$, while the knockoff filter with the OMP statistic has almost no power. The banded and the block diagonal pseudo knockoff filters with the half Lasso statistic are also considered. They control FDR but lose a lot of power for $\rho > 0$. Since the off-diagonal elements of $\Sigma^{-1}$ do not decay and $\Sigma^{-1}$ is not block diagonal or banded, there is no advantage of using these pseudo knockoff filters in this extreme example.

To understand why the knockoff filter with the OMP or the Lasso Path statistics performs
X has a reasonable amount of power since we force filters and the knockoff filter with the OMP statistic. The orthogonal pseudo knockoff filter still path is not computed exactly, but approximated by a fine grid of orthogonal pseudo knockoff filters. For the mildest case of correlated. We have computed the mean correlation of X is generated via the SDP construction). For the mildest case of q = 20% by varying the correlation ρ. The figures show the mean power and the mean FDR averaged over 200 trials.

Figure 6: Comparing the orthogonal pseudo knockoff filter with the half Lasso and least squares statistics with the knockoff filter with the OMP and the Lasso path statistics at a nominal FDR q = 20% by varying the correlation ρ. The figures show the mean power and the mean FDR.

 poorly in this example, we analyze the correlation between Xj and X̃j. Based on the second constraint of the knockoff filter [2], we use an argument similar to [19]. More specifically, we have vTΣ−1v ≤ 2vTD−1/2(diag(s))−1D−1/2v with v = (1, 1, .., 1)T ∈ Rp. This gives ∑p

i=1

1 / sidi ≥ ∑i,j

Σ−1

ij , where Σ−1 is defined in (41). By the construction of X, we have (Σ−1)ii = 1 and (Σ−1)ij ≈ ρ, ∀i ≠ j. Note that di ≥ 1. The lower bound of mean(s−1) is approximately equal to 1 / 2(1 + (p − 1)ρ) ≈ pp/2. If si generated by the SDP construction distributes evenly, we obtain si = O((pp)−1). For ρ ≠ 0 and p large enough, si is very small and thus Xj and X̃j are strongly correlated. We have computed the mean correlation of Xj, X̃j numerically (the knockoff matrix is generated via the SDP construction). For the mildest case of ρ = 0.1, the mean correlations of Xj, X̃j for the banded, the block diagonal pseudo knockoff filters, the knockoff filter, and the orthogonal pseudo knockoff filter are 0.976, 0.981, 0.971, and 0, respectively. The strong correlation between Xj, X̃j explains the weak power of the block diagonal and the banded pseudo knockoff filters and the knockoff filter with the OMP statistic. The orthogonal pseudo knockoff filter still has a reasonable amount of power since we force Xj, X̃j to be orthogonal by construction.

From the FDR result, we see that the Lasso path statistic is not robust. Note that the Lasso path is not computed exactly, but approximated by a fine grid of λ. Typically, the number of grid points to approximate λ is chosen to be 5p. Since Xj and X̃j are strongly correlated, this level of grid resolution for λ may not be fine enough to separate the entrance time of Xj and X̃j. From our simulations, we observe that Xj and X̃j enter into the model at the same λ, which leads to Wj = 0. In order to determine which one enters the model earlier, we need to refine the grid. However, refining the grid resolution leads to a considerable increase in the computational cost of the Lasso path statistic. To show that the FDR of the Lasso Path statistic is indeed under control as predicted by the knockoff theory in [3], we reduce the sample size to p = 100, n = 300 (sparsity k = 20 and k = 6), and increase the number of realizations to 1000 and implement the Lasso path statistic with the number of grid points for λ equal to 50p. Using this level of resolution, we observe that the mean FDR is controlled at q = 20%. However, the statistical power of the Lasso Path statistic is also greatly reduced and is less than 10% for large values of ρ (ρ ≥ 0.5). Based on the performance of these two knockoff statistics, we find that the OMP statistic is more robust.

Variance of the orthogonal pseudo knockoff filter with different statistics Although the orthogonal pseudo knockoff filter with the least squares statistic maintains a lot of power, its
mean FDR is more than the prescribed $q = 20\%$ (i.e. we lose the FDR control for the least squares statistic). Based on our construction of $X$, $\lambda_{\text{max}}(\Sigma^{-1})$ is of order $1 + (p-1)\rho \approx p\rho$. Therefore, the estimate of $\text{Var}(Z_1|\eta)$ in (17) is $O(p^2)$ if $N_\eta = S_0$ and $|S_0| \approx p$. Consequently, the upper bound in Theorem 4.1 is $O(\delta^{-2})$ and we may lose control of $Z_1/Z_2$ for some statistics. To understand the difference between the mean FDR of the half Lasso and the least squares statistic, we compute $\text{Var}(Z_1)$ numerically over 200 trials. The results are plotted in the figure below.

![Figure 7: Numerical computation of the variance of the orthogonal pseudo knockoff filter](image)

We focus on the order of $\text{Var}(Z_1)$. The left figure shows that $\text{Var}(Z_1)$ of the half Lasso statistic is $O(p)$ and the constant is about 0.1, while the right figure shows that $\text{Var}(Z_1)$ of the least squares statistic is $O(p^2)$ and the constant varies for different $\rho$. The results of $\rho = 0, 0.2, 0.4, 0.6, 0.8$ are qualitatively similar. The variance of the least squares obtained from our simulation matches well with our theoretical estimate and thus its FDR may lose control in the extreme example (Figure 6). The numerical variance of the half Lasso statistic, however, is order $O(p)$, which is much better than $O(p^2)$ in the estimate (17). Therefore, the mean-variance argument shows that the upper bound in (12) is $O((\delta^2 p)^{-1})$, which explains why we still have FDR control of the orthogonal pseudo knockoff filter with the half Lasso signed max statistic in this extreme example.

From the numerical results in this subsection and Section 3, we see that a half penalty in (19), e.g. the $l_1$ penalty $\lambda || \cdot ||_1$, reduces the variance of $Z_1$ significantly, which leads to robust performance of the orthogonal pseudo knockoff filter. We do not fully understand why a half Lasso penalty reduces the variance from $O(p^2)$ to $O(p)$ in the extreme example. From our numerical experiments, we observe that the combination of the orthogonal pseudo knockoff and the half Lasso signed max statistic seems to offer the most power among other pseudo knockoff filters. It would be worthwhile to further study the effect of a half penalty to take full advantage of the orthogonal pseudo knockoff filter.

5 Concluding remarks

In this paper, we introduce three classes of pseudo knockoff filters. These pseudo knockoff filters preserve some essential features of the original knockoff filter but offer more flexibility in constructing the knockoff matrix, especially when the features are highly correlated or when the inverse of the covariance matrix, $\Sigma^{-1}$, decays very slowly away from its main diagonal. We provide a partial analysis of the pseudo knockoff filters by investigating the expectation inequality (9), which is a variant of the corresponding expectation inequality (10) for the knockoff filter. We establish this expectation inequality for the block diagonal and the banded pseudo knockoff filters. For the orthogonal pseudo knockoff filter, we provide a probabilistic analysis based on the mean-variance argument. This analysis gives an upper bound on the the expectation of interest. In the case when
\(\Sigma^{-1}\) is diagonally dominated or when \(\Sigma^{-1}\) has some special structure, this probabilistic analysis provides a relatively tight upper bound for the expectation of interest. This analysis offers some partial explanation why the pseudo knockoff filters provide FDR control in the examples that we consider in this paper. We have also performed a number of numerical experiments to test the performance of the pseudo knockoff filters and compare them with the knockoff filter. In the case when the features are highly correlated and the non-sparse case (e.g. about 20\% non-null features), the orthogonal pseudo knockoff filter offers more power than the knockoff filter with the OMP or Lasso Path statistic. In the extreme case when \(\Sigma^{-1}\) decays very slowly away from its main diagonal, the knockoff filter with the OMP or the Lasso Path statistic tends to lose considerable power. The orthogonal pseudo knockoff filter still offers reasonably high power in this case. The study presented in this paper is still at a very preliminary stage and further study is required to fully understand the advantages and the limitations of the pseudo knockoff filters.

**Appendix**

**Verification of the construction (31) of \(\hat{X}\).** Let \(\hat{X}\) be constructed from (31). Direct calculations show that

\[
(X - \hat{X})^T(X - \hat{X}) = [2X\Sigma^{-1} - 2UCB^{-1}]^T[2X\Sigma^{-1} - 2UCB^{-1}]
= 4B^{-1}(\Sigma^{-1}X^TX\Sigma^{-1} + C^TU^TU\Sigma^{-1})B^{-1} = 4B^{-1}(\Sigma^{-1} + C^TC)B^{-1} = 4B^{-1}.
\]

\[
(X + \hat{X})^T(X - \hat{X}) = [X(2I - 2\Sigma^{-1}B^{-1}) + 2UCB^{-1}]^T[2X\Sigma^{-1}B^{-1} - 2UCB^{-1}]
= 4(I - \Sigma^{-1}B^{-1})^TX^TX\Sigma^{-1}B^{-1} - 4B^{-1}C^TU^TU\Sigma^{-1}B^{-1}
= 4(I - B^{-1}\Sigma^{-1})B^{-1} - 4B^{-1}C^TCB^{-1} = 4(I - B^{-1}\Sigma^{-1})B^{-1} - 4B^{-1}(B - \Sigma^{-1})B^{-1} = 0.
\]

Here, we use \(U^TX = X^TU = 0\). The first identity implies (29) and the second is exactly the orthogonal condition (10).

**Proof of Lemma 4.2** Conditional on \(\eta\), we can determine \(N_\eta = \{j \in S_0 : W_j \neq 0\}\). Recall that \(\xi\) and \(\eta\) are independent and \(\xi_{S_0} \overset{d}{=} -\xi_{S_0}\). We have \(E(1_{\xi_i > 0} | \eta) = E(1_{\xi_i > 0}) = 1/2, i \in S_0\) and for any \(i, j \in N_\eta\),

\[
E(1_{\xi_i > 0}1_{\xi_j < 0}) - \frac{1}{4} + E(1_{\xi_i > 0}1_{\xi_j > 0}) - \frac{1}{4} = E(1_{\xi_i > 0}) - \frac{1}{2} = 0.
\]

Similarly, \(E(1_{\xi_i < 0}1_{\xi_j > 0}) - \frac{1}{4} = -(E(1_{\xi_i > 0}1_{\xi_j > 0}) - \frac{1}{4}), \forall i, j \in S_0\). Meanwhile, the symmetry of \(\xi_{S_0}\) implies \(E(1_{\xi_i < 0}1_{\xi_j < 0}) = E(1_{\xi_i > 0}1_{\xi_j > 0})\). Therefore, we obtain

\[
\text{Cov}(Y_i, Y_j | \eta) = E(Y_iY_j | \eta) - E(Y_i | \eta)E(Y_j | \eta) = E(Y_iY_j | \eta) - \frac{1}{4}
= E(1_{f_i(\eta)} > 01_{\xi_i > 0} + 1_{f_i(\eta)} < 01_{\xi_i < 0} \cdot 1_{f_j(\eta)} > 01_{\xi_j > 0} + 1_{f_j(\eta)} < 01_{\xi_j < 0} | \eta) - \frac{1}{4}
= 1_{f_i(\eta)} > 01_{f_j(\eta)} > 0 \left[ E(1_{\xi_i > 0}1_{\xi_j > 0}) - \frac{1}{4} \right] + 1_{f_i(\eta)} > 01_{f_j(\eta)} < 0 \left[ E(1_{\xi_i > 0}1_{\xi_j < 0}) - \frac{1}{4} \right]
+ 1_{f_i(\eta)} < 01_{f_j(\eta)} > 0 \left[ E(1_{\xi_i < 0}1_{\xi_j > 0}) - \frac{1}{4} \right] + 1_{f_i(\eta)} < 01_{f_j(\eta)} < 0 \left[ E(1_{\xi_i < 0}1_{\xi_j < 0}) - \frac{1}{4} \right],
\]

where \(w_i \triangleq 1_{f_i(\eta)} > 0 - 1_{f_i(\eta)} < 0\). By definition, \(w_i = 1\) or \(-1\). From \(\text{Cov}(\xi) = B = 2\Sigma^{-1}\), we know that the joint distribution of \((\xi_i, \xi_j)\) is \(\left(\begin{array}{c} \xi_i \\ \xi_j \end{array}\right) \sim N\left(0, \begin{pmatrix} B_{ii} & B_{ij} \\ B_{ji} & B_{jj} \end{pmatrix}\right)\). Since normalizing
\( \xi_i, \xi_j \) does not change their sign, we assume that \( (\xi_i, \xi_j) \sim N \left(0, \begin{pmatrix} \mu_{ij} & 1 \\ \mu_{ij} & 1 \end{pmatrix} \right) \), where \( \mu_{ij} = B_{ij}/(B_{ii}^{1/2}B_{jj}^{1/2}) = (\Sigma^{-1})_{ij} \) (see (41)). Define
\[
\mu = \mu_{ij} = (\Sigma^{-1})_{ij},
\]
and let \( P(\xi_i, \xi_j) \) and \( P_s(\cdot) \) be the probability distribution function of \((\xi_i, \xi_j) \) and the standard normal distribution, respectively.

Using \( 0 \leq e^x - 1 - x \leq \frac{x^2}{2}(e^x 1_{x>0} + 1) \) by taking \( x \triangleq -\frac{\mu^2 \xi_i^2 + \mu^2 \xi_j^2 - 2 \mu \xi_i \xi_j}{2(1 - \mu^2)} \), we expand \( P(\xi_i, \xi_j) - P_s(\xi_i)P_s(\xi_j) \) up to \( \mu^2 \)
\[
[P(\xi_i, \xi_j) - P_s(\xi_i)P_s(\xi_j)]w_iw_j = \frac{P_s(\xi_i)P_s(\xi_j)}{\sqrt{1 - \mu^2}} (1 + x - \sqrt{1 - \mu^2})w_iw_j
\]
\[
\leq \frac{P_s(\xi_i)P_s(\xi_j)}{\sqrt{1 - \mu^2}} (1 + x - \sqrt{1 - \mu^2})w_iw_j + \frac{x^2}{2}
\]
\[
\leq \frac{P_s(\xi_i)P_s(\xi_j)}{\sqrt{1 - \mu^2}} (1 + x - \sqrt{1 - \mu^2})w_iw_j + \frac{x^2}{2}(e^x 1_{x>0} + 1)
\]
\[
= \frac{P_s(\xi_i)P_s(\xi_j)}{\sqrt{1 - \mu^2}} (1 + x - \sqrt{1 - \mu^2})w_iw_j + \frac{x^2}{2} + P(\xi_i, \xi_j)\frac{x^2}{2}1_{x>0}.
\]

Integrating both sides with respect to \( \xi_i, \xi_j \) in the region \( \xi_i, \xi_j > 0 \) gives
\[
\left(E(1_{\xi_i>0}1_{\xi_j>0}) - \frac{1}{4}\right) w_iw_j \leq \int_{\xi_i,\xi_j>0} \frac{P_s(\xi_i)P_s(\xi_j)}{\sqrt{1 - \mu^2}} (1 + x - \sqrt{1 - \mu^2})w_iw_j + \frac{x^2}{2} d\xi_i d\xi_j
\]
\[
+ \int_{\xi_i>0,\xi_j>0} P(\xi_i, \xi_j)\frac{x^2}{2}1_{x>0} d\xi_i d\xi_j \triangleq I + \Pi + \Pi I.
\]

Since \( P_s(\cdot) \) is standard Gaussian distribution and \( x = -\frac{\mu^2 \xi_i^2 + \mu^2 \xi_j^2 - 2 \mu \xi_i \xi_j}{2(1 - \mu^2)} \), we can calculate all the moments in \( I, \Pi \) explicitly. For \( I \), we have
\[
I = \left(\frac{1}{4}(\frac{1}{\sqrt{1 - \mu^2}} - 1) + \frac{\mu}{2\pi(1 - \mu^2)^{3/2}} - \frac{1}{4(1 - \mu^2)^{3/2}}\right) w_iw_j
\]
\[
\leq \frac{\mu w_iw_j}{2\pi} + \frac{\mu}{2\pi(1 - \mu^2)^{3/2}} - \frac{1}{4(1 - \mu^2)^{3/2}}
\]
\[
= \frac{\mu w_iw_j}{2\pi} + \frac{\mu}{2\pi(1 - \mu^2)^{3/2}} - \frac{1}{4(1 - \mu^2)^{3/2}} \triangleq \frac{\mu w_iw_j}{2\pi} + c_1(\mu)\mu^2,
\]
where \( c_1(\mu) \geq 0 \) collects the coefficients of \( \mu^2 \) and is bounded near \( \mu = 0 \). We use \( E(\xi_1 1_{\xi>0}) = 1/\sqrt{2\pi}, E(\xi_2^2 1_{\xi>0}) = 1 \) for the standard Gaussian \( \xi \) to obtain the first equality, and \(|w_i| = |w_j| = 1 \) to obtain the inequality. For the second term, we get
\[
\Pi = \frac{\mu^2}{8(1 - \mu^2)^{5/2}} \int_{\xi_i,\xi_j>0} P_s(\xi_i)P_s(\xi_j)(2\xi_i\xi_j - \mu(\xi_i^2 + \xi_j^2))^2 d\xi_i d\xi_j
\]
\[
= \frac{\mu^2}{8(1 - \mu^2)^{5/2}} \int_{\xi_i,\xi_j>0} P_s(\xi_i)P_s(\xi_j)(2\xi_i\xi_j - \mu(\xi_i^2 + \xi_j^2))^2 d\xi_i d\xi_j
\]
\[
\triangleq c_2(\mu)\mu^2,
\]
where \( c_2(\mu) = \frac{1}{8(1 - \mu^2)^{5/2}} \geq 0 \) is bounded near \( \mu = 0 \). Since \( \xi_i, \xi_j > 0 \) and \( x = -\frac{\mu^2 \xi_i^2 + \mu^2 \xi_j^2 - 2 \mu \xi_i \xi_j}{2(1 - \mu^2)} \), \( \mu \leq 0 \) implies \( x \leq 0 \), or equivalently \( 1_{x>0} \leq 1_{\mu>0} \). Note that
\[
x = -\frac{\mu^2 \xi_i^2 + \mu^2 \xi_j^2 - 2 \mu \xi_i \xi_j}{2(1 - \mu^2)} \leq -\frac{2\mu^2 \xi_i \xi_j - 2\mu \xi_i \xi_j}{2(1 - \mu^2)} = \frac{|\mu| \xi_i \xi_j}{(1 + |\mu|)}, \quad \forall \xi_i, \xi_j > 0.
For $\xi_i, \xi_j > 0$, we have $x^2 \mathbf{1}_{x>0} \leq \left(\frac{\mu |\xi_i|}{1+|\mu|}\right)^2 \mathbf{1}_{\mu>0}$. Therefore, we obtain

$$
\text{III} = \frac{1}{2} E(x^2 \mathbf{1}_{x>0} \mathbf{1}_{\xi_i, \xi_j>0}) \leq \frac{1}{2} \frac{|\mu^2 \mathbf{1}_{\mu>0}|}{(1 + |\mu|)^2} E(\xi_i^2 \xi_j \mathbf{1}_{\xi_i, \xi_j>0}) \\
\leq \frac{1}{2} \frac{|\mu^2 \mathbf{1}_{\mu>0}|}{(1 + |\mu|)^2} (E(\xi_i^4 \mathbf{1}_{\xi_i>0}) E(\xi_j^4 \mathbf{1}_{\xi_j>0}))^{1/2} = \frac{1}{2} \frac{|\mu^2 \mathbf{1}_{\mu>0}|}{(1 + |\mu|)^2} \frac{3}{2} \triangleq \mathbf{1}_{\mu>0} c_3(\mu) \mu^2,
$$

(59)

where $c_3(\mu) = \frac{3}{4(1 + |\mu|)^2}$ is bounded near $\mu = 0$. Combining (56), (57), (58) and (59), we yield

$$
\text{Cov}(Y_i, Y_j|\eta) = \left[E(\mathbf{1}_{\xi_i>0} \mathbf{1}_{\xi_j>0}) - \frac{1}{4}\right] w_i w_j \leq \frac{\mu}{2 \pi} w_i w_j + (c(\mu) + c_2(\mu) + c_3(\mu)) \mathbf{1}_{\mu>0}) \mu^2 \triangleq \frac{\mu}{2 \pi} w_i w_j + c(\mu) \mu^2.
$$

Here, $c(\mu) = c_1(\mu) + c_2(\mu) + c_3(\mu) \mathbf{1}_{\mu>0}$. Since $c_i(\mu)$ is a non-negative and an explicit function of $\mu$, it is not difficult to show that $c(\mu) < \frac{\mu}{2}$ for $|\mu| < \frac{1}{2}$. For $|\mu| > 1/2$, we use the estimate $\text{Cov}(Y_i, Y_j|\eta) \leq 1/4 \leq -1/2 \pi + \frac{3}{2} \mu^2$. Finally, we conclude

$$
\text{Cov}(Y_i, Y_j|\eta) \leq \left(\frac{\mu}{2 \pi} w_i w_j + c(\mu) \mu^2\right) \wedge \frac{1}{4} \leq \frac{\mu}{2 \pi} w_i w_j + \frac{3}{2} \mu^2,
$$

where $\mu = (\Sigma^{-1})_{ij}$ is defined in (55). This proves Lemma 4.2.

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